



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 04:58 pm GMT

PDB ID : 1W85  
Title : The crystal structure of pyruvate dehydrogenase E1 bound to the peripheral subunit binding domain of E2  
Authors : Frank, R.A.W.; Pratap, J.V.; Pei, X.Y.; Perham, R.N.; Luisi, B.F.  
Deposited on : 2004-09-16  
Resolution : 2.00 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

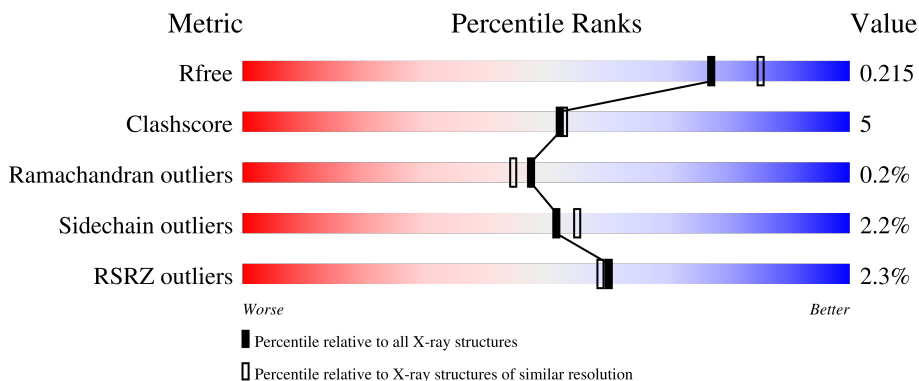
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	368	 4% 89% 7% ..
1	C	368	 % 90% 8% ..
1	E	368	 4% 84% 10% . 5%
1	G	368	 2% 90% 8% ..
2	B	324	 86% 13% .

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Mol	Chain	Length	Quality of chain
2	D	324	
2	F	324	
2	H	324	
3	I	49	
3	J	49	

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
6	TPP	A	1370	-	-	X	-
6	TPP	C	1370	-	-	X	-
6	TPP	E	1370	-	-	X	-
6	TPP	G	1370	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 23509 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, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	Total 2771	C 1777	N 472	O 514	S 8	0	0	1
1	C	365	Total 2877	C 1841	N 490	O 538	S 8	0	0	0
1	E	350	Total 2695	C 1723	N 461	O 503	S 8	0	0	0
1	G	364	Total 2854	C 1827	N 484	O 535	S 8	0	0	0

- Molecule 2 is a protein called PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	324	Total 2470	C 1573	N 422	O 467	S 8	0	0	0
2	D	324	Total 2483	C 1583	N 421	O 471	S 8	0	0	0
2	F	324	Total 2473	C 1576	N 422	O 467	S 8	0	0	0
2	H	324	Total 2483	C 1583	N 421	O 471	S 8	0	0	0

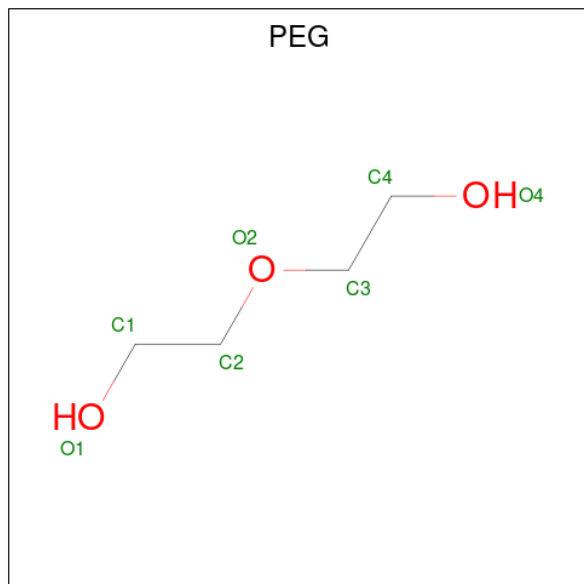
- Molecule 3 is a protein called DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	42	Total 302	C 189	N 56	O 56	S 1	0	0	0
3	J	35	Total 233	C 143	N 44	O 45	S 1	0	0	1

- Molecule 4 is MAGNESIUM ION (three-letter code: 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	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0

- Molecule 6 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ).



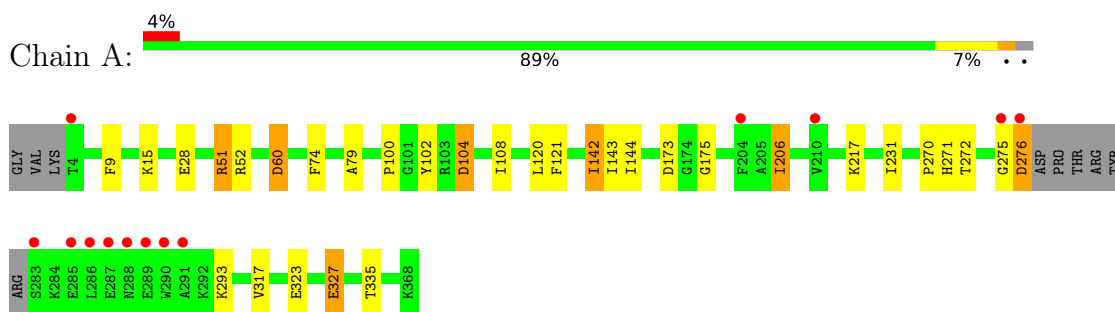
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	198	Total 198	O 198	0	0
8	C	282	Total 282	O 282	0	0
8	D	241	Total 241	O 241	0	0
8	E	137	Total 137	O 137	0	0
8	F	169	Total 169	O 169	0	0
8	G	234	Total 234	O 234	0	0
8	H	227	Total 227	O 227	0	0
8	I	12	Total 12	O 12	0	0
8	J	9	Total 9	O 9	0	0

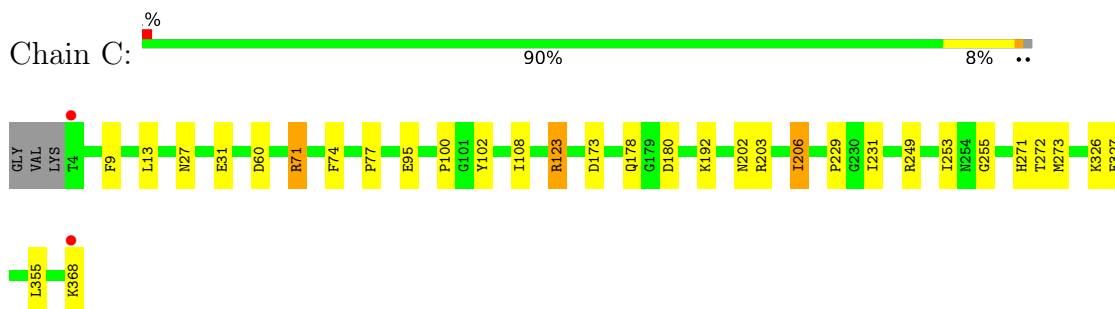
### 3 Residue-property plots [i](#)

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.

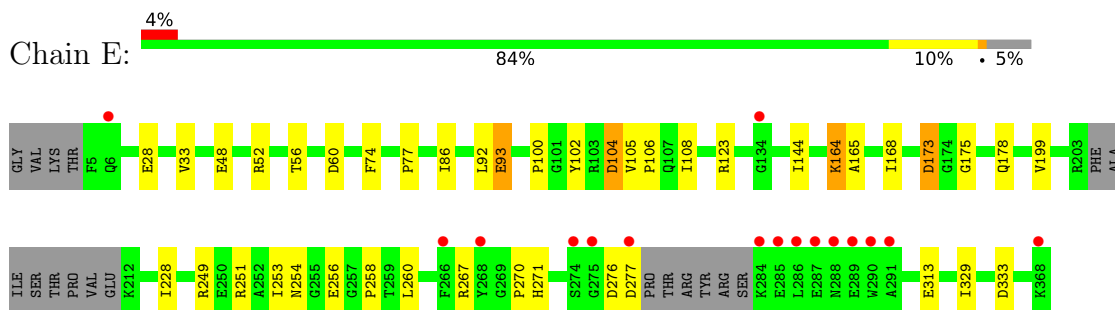
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



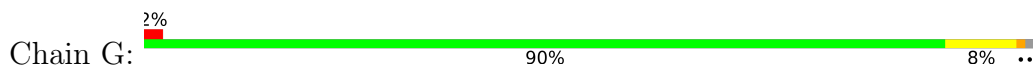
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



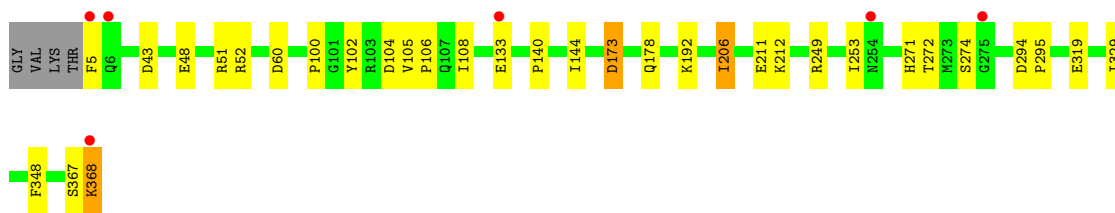
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT

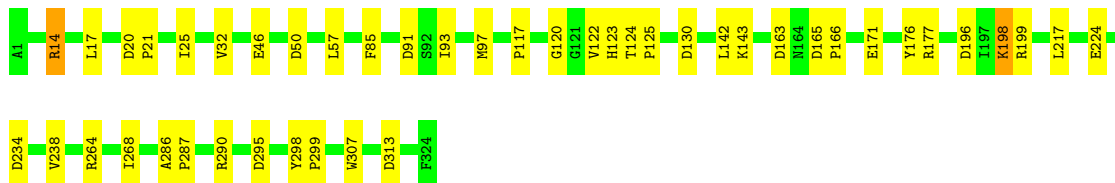






- Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT

Chain B: 86% 13%



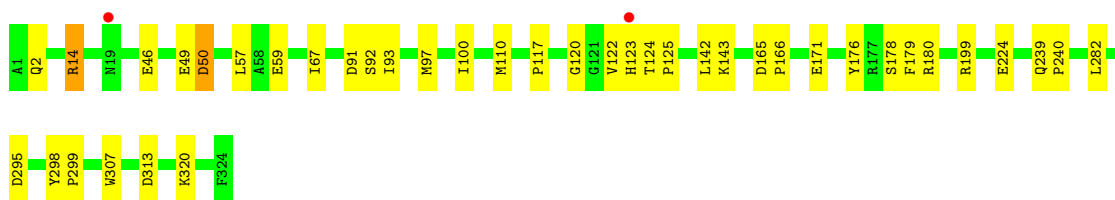
- Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT

Chain D: 89% 11%



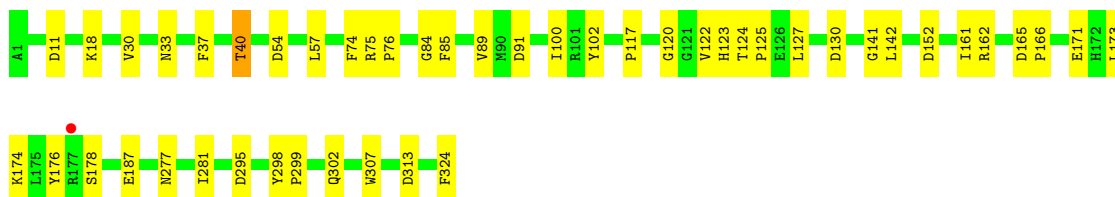
- Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT

Chain F: 88% 12%

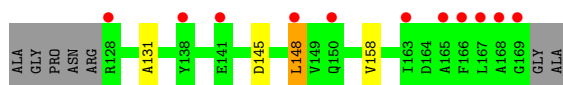
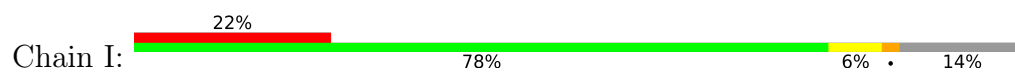


- Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT

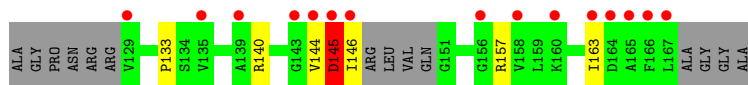
Chain H: 85% 14%



- Molecule 3: DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE



• Molecule 3: DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.27Å 232.33Å 91.92Å 90.00° 90.81° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.00) 94.8 (20.00-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.176 , 0.215 0.177 , 0.215	Depositor DCC
$R_{free}$ test set	9031 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtrriage
Anisotropy	0.586	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K, TPP, PEG, 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	0.65	1/2831 (0.0%)	0.71	6/3832 (0.2%)
1	C	0.69	0/2940	0.71	4/3972 (0.1%)
1	E	0.55	0/2750	0.66	6/3712 (0.2%)
1	G	0.60	0/2917	0.68	4/3945 (0.1%)
2	B	0.68	2/2516 (0.1%)	0.79	8/3415 (0.2%)
2	D	0.71	0/2529	0.79	8/3430 (0.2%)
2	F	0.59	0/2519	0.72	5/3419 (0.1%)
2	H	0.63	0/2529	0.76	6/3430 (0.2%)
3	I	0.50	0/304	0.68	0/407
3	J	0.55	0/233	0.85	1/312 (0.3%)
All	All	0.64	3/22068 (0.0%)	0.73	48/29874 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	ARG	CD-NE	8.95	1.61	1.46
1	A	52	ARG	CZ-NH2	5.64	1.40	1.33
2	B	199	ARG	CZ-NH2	-5.22	1.26	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	ARG	NE-CZ-NH2	-13.95	113.32	120.30
2	B	199	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	A	52	ARG	NE-CZ-NH2	-7.75	116.42	120.30
2	H	295	ASP	CB-CG-OD2	7.50	125.05	118.30
2	D	54	ASP	CB-CG-OD2	6.62	124.26	118.30
2	H	11	ASP	CB-CG-OD2	6.59	124.23	118.30
1	G	60	ASP	CB-CG-OD2	6.52	124.17	118.30
2	D	91	ASP	CB-CG-OD2	6.42	124.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	H	313	ASP	CB-CG-OD2	6.25	123.92	118.30
1	C	123	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	H	54	ASP	CB-CG-OD2	6.19	123.87	118.30
2	F	313	ASP	CB-CG-OD2	6.13	123.81	118.30
1	G	173	ASP	CB-CG-OD2	6.04	123.74	118.30
2	F	91	ASP	CB-CG-OD2	6.04	123.73	118.30
2	F	50	ASP	CB-CG-OD2	6.02	123.72	118.30
2	B	50	ASP	CB-CG-OD2	5.98	123.69	118.30
2	B	91	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	276	ASP	CB-CG-OD2	5.90	123.61	118.30
1	G	104	ASP	CB-CG-OD2	5.88	123.60	118.30
2	B	295	ASP	CB-CG-OD2	5.88	123.59	118.30
2	B	234	ASP	CB-CG-OD2	5.87	123.58	118.30
2	D	29	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	142	ILE	CG1-CB-CG2	-5.76	98.73	111.40
1	C	180	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	60	ASP	CB-CG-OD2	5.62	123.35	118.30
1	E	173	ASP	CB-CG-OD2	5.56	123.30	118.30
2	D	295	ASP	CB-CG-OD2	5.55	123.29	118.30
2	F	165	ASP	CB-CG-OD2	5.53	123.28	118.30
1	E	277	ASP	CB-CG-OD2	5.53	123.27	118.30
2	D	313	ASP	CB-CG-OD2	5.47	123.23	118.30
1	E	60	ASP	CB-CG-OD2	5.45	123.21	118.30
1	E	104	ASP	CB-CG-OD2	5.45	123.20	118.30
1	E	333	ASP	CB-CG-OD2	5.43	123.19	118.30
2	D	11	ASP	CB-CG-OD2	5.43	123.19	118.30
2	D	203	ASP	CB-CG-OD2	5.41	123.17	118.30
1	E	276	ASP	CB-CG-OD2	5.40	123.16	118.30
3	J	145	ASP	CB-CG-OD2	5.38	123.14	118.30
2	B	313	ASP	CB-CG-OD2	5.35	123.12	118.30
2	B	163	ASP	CB-CG-OD2	5.34	123.10	118.30
2	D	152	ASP	CB-CG-OD2	5.32	123.08	118.30
1	G	43	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	104	ASP	CB-CG-OD2	5.23	123.00	118.30
2	F	295	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	51	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	H	152	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	60	ASP	CB-CG-OD2	5.10	122.89	118.30
2	H	91	ASP	CB-CG-OD2	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2771	0	2713	34	0
1	C	2877	0	2845	30	0
1	E	2695	0	2630	32	0
1	G	2854	0	2806	23	0
2	B	2470	0	2476	26	0
2	D	2483	0	2504	24	0
2	F	2473	0	2485	28	0
2	H	2483	0	2504	34	0
3	I	302	0	300	2	0
3	J	233	0	218	8	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	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	7	0	10	0	0
5	C	7	0	10	0	0
5	G	7	0	10	0	0
6	A	26	0	16	18	0
6	C	26	0	16	10	0
6	E	26	0	16	11	0
6	G	26	0	16	12	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	A	224	0	0	1	0
8	B	198	0	0	2	0
8	C	282	0	0	6	0
8	D	241	0	0	3	0
8	E	137	0	0	0	0
8	F	169	0	0	4	0
8	G	234	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	227	0	0	2	0
8	I	12	0	0	0	0
8	J	9	0	0	0	0
All	All	23509	0	21575	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (238) 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)
3:J:145:ASP:O	3:J:146:ILE:HG22	1.42	1.14
2:F:50:ASP:HB3	8:F:2025:HOH:O	1.69	0.92
3:J:145:ASP:O	3:J:146:ILE:CG2	2.18	0.89
6:A:1370:TPP:H2	6:A:1370:TPP:HN42	1.37	0.87
6:E:1370:TPP:H2	6:E:1370:TPP:HN42	1.40	0.86
1:C:77:PRO:HG3	1:C:273:MET:HE3	1.58	0.85
2:H:33:ASN:HB2	8:H:2020:HOH:O	1.79	0.82
2:F:143:LYS:HE3	8:F:2097:HOH:O	1.81	0.80
2:B:299:PRO:HG3	2:B:307:TRP:CD2	2.17	0.79
1:A:102:TYR:OH	6:A:1370:TPP:H72	1.82	0.79
2:D:50:ASP:HB3	8:D:2039:HOH:O	1.82	0.78
1:A:100:PRO:HG2	1:A:108:ILE:HG21	1.67	0.77
1:A:120:LEU:HD11	1:A:335:THR:HG21	1.67	0.76
2:D:299:PRO:HG3	2:D:307:TRP:CD2	2.21	0.75
2:F:67:ILE:HG12	2:F:110:MET:CE	2.16	0.75
8:F:2148:HOH:O	3:J:133:PRO:HB3	1.88	0.73
2:B:125:PRO:HG3	1:C:74:PHE:CD1	2.24	0.73
1:C:77:PRO:CG	1:C:273:MET:CE	2.67	0.72
6:C:1370:TPP:H2	6:C:1370:TPP:HN42	1.54	0.72
2:H:299:PRO:HG3	2:H:307:TRP:CD2	2.24	0.72
1:C:102:TYR:OH	6:C:1370:TPP:H71	1.89	0.72
1:A:74:PHE:CD1	2:D:125:PRO:HG3	2.25	0.72
1:C:71:ARG:HD2	8:C:2127:HOH:O	1.89	0.72
1:A:323:GLU:O	1:A:327:GLU:HG2	1.89	0.71
1:G:102:TYR:OH	6:G:1370:TPP:H71	1.90	0.71
2:B:32:VAL:HG23	8:B:2023:HOH:O	1.91	0.70
1:G:367:SER:O	1:G:368:LYS:HB2	1.90	0.70
1:A:206:ILE:HG13	6:A:1370:TPP:H62	1.74	0.69
6:C:1370:TPP:HN42	6:C:1370:TPP:C2	2.06	0.69
1:E:74:PHE:CD1	2:H:125:PRO:HG3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:HIS:CE1	6:G:1370:TPP:S1	2.86	0.68
1:C:77:PRO:HG3	1:C:273:MET:CE	2.25	0.67
1:C:100:PRO:HG3	1:C:108:ILE:CG2	2.24	0.66
2:F:299:PRO:HG3	2:F:307:TRP:CD2	2.30	0.66
6:G:1370:TPP:HN42	6:G:1370:TPP:H2	1.60	0.66
2:F:67:ILE:HG12	2:F:110:MET:HE2	1.77	0.66
1:C:271:HIS:CE1	6:C:1370:TPP:H62	2.31	0.66
2:B:298:TYR:CG	2:B:299:PRO:HD2	2.32	0.65
2:F:67:ILE:HA	2:F:110:MET:HE1	1.78	0.65
2:D:298:TYR:CG	2:D:299:PRO:HD2	2.32	0.65
6:A:1370:TPP:HN42	6:A:1370:TPP:C2	2.08	0.65
2:B:299:PRO:HG3	2:B:307:TRP:CG	2.31	0.65
1:A:206:ILE:CG1	6:A:1370:TPP:H62	2.27	0.64
1:E:102:TYR:HE2	1:E:144:ILE:HD11	1.60	0.64
1:A:100:PRO:HB3	1:A:104:ASP:HB2	1.79	0.64
2:H:298:TYR:CG	2:H:299:PRO:HD2	2.32	0.63
1:E:102:TYR:HE2	1:E:144:ILE:CD1	2.12	0.63
1:E:165:ALA:N	1:E:253:ILE:HD11	2.14	0.63
1:A:102:TYR:OH	6:A:1370:TPP:S1	2.55	0.63
2:H:298:TYR:CD1	2:H:299:PRO:HD2	2.33	0.63
2:D:298:TYR:CD1	2:D:299:PRO:HD2	2.34	0.62
2:D:299:PRO:HG3	2:D:307:TRP:CG	2.34	0.62
1:E:102:TYR:OH	6:E:1370:TPP:S1	2.55	0.62
1:E:123:ARG:O	2:H:302:GLN:NE2	2.27	0.62
1:G:144:ILE:HD12	6:G:1370:TPP:C4'	2.30	0.62
2:F:299:PRO:HG3	2:F:307:TRP:CG	2.35	0.61
1:C:100:PRO:HG3	1:C:108:ILE:HG21	1.81	0.61
1:C:77:PRO:HG2	1:C:273:MET:CE	2.30	0.61
6:E:1370:TPP:HN42	6:E:1370:TPP:C2	2.12	0.60
3:I:145:ASP:HB3	3:I:148:LEU:HD22	1.82	0.60
2:H:299:PRO:HG3	2:H:307:TRP:CG	2.37	0.60
1:E:144:ILE:CG2	1:E:175:GLY:HA2	2.31	0.59
1:E:271:HIS:NE2	6:E:1370:TPP:S1	2.69	0.59
1:A:9:PHE:HZ	1:C:231:ILE:HD11	1.66	0.59
1:A:100:PRO:HG2	1:A:108:ILE:CG2	2.33	0.58
1:A:206:ILE:HG13	6:A:1370:TPP:C6	2.32	0.58
3:J:144:VAL:HG12	3:J:145:ASP:H	1.68	0.58
1:G:271:HIS:CE1	6:G:1370:TPP:H62	2.39	0.58
2:B:14:ARG:NH1	2:B:46:GLU:OE1	2.36	0.58
1:C:77:PRO:CG	1:C:273:MET:HE3	2.29	0.58
2:F:298:TYR:CG	2:F:299:PRO:HD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:HIS:CE1	6:A:1370:TPP:S1	2.98	0.57
1:A:51:ARG:HG2	1:A:317:VAL:HG21	1.86	0.57
2:F:67:ILE:HG12	2:F:110:MET:HE1	1.84	0.57
6:G:1370:TPP:HN42	6:G:1370:TPP:C2	2.17	0.57
1:A:102:TYR:HH	6:A:1370:TPP:H72	1.67	0.56
1:A:271:HIS:HE1	6:A:1370:TPP:S1	2.28	0.56
2:B:264:ARG:NH2	2:B:290:ARG:O	2.38	0.56
2:D:174:LYS:HE3	8:D:2129:HOH:O	2.04	0.56
1:C:271:HIS:CE1	6:C:1370:TPP:S1	2.99	0.55
2:F:49:GLU:OE2	1:G:212:LYS:NZ	2.39	0.55
2:F:120:GLY:HA3	2:F:298:TYR:OH	2.07	0.55
2:H:277:ASN:O	2:H:281:ILE:HB	2.07	0.54
1:E:100:PRO:HB3	1:E:104:ASP:HB2	1.89	0.54
2:B:298:TYR:CD1	2:B:299:PRO:HD2	2.42	0.54
2:D:207:ILE:HA	2:D:233:VAL:HG13	1.88	0.54
1:E:102:TYR:CZ	6:E:1370:TPP:S1	3.01	0.54
1:E:102:TYR:CE2	1:E:144:ILE:HD11	2.42	0.54
1:C:192:LYS:HE2	1:C:255:GLY:O	2.08	0.53
2:H:324:PHE:O	3:J:157:ARG:NH2	2.36	0.53
2:B:298:TYR:CD2	2:B:299:PRO:HD2	2.44	0.53
1:G:48:GLU:OE2	1:G:52:ARG:HD2	2.07	0.53
1:A:270:PRO:HB3	1:A:276:ASP:O	2.09	0.53
1:A:100:PRO:CG	1:A:108:ILE:CG2	2.87	0.53
3:J:145:ASP:C	3:J:146:ILE:HG22	2.22	0.52
2:B:122:VAL:HG23	2:B:124:THR:HG23	1.91	0.52
1:E:92:LEU:HD11	1:E:168:ILE:HG21	1.91	0.52
2:H:30:VAL:HB	2:H:40:THR:HG21	1.91	0.52
2:D:122:VAL:HG23	2:D:124:THR:HG23	1.91	0.52
3:I:131:ALA:HB2	3:I:158:VAL:HG22	1.91	0.52
2:H:40:THR:HG22	8:H:2052:HOH:O	2.09	0.52
2:F:2:GLN:HG3	2:F:180:ARG:HB3	1.91	0.52
2:H:117:PRO:HA	2:H:171:GLU:O	2.10	0.52
2:F:298:TYR:CD1	2:F:299:PRO:HD2	2.45	0.51
1:G:271:HIS:NE2	6:G:1370:TPP:S1	2.83	0.51
1:C:123:ARG:NH2	8:C:2127:HOH:O	2.42	0.51
1:E:100:PRO:HG2	1:E:108:ILE:HG21	1.92	0.51
1:A:28:GLU:OE2	1:A:293:LYS:HE2	2.10	0.51
1:C:95:GLU:HG2	8:C:2099:HOH:O	2.11	0.51
1:E:28:GLU:CD	1:E:28:GLU:H	2.13	0.50
2:H:120:GLY:HA3	2:H:298:TYR:OH	2.10	0.50
2:B:124:THR:HB	2:B:125:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:VAL:HG23	2:F:124:THR:HG23	1.93	0.50
1:G:51:ARG:HD2	8:G:2198:HOH:O	2.11	0.50
1:A:100:PRO:CG	1:A:108:ILE:HG21	2.41	0.50
1:C:27:ASN:OD1	1:C:31:GLU:HG3	2.10	0.50
1:G:100:PRO:HG2	1:G:108:ILE:HG21	1.93	0.50
6:A:1370:TPP:O2B	6:A:1370:TPP:H71	2.12	0.49
6:E:1370:TPP:H72	2:H:57:LEU:CD1	2.42	0.49
1:G:102:TYR:HA	1:G:140:PRO:HB3	1.94	0.49
1:E:56:THR:HG21	1:E:86:ILE:HD11	1.94	0.49
2:F:117:PRO:HA	2:F:171:GLU:O	2.13	0.49
2:H:75:ARG:HD3	2:H:161:ILE:O	2.13	0.49
8:F:2145:HOH:O	2:H:277:ASN:HB3	2.12	0.49
1:E:123:ARG:O	2:H:302:GLN:HG2	2.13	0.48
2:H:162:ARG:NH2	2:H:187:GLU:OE1	2.44	0.48
2:D:142:LEU:HD23	2:D:166:PRO:HB2	1.96	0.48
2:B:198:LYS:HB3	2:B:217:LEU:HD21	1.94	0.48
1:C:203:ARG:HD3	8:C:2178:HOH:O	2.13	0.48
6:E:1370:TPP:C5'	2:H:85:PHE:CE2	2.96	0.48
2:H:37:PHE:CZ	2:H:173:LEU:HD22	2.49	0.48
1:E:165:ALA:N	1:E:253:ILE:CD1	2.77	0.48
1:E:164:LYS:C	1:E:253:ILE:CD1	2.82	0.48
1:A:102:TYR:CZ	6:A:1370:TPP:S1	3.07	0.47
2:B:57:LEU:HD11	6:C:1370:TPP:H72	1.97	0.47
2:B:120:GLY:HA3	2:B:298:TYR:OH	2.14	0.47
1:E:251:ARG:HG3	1:E:256:GLU:HB2	1.97	0.47
1:G:271:HIS:CD2	1:G:272:THR:HG23	2.49	0.47
1:C:100:PRO:CG	1:C:108:ILE:HG21	2.43	0.47
1:C:368:LYS:HA	8:C:2276:HOH:O	2.13	0.47
2:F:57:LEU:HD11	6:G:1370:TPP:CM4	2.45	0.47
6:A:1370:TPP:C2	6:A:1370:TPP:N4'	2.77	0.47
1:E:100:PRO:HG3	1:E:108:ILE:CG2	2.44	0.47
1:E:178:GLN:NE2	6:E:1370:TPP:HM23	2.30	0.47
2:B:286:ALA:HB1	2:B:287:PRO:HD2	1.97	0.47
2:D:277:ASN:O	2:D:281:ILE:HB	2.15	0.46
2:D:117:PRO:HA	2:D:171:GLU:O	2.15	0.46
1:E:144:ILE:HG21	1:E:175:GLY:HA2	1.97	0.46
1:C:206:ILE:HG13	6:C:1370:TPP:H61	1.98	0.46
1:C:271:HIS:CD2	1:C:272:THR:HG23	2.51	0.46
2:D:320:LYS:HE3	2:D:320:LYS:HB2	1.70	0.46
6:E:1370:TPP:H2	6:E:1370:TPP:N4'	2.19	0.46
1:G:100:PRO:HG3	1:G:108:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ASP:HB3	2:B:166:PRO:CD	2.46	0.45
6:C:1370:TPP:C2	6:C:1370:TPP:N4'	2.78	0.45
1:A:271:HIS:CD2	1:A:272:THR:HG23	2.51	0.45
1:E:228:ILE:HG21	1:E:258:PRO:HG2	1.96	0.45
2:H:122:VAL:HG23	2:H:124:THR:HG23	1.98	0.45
2:B:85:PHE:CE2	6:C:1370:TPP:C5'	2.99	0.45
2:B:17:LEU:HD11	2:B:25:ILE:HD12	1.99	0.45
1:C:202:ASN:O	1:C:203:ARG:HB2	2.17	0.45
1:A:121:PHE:HA	8:A:2105:HOH:O	2.16	0.45
1:G:249:ARG:O	1:G:253:ILE:HG23	2.16	0.45
2:D:120:GLY:HA3	2:D:298:TYR:OH	2.17	0.45
6:E:1370:TPP:C2	6:E:1370:TPP:N4'	2.78	0.45
2:F:93:ILE:HA	2:F:97:MET:HG2	1.99	0.45
1:G:294:ASP:HA	1:G:295:PRO:HD2	1.89	0.45
2:F:124:THR:HB	2:F:125:PRO:HD2	1.98	0.44
2:D:14:ARG:NH1	8:D:2010:HOH:O	2.50	0.44
2:D:286:ALA:HB1	2:D:287:PRO:HD2	2.00	0.44
2:F:67:ILE:CG1	2:F:110:MET:HE1	2.48	0.44
1:E:93:GLU:HG3	1:E:249:ARG:NH2	2.32	0.44
1:G:133:GLU:HG2	8:G:2105:HOH:O	2.18	0.44
1:E:164:LYS:C	1:E:253:ILE:HD11	2.37	0.44
2:F:299:PRO:HA	2:H:102:TYR:OH	2.18	0.44
2:F:59:GLU:OE2	6:G:1370:TPP:N1'	2.51	0.44
2:B:93:ILE:HA	2:B:97:MET:HG2	2.00	0.44
1:A:231:ILE:HD11	1:C:9:PHE:HZ	1.83	0.43
6:E:1370:TPP:H72	2:H:57:LEU:HD11	2.00	0.43
1:G:319:GLU:HG2	8:G:2194:HOH:O	2.18	0.43
2:B:238:VAL:HB	2:B:268:ILE:HG12	1.99	0.43
1:C:355:LEU:HD23	1:C:355:LEU:HA	1.84	0.43
2:F:199:ARG:NH2	2:F:224:GLU:OE1	2.52	0.43
1:A:102:TYR:OH	6:A:1370:TPP:O2B	2.36	0.43
1:A:206:ILE:HG12	6:A:1370:TPP:H62	2.00	0.43
2:B:298:TYR:CG	2:B:299:PRO:CD	3.00	0.43
1:C:249:ARG:O	1:C:253:ILE:HG12	2.19	0.43
2:D:298:TYR:CG	2:D:299:PRO:CD	2.99	0.43
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.76	0.43
2:F:14:ARG:NH1	2:F:46:GLU:OE1	2.47	0.43
1:A:142:ILE:HG21	2:D:126:GLU:O	2.19	0.43
2:H:324:PHE:C	3:J:157:ARG:HH22	2.21	0.43
1:A:60:ASP:OD2	1:A:79:ALA:HB2	2.19	0.42
2:F:92:SER:O	2:F:97:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1370:TPP:N1'	2:D:59:GLU:OE2	2.51	0.42
2:B:117:PRO:HA	2:B:171:GLU:O	2.18	0.42
2:D:174:LYS:O	2:D:178:SER:HB3	2.18	0.42
1:E:164:LYS:HD2	1:E:164:LYS:HA	1.82	0.42
1:C:178:GLN:NE2	6:C:1370:TPP:HM23	2.34	0.42
2:H:142:LEU:HD23	2:H:166:PRO:HB2	2.01	0.42
1:A:143:ILE:HG23	6:A:1370:TPP:HM21	2.01	0.42
1:E:100:PRO:CG	1:E:108:ILE:HG21	2.50	0.42
2:F:178:SER:OG	2:F:179:PHE:HD1	2.03	0.42
2:D:124:THR:HB	2:D:125:PRO:HD2	2.01	0.42
1:E:105:VAL:N	1:E:106:PRO:CD	2.83	0.42
2:H:89:VAL:HG22	2:H:89:VAL:O	2.19	0.42
2:H:299:PRO:HG3	2:H:307:TRP:CE3	2.53	0.42
2:H:74:PHE:O	2:H:76:PRO:HD3	2.19	0.42
2:H:84:GLY:HA3	2:H:127:LEU:O	2.20	0.42
2:H:174:LYS:O	2:H:178:SER:HB3	2.20	0.42
3:J:144:VAL:HG21	3:J:163:ILE:HG23	2.02	0.42
1:G:348:PHE:CZ	2:H:141:GLY:HA2	2.55	0.41
2:B:142:LEU:HD23	2:B:166:PRO:HB2	2.03	0.41
1:G:100:PRO:CG	1:G:108:ILE:HG21	2.50	0.41
1:G:105:VAL:N	1:G:106:PRO:CD	2.83	0.41
1:A:142:ILE:HG13	2:D:126:GLU:HB3	2.02	0.41
1:E:199:VAL:HG23	1:E:260:LEU:HD11	2.01	0.41
1:G:178:GLN:NE2	6:G:1370:TPP:HM23	2.36	0.41
2:D:298:TYR:CD2	2:D:299:PRO:HD2	2.55	0.41
1:A:9:PHE:CD1	1:C:229:PRO:HB3	2.55	0.41
2:B:299:PRO:HG3	2:B:307:TRP:CE3	2.52	0.41
2:H:37:PHE:CZ	2:H:173:LEU:CD2	3.03	0.41
6:A:1370:TPP:CM4	2:D:57:LEU:HD11	2.50	0.41
2:B:20:ASP:HA	2:B:21:PRO:HD2	1.87	0.41
1:E:93:GLU:HG3	1:E:249:ARG:CZ	2.51	0.41
1:G:102:TYR:HH	6:G:1370:TPP:H71	1.83	0.41
1:A:144:ILE:CG2	1:A:175:GLY:HA2	2.51	0.41
1:A:231:ILE:HD11	1:C:9:PHE:CZ	2.56	0.40
2:H:165:ASP:HB3	2:H:166:PRO:CD	2.51	0.40
2:B:143:LYS:HE3	8:B:2103:HOH:O	2.21	0.40
2:F:239:GLN:HA	2:F:240:PRO:HA	1.87	0.40
1:E:48:GLU:OE2	1:E:52:ARG:HD2	2.22	0.40
2:F:97:MET:CB	2:F:110:MET:HE3	2.52	0.40
2:H:100:ILE:HA	2:H:100:ILE:HD13	1.84	0.40
1:G:271:HIS:HE1	6:G:1370:TPP:S1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:NH2	8:C:2075:HOH:O	2.52	0.40
1:E:77:PRO:HG2	1:E:270:PRO:HD2	2.03	0.40
2:F:142:LEU:HD23	2:F:166:PRO:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	355/368 (96%)	346 (98%)	7 (2%)	2 (1%)	25 19
1	C	363/368 (99%)	354 (98%)	8 (2%)	1 (0%)	41 37
1	E	344/368 (94%)	337 (98%)	7 (2%)	0	100 100
1	G	362/368 (98%)	351 (97%)	10 (3%)	1 (0%)	41 37
2	B	322/324 (99%)	315 (98%)	7 (2%)	0	100 100
2	D	322/324 (99%)	314 (98%)	8 (2%)	0	100 100
2	F	322/324 (99%)	314 (98%)	8 (2%)	0	100 100
2	H	322/324 (99%)	314 (98%)	8 (2%)	0	100 100
3	I	40/49 (82%)	39 (98%)	1 (2%)	0	100 100
3	J	31/49 (63%)	26 (84%)	4 (13%)	1 (3%)	4 1
All	All	2783/2866 (97%)	2710 (97%)	68 (2%)	5 (0%)	47 44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	206	ILE
3	J	140	ARG
1	A	206	ILE
1	A	275	GLY

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Mol	Chain	Res	Type
1	G	206	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	279/304 (92%)	276 (99%)	3 (1%)	73 78
1	C	296/304 (97%)	292 (99%)	4 (1%)	67 72
1	E	270/304 (89%)	262 (97%)	8 (3%)	41 41
1	G	292/304 (96%)	284 (97%)	8 (3%)	44 46
2	B	258/263 (98%)	250 (97%)	8 (3%)	40 40
2	D	262/263 (100%)	258 (98%)	4 (2%)	65 69
2	F	259/263 (98%)	253 (98%)	6 (2%)	50 53
2	H	262/263 (100%)	257 (98%)	5 (2%)	57 61
3	I	28/36 (78%)	27 (96%)	1 (4%)	35 34
3	J	21/36 (58%)	20 (95%)	1 (5%)	25 22
All	All	2227/2340 (95%)	2179 (98%)	48 (2%)	52 55

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	173	ASP
1	A	327	GLU
2	B	14	ARG
2	B	123	HIS
2	B	130	ASP
2	B	176	TYR
2	B	177	ARG
2	B	196	ASP
2	B	198	LYS
2	B	224	GLU
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	173	ASP
1	C	326	LYS
1	C	327	GLU
2	D	123	HIS
2	D	130	ASP
2	D	176	TYR
2	D	277	ASN
1	E	33	VAL
1	E	93	GLU
1	E	164	LYS
1	E	173	ASP
1	E	254	ASN
1	E	267	ARG
1	E	313	GLU
1	E	329	ILE
2	F	14	ARG
2	F	100	ILE
2	F	123	HIS
2	F	176	TYR
2	F	282	LEU
2	F	320	LYS
1	G	5	PHE
1	G	173	ASP
1	G	192	LYS
1	G	206	ILE
1	G	211	GLU
1	G	274	SER
1	G	329	ILE
1	G	368	LYS
2	H	18	LYS
2	H	40	THR
2	H	123	HIS
2	H	130	ASP
2	H	176	TYR
3	I	148	LEU
3	J	145	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	123	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	PEG	C	1369	-	6,6,6	0.51	0	5,5,5	0.25	0
6	TPP	G	1370	4	22,27,27	2.36	6 (27%)	29,40,40	1.69	8 (27%)
6	TPP	C	1370	4	22,27,27	2.41	6 (27%)	29,40,40	1.74	6 (20%)
6	TPP	E	1370	4	22,27,27	2.43	7 (31%)	29,40,40	1.97	9 (31%)
6	TPP	A	1370	4	22,27,27	2.31	6 (27%)	29,40,40	1.98	9 (31%)
5	PEG	A	1369	-	6,6,6	0.48	0	5,5,5	0.21	0
5	PEG	G	1369	-	6,6,6	0.47	0	5,5,5	0.22	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	PEG	C	1369	-	-	1/4/4/4	-
6	TPP	G	1370	4	-	1/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TPP	C	1370	4	-	3/16/17/17	0/2/2/2
6	TPP	E	1370	4	-	5/16/17/17	0/2/2/2
6	TPP	A	1370	4	-	6/16/17/17	0/2/2/2
5	PEG	A	1369	-	-	3/4/4/4	-
5	PEG	G	1369	-	-	3/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1370	TPP	C4-N3	-7.65	1.33	1.39
6	G	1370	TPP	C4-N3	-7.02	1.33	1.39
6	C	1370	TPP	C4-N3	-6.82	1.33	1.39
6	A	1370	TPP	C4-N3	-6.69	1.33	1.39
6	C	1370	TPP	C5'-C4'	5.26	1.51	1.42
6	G	1370	TPP	C5'-C4'	4.91	1.51	1.42
6	A	1370	TPP	C2-N3	-4.74	1.26	1.36
6	A	1370	TPP	C5'-C4'	4.34	1.50	1.42
6	E	1370	TPP	C5'-C4'	4.31	1.50	1.42
6	C	1370	TPP	C2-N3	-3.98	1.27	1.36
6	G	1370	TPP	C2-N3	-3.95	1.27	1.36
6	E	1370	TPP	C2-N3	-3.92	1.27	1.36
6	C	1370	TPP	C7'-N3	-2.86	1.43	1.48
6	G	1370	TPP	C4'-N3'	2.83	1.39	1.35
6	C	1370	TPP	C6-C5	2.78	1.52	1.50
6	E	1370	TPP	PB-O1B	2.72	1.59	1.50
6	E	1370	TPP	C6-C5	2.58	1.52	1.50
6	A	1370	TPP	C7'-N3	-2.54	1.44	1.48
6	A	1370	TPP	PA-O1A	2.36	1.59	1.50
6	E	1370	TPP	PA-O1A	2.33	1.59	1.50
6	G	1370	TPP	PA-O1A	2.24	1.58	1.50
6	A	1370	TPP	C6-C5	2.19	1.51	1.50
6	G	1370	TPP	C7'-N3	-2.09	1.44	1.48
6	C	1370	TPP	PA-O1A	2.08	1.58	1.50
6	E	1370	TPP	C4'-N3'	2.06	1.38	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1370	TPP	C6-C5-C4	-6.13	122.51	127.43
6	E	1370	TPP	C6-C5-C4	-5.76	122.81	127.43
6	C	1370	TPP	C6-C5-C4	-3.90	124.30	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1370	TPP	C6'-N1'-C2'	3.70	122.26	115.96
6	C	1370	TPP	C7'-N3-C2	-3.65	118.75	125.35
6	A	1370	TPP	C6'-N1'-C2'	3.62	122.12	115.96
6	A	1370	TPP	C7'-N3-C2	-3.50	119.03	125.35
6	E	1370	TPP	C6'-N1'-C2'	3.46	121.85	115.96
6	E	1370	TPP	PA-O3A-PB	-3.20	121.85	132.83
6	G	1370	TPP	C6-C5-C4	-3.19	124.87	127.43
6	G	1370	TPP	C7'-N3-C2	-3.09	119.76	125.35
6	C	1370	TPP	C6'-N1'-C2'	3.08	121.21	115.96
6	E	1370	TPP	O3B-PB-O2B	3.05	119.30	107.64
6	E	1370	TPP	N4'-C4'-N3'	2.96	121.21	117.03
6	G	1370	TPP	N4'-C4'-N3'	2.89	121.11	117.03
6	A	1370	TPP	N4'-C4'-N3'	2.86	121.07	117.03
6	C	1370	TPP	C5'-C4'-N3'	-2.84	116.78	121.24
6	A	1370	TPP	C5'-C4'-N3'	-2.75	116.92	121.24
6	E	1370	TPP	C7'-N3-C2	-2.48	120.87	125.35
6	A	1370	TPP	C5'-C6'-N1'	-2.40	119.83	123.82
6	E	1370	TPP	N1'-C2'-N3'	-2.25	121.66	125.54
6	G	1370	TPP	PA-O3A-PB	-2.24	125.14	132.83
6	E	1370	TPP	C5'-C4'-N3'	-2.24	117.72	121.24
6	A	1370	TPP	N1'-C2'-N3'	-2.20	121.76	125.54
6	G	1370	TPP	N1'-C2'-N3'	-2.15	121.83	125.54
6	E	1370	TPP	C5'-C6'-N1'	-2.14	120.25	123.82
6	C	1370	TPP	N4'-C4'-N3'	2.13	120.05	117.03
6	A	1370	TPP	CM2-C2'-N3'	2.09	120.42	117.15
6	G	1370	TPP	C5'-C6'-N1'	-2.09	120.34	123.82
6	G	1370	TPP	CM2-C2'-N3'	2.02	120.31	117.15
6	A	1370	TPP	C2'-N3'-C4'	2.02	121.22	118.08
6	C	1370	TPP	C5'-C7'-N3	-2.01	109.93	113.28

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1370	TPP	C4'-C5'-C7'-N3
6	A	1370	TPP	C4-C5-C6-C7
6	A	1370	TPP	C5-C6-C7-O7
6	A	1370	TPP	C7-O7-PA-O1A
6	A	1370	TPP	C7-O7-PA-O2A
6	A	1370	TPP	C7-O7-PA-O3A
6	C	1370	TPP	C4'-C5'-C7'-N3
6	C	1370	TPP	PB-O3A-PA-O7

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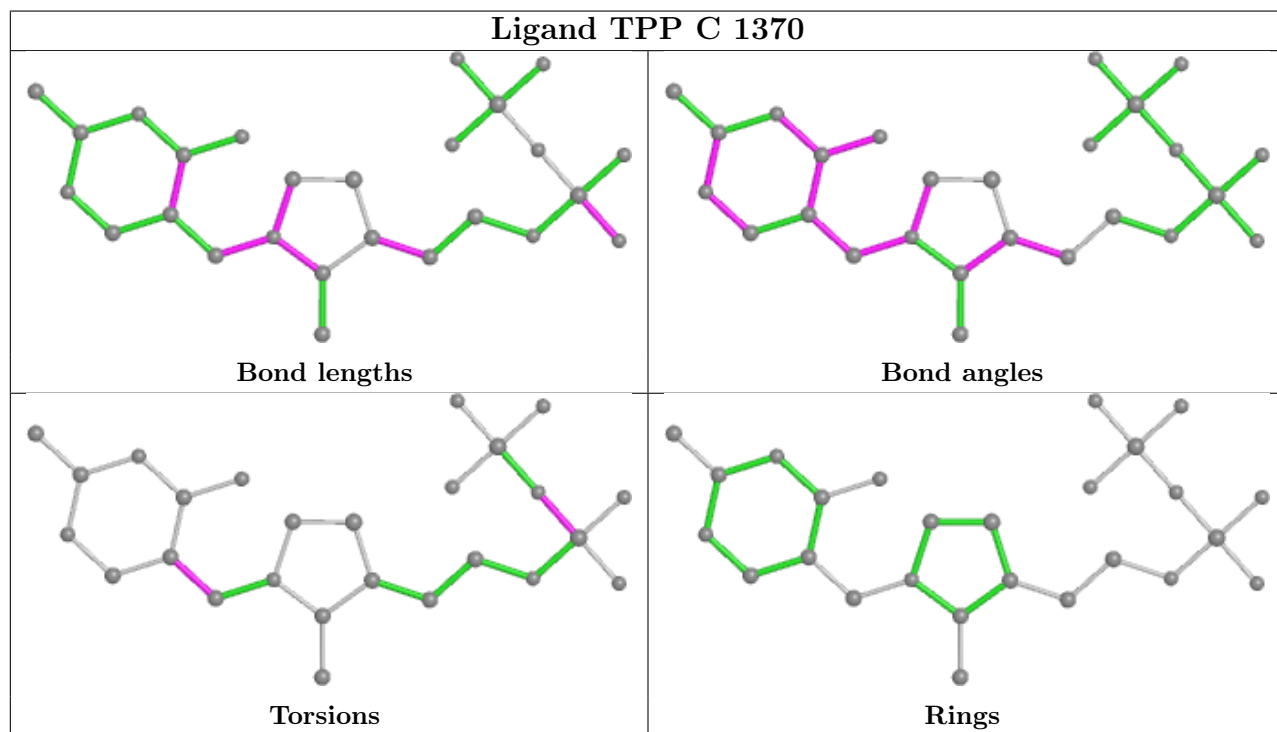
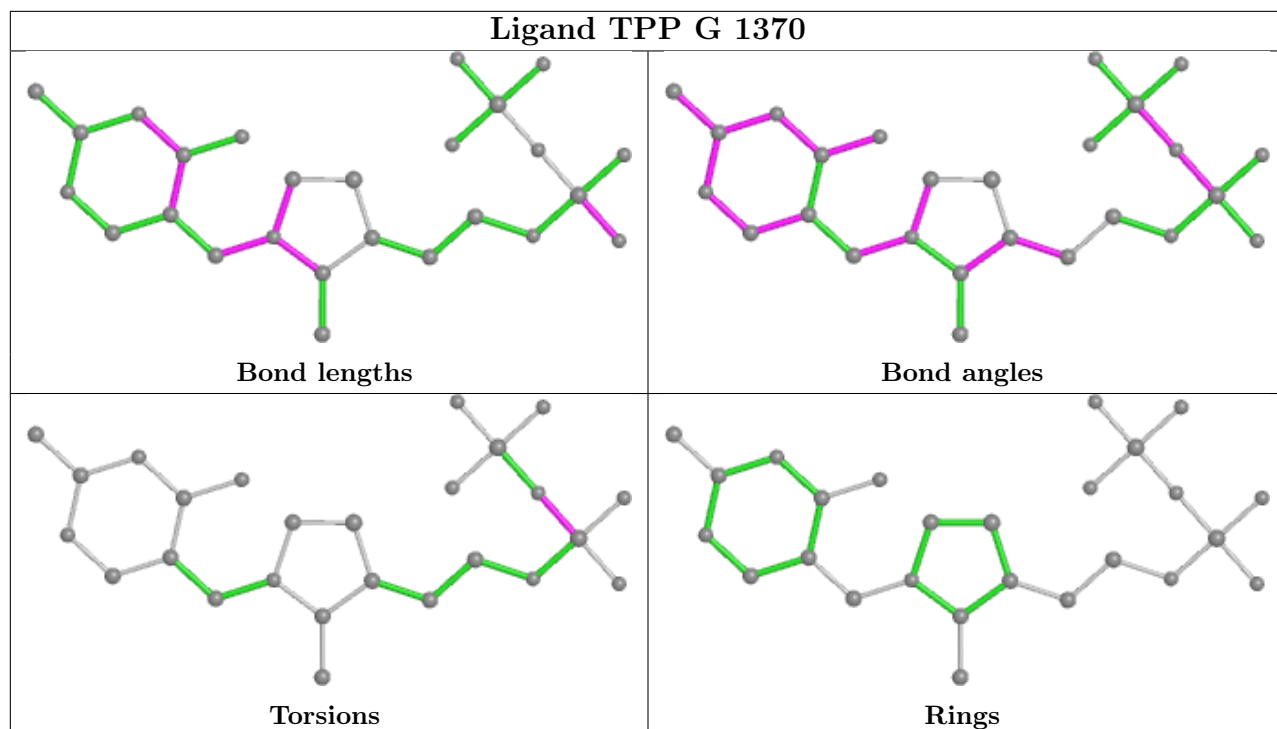
Mol	Chain	Res	Type	Atoms
6	E	1370	TPP	C5-C6-C7-O7
6	E	1370	TPP	C7-O7-PA-O1A
6	E	1370	TPP	C7-O7-PA-O2A
6	E	1370	TPP	PB-O3A-PA-O7
5	A	1369	PEG	O1-C1-C2-O2
5	A	1369	PEG	O2-C3-C4-O4
5	G	1369	PEG	O1-C1-C2-O2
5	G	1369	PEG	O2-C3-C4-O4
6	G	1370	TPP	PB-O3A-PA-O7
6	E	1370	TPP	C7-O7-PA-O3A
5	C	1369	PEG	C4-C3-O2-C2
5	G	1369	PEG	C1-C2-O2-C3
5	A	1369	PEG	C1-C2-O2-C3
6	C	1370	TPP	C6'-C5'-C7'-N3

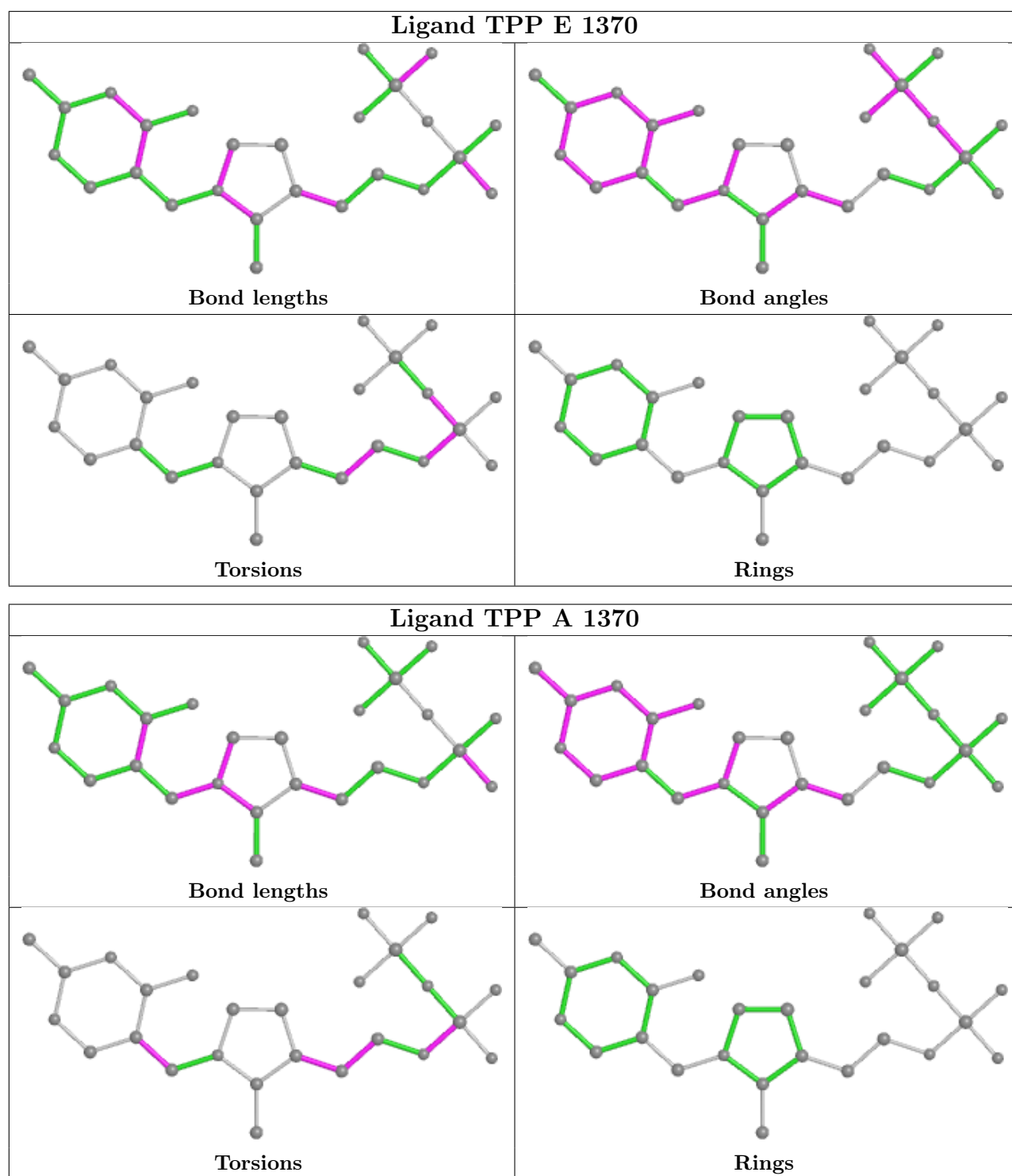
There are no ring outliers.

4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1370	TPP	12	0
6	C	1370	TPP	10	0
6	E	1370	TPP	11	0
6	A	1370	TPP	18	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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/368 (97%)	-0.18	13 (3%) 42 42	11, 19, 34, 47	2 (0%)
1	C	365/368 (99%)	-0.35	2 (0%) 91 90	8, 17, 29, 37	2 (0%)
1	E	350/368 (95%)	0.15	16 (4%) 32 31	18, 27, 42, 48	1 (0%)
1	G	364/368 (98%)	-0.18	6 (1%) 72 70	14, 21, 31, 43	1 (0%)
2	B	324/324 (100%)	-0.41	0 100 100	11, 17, 26, 31	0
2	D	324/324 (100%)	-0.47	0 100 100	10, 15, 22, 25	0
2	F	324/324 (100%)	-0.21	2 (0%) 89 88	15, 22, 32, 36	0
2	H	324/324 (100%)	-0.36	1 (0%) 94 93	13, 18, 25, 28	0
3	I	42/49 (85%)	1.37	11 (26%) 0 0	34, 49, 55, 57	0
3	J	35/49 (71%)	1.99	15 (42%) 0 0	43, 56, 63, 63	0
All	All	2811/2866 (98%)	-0.19	66 (2%) 60 59	8, 20, 38, 63	6 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	LEU	6.0
1	E	290	TRP	5.6
3	J	163	ILE	5.3
3	J	164	ASP	4.0
1	E	286	LEU	4.0
1	E	291	ALA	3.9
1	A	290	TRP	3.9
3	J	146	ILE	3.9
3	J	156	GLY	3.7
1	G	368	LYS	3.7
1	A	287	GLU	3.6
1	A	4	THR	3.6
1	E	275	GLY	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	J	129	VAL	3.5
1	G	5	PHE	3.5
1	E	284	LYS	3.4
3	I	168	ALA	3.4
3	I	148	LEU	3.4
1	E	287	GLU	3.4
1	E	289	GLU	3.4
3	I	167	LEU	3.4
3	J	166	PHE	3.3
3	J	143	GLY	3.3
1	E	368	LYS	3.2
3	J	145	ASP	3.0
1	C	4	THR	2.9
1	A	204	PHE	2.9
3	J	139	ALA	2.8
3	J	165	ALA	2.8
1	E	288	ASN	2.8
3	I	169	GLY	2.8
3	J	158	VAL	2.7
1	A	276	ASP	2.7
1	A	283	SER	2.7
1	A	275	GLY	2.7
2	F	123	HIS	2.6
3	I	128	ARG	2.6
3	J	144	VAL	2.6
1	E	266	PHE	2.6
3	I	163	ILE	2.6
1	G	6	GLN	2.6
1	C	368	LYS	2.6
1	A	289	GLU	2.5
1	E	285	GLU	2.5
1	E	277	ASP	2.5
1	E	134	GLY	2.5
1	A	288	ASN	2.4
1	E	274	SER	2.4
3	I	141	GLU	2.4
1	A	210	VAL	2.4
3	I	166	PHE	2.3
1	G	254	ASN	2.3
1	E	6	GLN	2.3
3	J	160	LYS	2.3
3	J	167	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	150	GLN	2.3
1	E	268	TYR	2.2
1	G	275	GLY	2.2
2	H	177	ARG	2.2
1	A	285	GLU	2.2
1	G	133	GLU	2.1
1	A	291	ALA	2.1
3	I	138	TYR	2.1
3	J	135	VAL	2.0
2	F	19	ASN	2.0
3	I	165	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

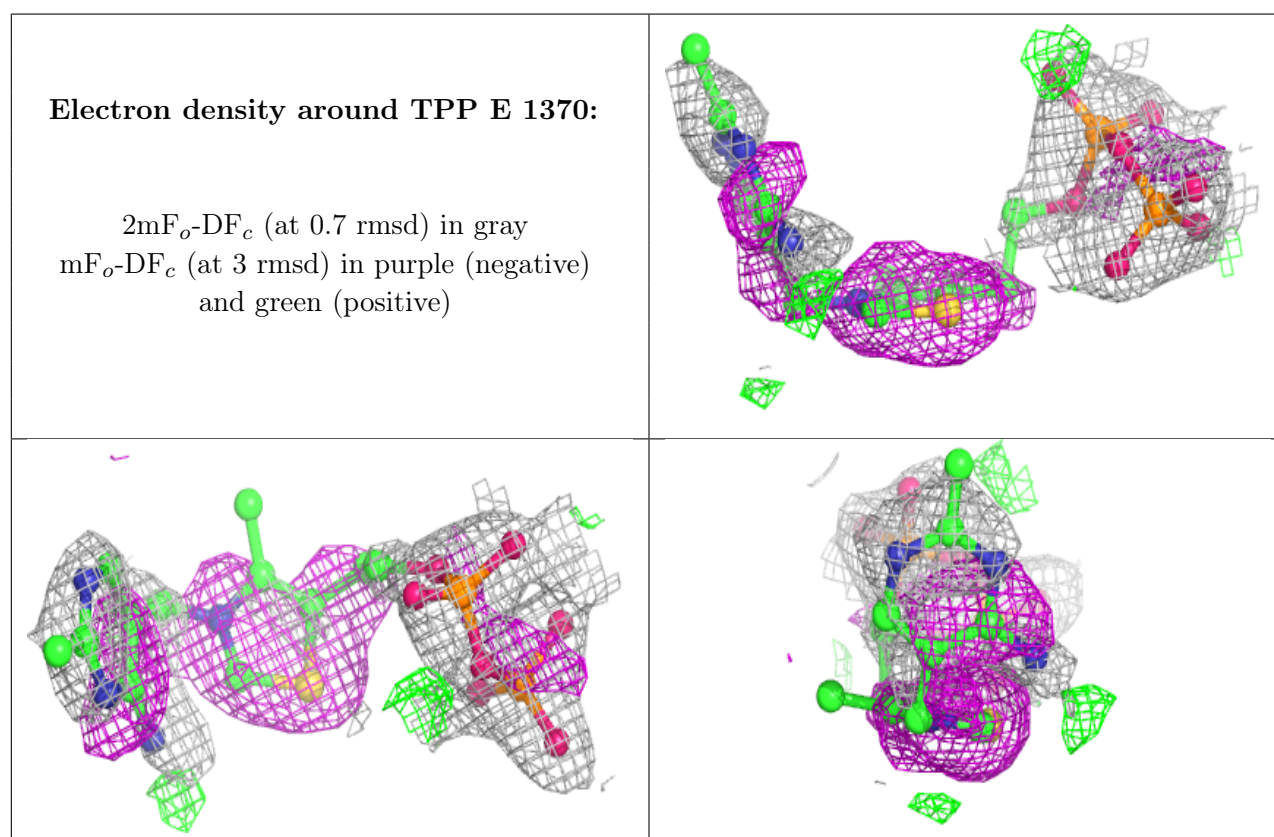
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	TPP	E	1370	26/26	0.78	0.38	42,44,45,45	0
5	PEG	C	1369	7/7	0.82	0.18	53,53,54,54	0
6	TPP	A	1370	26/26	0.83	0.27	34,38,38,39	0
6	TPP	C	1370	26/26	0.85	0.24	20,30,31,31	0
5	PEG	A	1369	7/7	0.85	0.15	51,51,51,51	0
6	TPP	G	1370	26/26	0.85	0.26	25,33,34,34	0
5	PEG	G	1369	7/7	0.89	0.13	42,42,42,42	0
4	MG	E	1368	1/1	0.97	0.04	24,24,24,24	0
4	MG	F	1326	1/1	0.99	0.07	14,14,14,14	0
4	MG	B	1326	1/1	0.99	0.04	15,15,15,15	0
4	MG	C	1368	1/1	0.99	0.12	7,7,7,7	0
4	MG	A	1368	1/1	0.99	0.04	20,20,20,20	0

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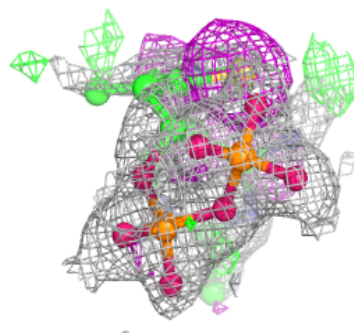
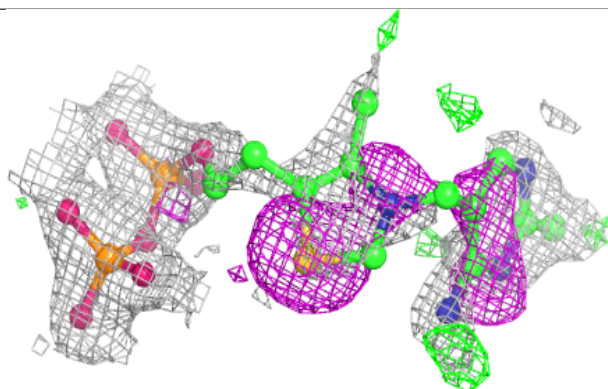
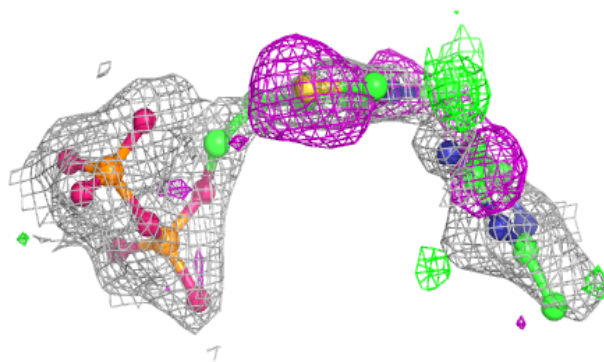
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	K	F	1325	1/1	0.99	0.03	28,28,28,28	0
7	K	H	1325	1/1	0.99	0.04	21,21,21,21	0
7	K	D	1325	1/1	1.00	0.04	19,19,19,19	0
4	MG	G	1368	1/1	1.00	0.10	9,9,9,9	0
7	K	B	1325	1/1	1.00	0.04	18,18,18,18	0

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.

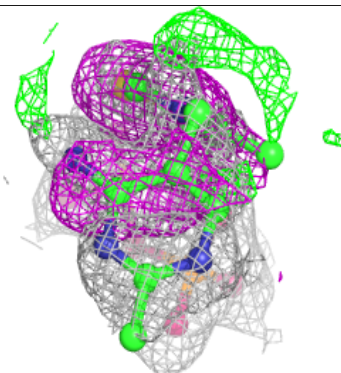
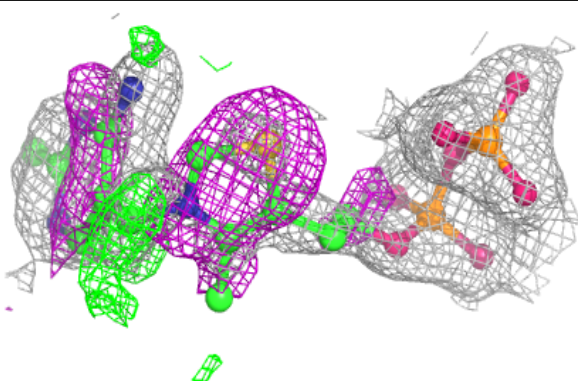
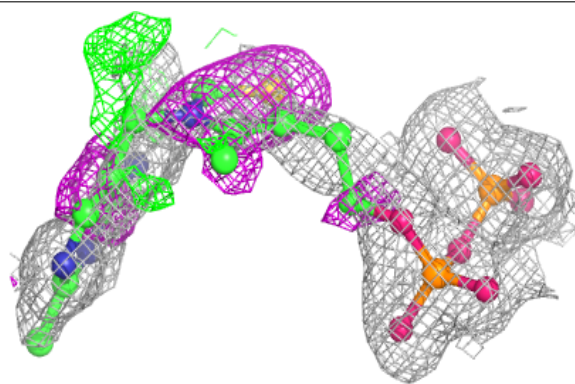


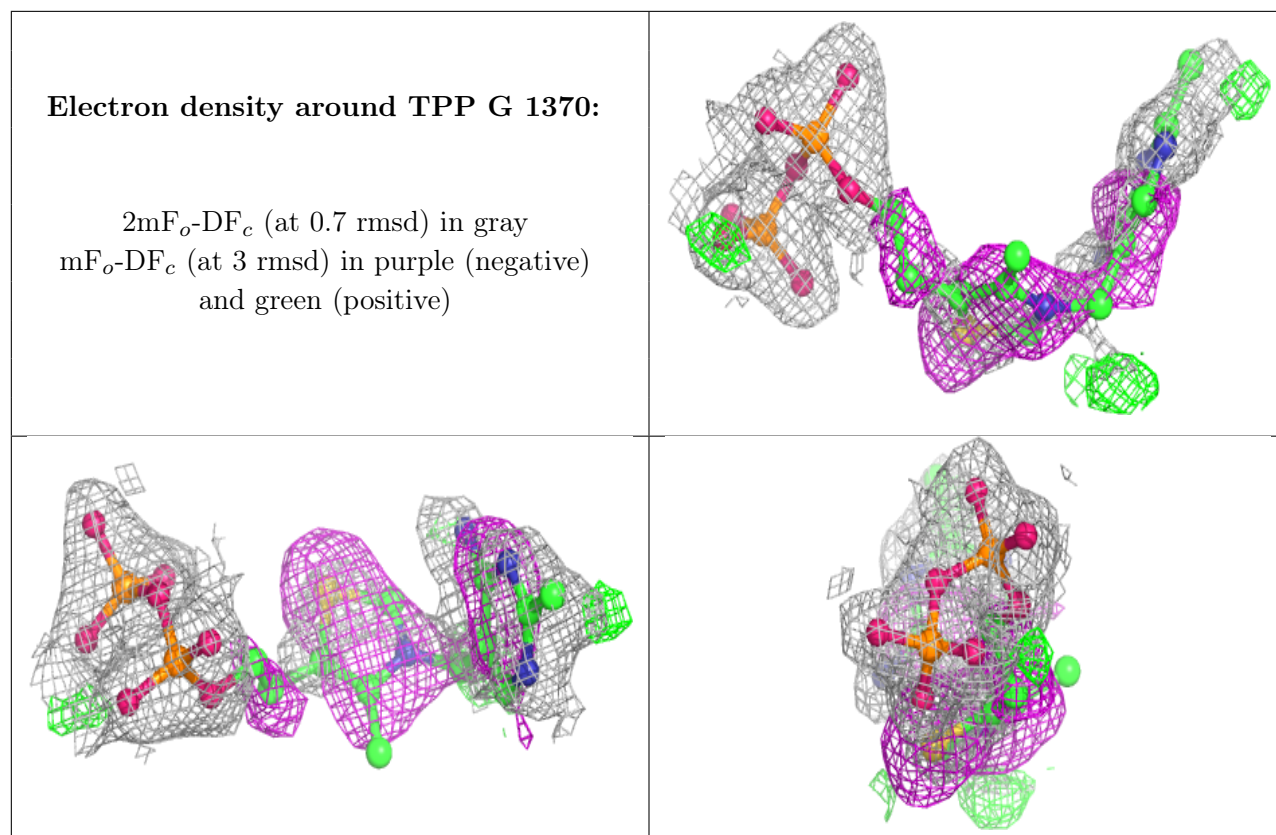
**Electron density around TPP A 1370:**

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

**Electron density around TPP 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.