



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:07 PM UTC

PDB ID : 1W85 / pdb_00001w85
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

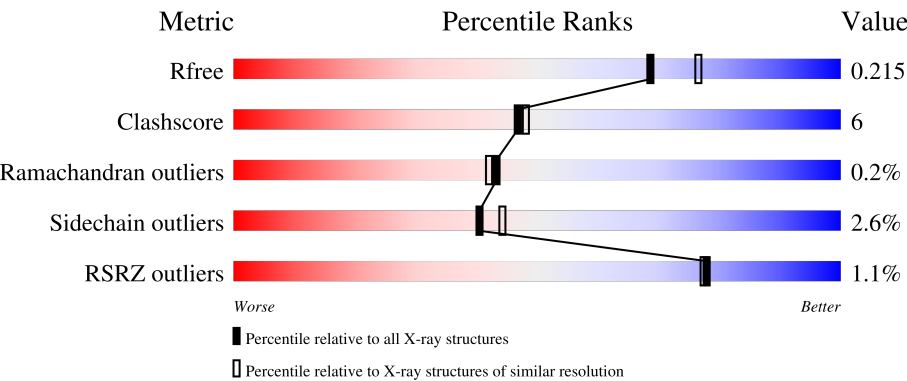
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	% 88%9%..
1	C	368	89%9%..
1	E	368	% 83%11%.5%
1	G	368	90%8%..
2	B	324	88%11%.

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Mol	Chain	Length	Quality of chain
2	D	324	 92% 7% .
2	F	324	 88% 11%
2	H	324	 88% 12%
3	I	49	 16% 78% . . 14%
3	J	49	 24% 55% 12% . 29%

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

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

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

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

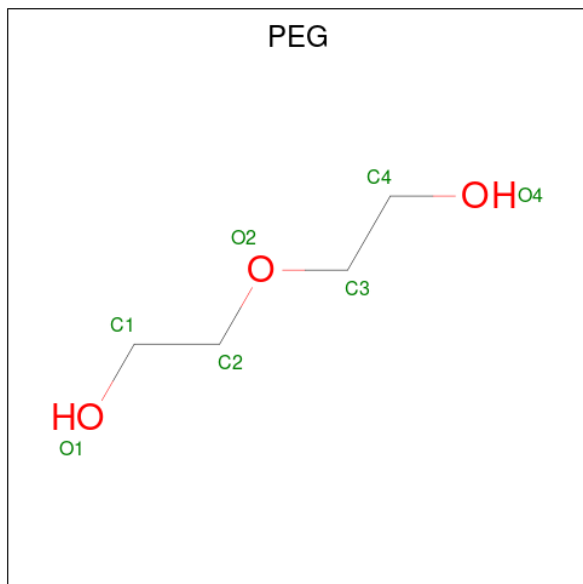
- Molecule 3 is a protein called DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE.

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

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

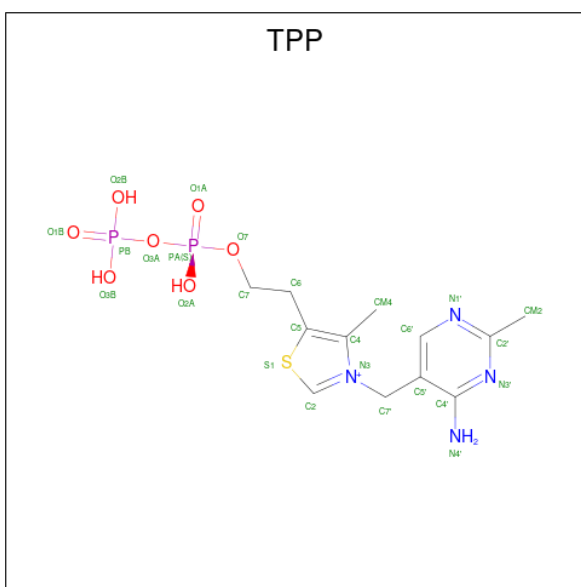
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
6	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
6	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
6	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	224	Total O 224 224	0	0

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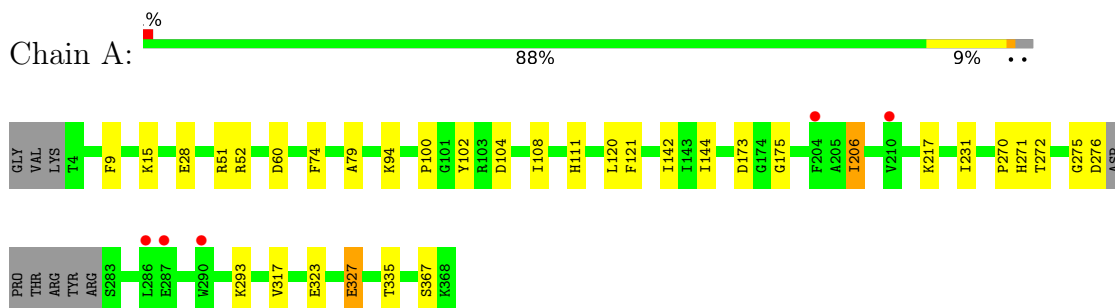
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	198	Total 198	O 198	0	0
8	C	282	Total 282	O 282	0	0
8	D	241	Total 241	O 241	0	0
8	E	137	Total 137	O 137	0	0
8	F	169	Total 169	O 169	0	0
8	G	234	Total 234	O 234	0	0
8	H	227	Total 227	O 227	0	0
8	I	12	Total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

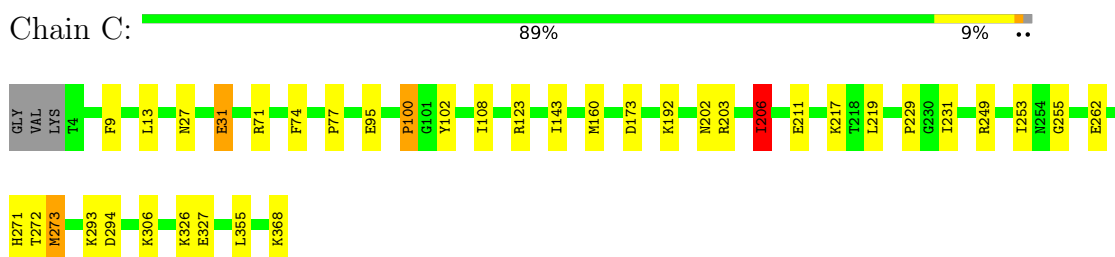
3 Residue-property plots

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.

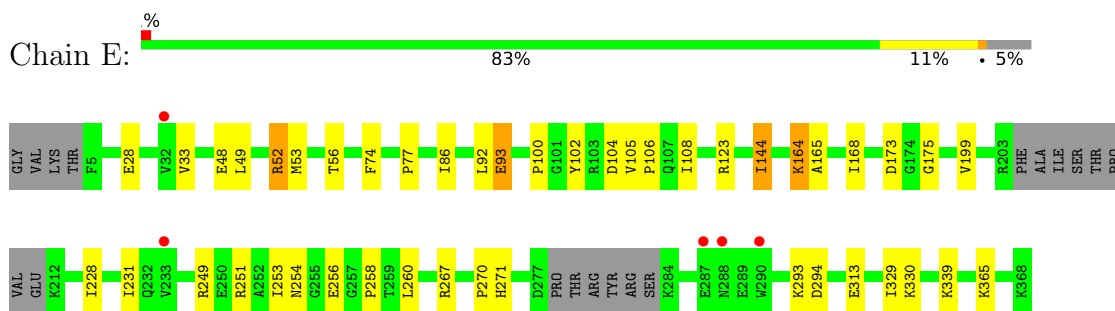
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



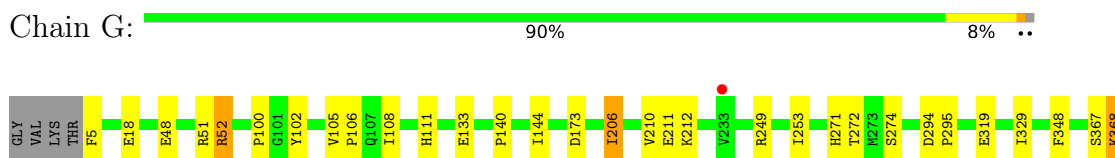
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



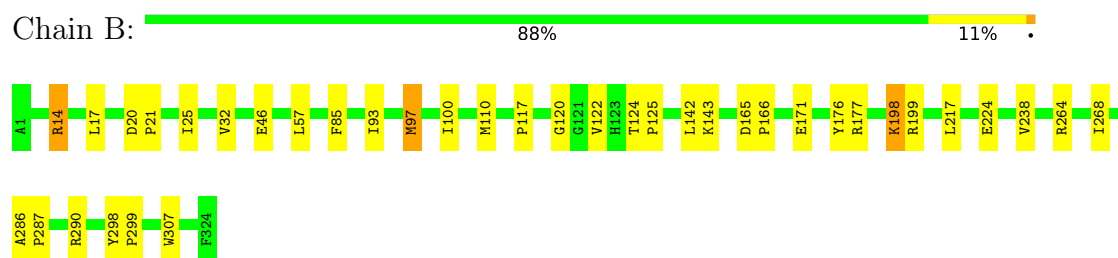
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



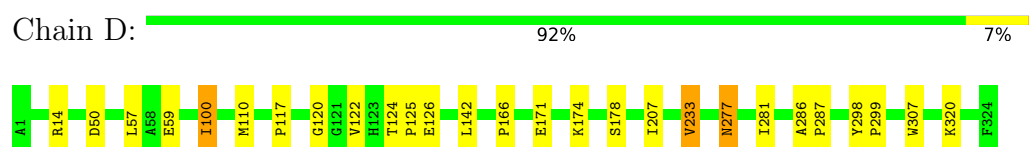
- Molecule 1: PYRUVATE DEHYDROGENASE E1 COMPONENT, ALPHA SUBUNIT



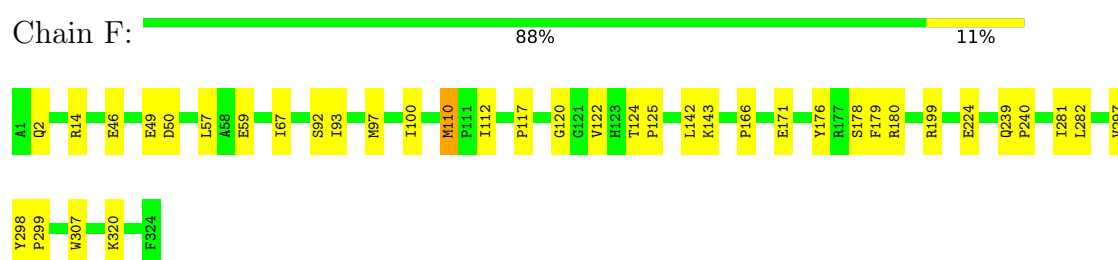
• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



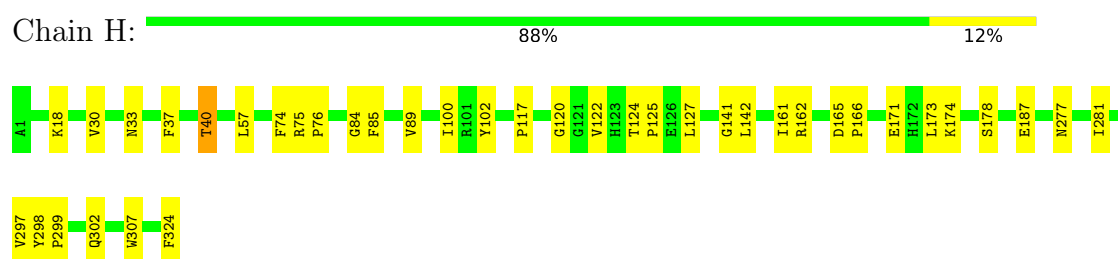
• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



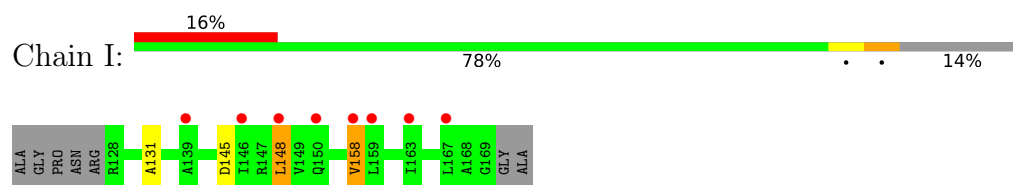
• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT

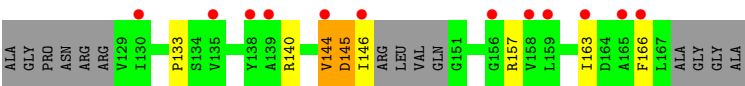


• Molecule 3: DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE



• Molecule 3: DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 94.6 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.01Å)	Xtriage
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 (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23509	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, K, TPP, 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	0.81	2/2831 (0.1%)	0.88	1/3832 (0.0%)
1	C	0.83	1/2940 (0.0%)	0.87	1/3972 (0.0%)
1	E	0.67	0/2750	0.86	0/3712
1	G	0.73	0/2917	0.87	0/3945
2	B	0.86	3/2516 (0.1%)	0.89	1/3415 (0.0%)
2	D	0.87	0/2529	0.91	0/3430
2	F	0.78	1/2519 (0.0%)	0.86	0/3419
2	H	0.80	0/2529	0.88	0/3430
3	I	0.67	0/304	0.83	0/407
3	J	0.77	1/233 (0.4%)	1.02	0/312
All	All	0.79	8/22068 (0.0%)	0.88	3/29874 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	ARG	CD-NE	11.01	1.61	1.46
2	F	110	MET	SD-CE	-8.86	1.57	1.79
1	C	273	MET	SD-CE	-7.06	1.61	1.79
3	J	166	PHE	C-N	-6.81	1.23	1.33
2	B	97	MET	SD-CE	-6.50	1.63	1.79
1	A	367	SER	C-N	-6.42	1.24	1.33
2	B	199	ARG	CZ-NH2	-5.53	1.26	1.33
1	A	52	ARG	CZ-NH2	5.33	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	ARG	NE-CZ-NH2	-6.53	113.32	119.20
1	C	100	PRO	CB-CA-C	-5.36	103.93	110.95
1	A	367	SER	O-C-N	-5.03	114.95	123.00

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	2771	0	2713	33	0
1	C	2877	0	2845	33	0
1	E	2695	0	2630	33	0
1	G	2854	0	2806	21	0
2	B	2470	0	2476	29	0
2	D	2483	0	2504	27	0
2	F	2473	0	2485	31	0
2	H	2483	0	2504	35	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	1	0
5	G	7	0	10	0	0
6	A	26	0	16	19	0
6	C	26	0	16	12	0
6	E	26	0	16	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	234	0	0	3	0
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	249	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 6.

All (249) 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	1.59	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
2:F:67:ILE:HG12	2:F:110:MET:HE1	1.64	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
2:F:57:LEU:HD11	6:G:1370:TPP:HM43	1.71	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:LEU:CD1	6:G:1370:TPP:HM43	2.22	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
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
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: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:F:67:ILE:HA	2:F:110:MET:HE1	1.78	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:102:TYR:OH	6:E:1370:TPP:S1	2.55	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: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
2:B:57:LEU:HD11	6:C:1370:TPP:HM43	1.83	0.59
2:F:67:ILE:CG1	2:F:110:MET:HE1	2.31	0.59
1:A:100:PRO:HG2	1:A:108:ILE:CG2	2.33	0.58
1:C:77:PRO:CG	1:C:273:MET:HE3	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG13	6:A:1370:TPP:C6	2.32	0.58
6:A:1370:TPP:HM43	2:D:57:LEU:CD1	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
2:F:298:TYR:CG	2:F:299:PRO:HD2	2.39	0.58
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
3:J:145:ASP:C	3:J:146:ILE:HG22	2.22	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
6:A:1370:TPP:HM43	2:D:57:LEU:HD11	1.87	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:E:28:GLU:CD	1:E:28:GLU:H	2.13	0.55
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
2:F:110:MET:HE3	2:F:112:ILE:HD12	1.90	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
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
1:E:164:LYS:C	1:E:253:ILE:CD1	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:57:LEU:CD1	6:C:1370:TPP:HM43	2.41	0.51
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
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:49:LEU:HG	1:E:53:MET:HE2	1.95	0.48
1:E:164:LYS:C	1:E:253:ILE:HD11	2.37	0.48
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
2:D:100:ILE:HD12	2:D:110:MET:HE3	1.95	0.48
1:E:165:ALA:N	1:E:253:ILE:CD1	2.77	0.48
1:C:143:ILE:HG23	6:C:1370:TPP:HM23	1.95	0.48
1:C:160:MET:HE2	5:C:1369:PEG:H22	1.96	0.48
1:A:102:TYR:CZ	6:A:1370:TPP:S1	3.07	0.47
2:H:324:PHE:C	3:J:157:ARG:HH22	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LYS:HA	8:C:2276:HOH:O	2.13	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
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
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:57:LEU:HD11	6:G:1370:TPP:CM4	2.45	0.44
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
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
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:67:ILE:HG12	2:F:110:MET:HE2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:H:142:LEU:HD23	2:H:166:PRO:HB2	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
1:C:219:LEU:HB2	1:C:262:GLU:CD	2.45	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
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
2:H:297:VAL:O	2:H:298:TYR:C	2.64	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
2:B:100:ILE:HG21	2:B:110:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLU:HG3	1:E:249:ARG:CZ	2.51	0.41
2:F:297:VAL:O	2:F:298:TYR:C	2.64	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
1:C:293:LYS:O	1:C:294:ASP:C	2.64	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
1:E:293:LYS:O	1:E:294:ASP:C	2.64	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: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
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%)	21	17
1	C	363/368 (99%)	354 (98%)	8 (2%)	1 (0%)	36	35
1	E	344/368 (94%)	337 (98%)	7 (2%)	0	100	100
1	G	362/368 (98%)	351 (97%)	10 (3%)	1 (0%)	36	35
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
3	J	31/49 (63%)	26 (84%)	4 (13%)	1 (3%)	3	1
All	All	2783/2866 (97%)	2710 (97%)	68 (2%)	5 (0%)	43	42

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
1	G	206	ILE

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	279/304 (92%)	274 (98%)	5 (2%)	51	58
1	C	296/304 (97%)	287 (97%)	9 (3%)	36	38
1	E	270/304 (89%)	256 (95%)	14 (5%)	21	18
1	G	292/304 (96%)	281 (96%)	11 (4%)	29	29
2	B	258/263 (98%)	253 (98%)	5 (2%)	50	56
2	D	262/263 (100%)	259 (99%)	3 (1%)	65	73
2	F	259/263 (98%)	254 (98%)	5 (2%)	50	56
2	H	262/263 (100%)	260 (99%)	2 (1%)	73	80
3	I	28/36 (78%)	26 (93%)	2 (7%)	13	10
3	J	21/36 (58%)	19 (90%)	2 (10%)	8	5
All	All	2227/2340 (95%)	2169 (97%)	58 (3%)	40	44

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	94	LYS
1	A	111	HIS
1	A	173	ASP
1	A	327	GLU
2	B	14	ARG
2	B	176	TYR
2	B	177	ARG
2	B	198	LYS
2	B	224	GLU
1	C	13	LEU
1	C	31	GLU
1	C	173	ASP
1	C	206	ILE
1	C	211	GLU
1	C	217	LYS
1	C	306	LYS
1	C	326	LYS
1	C	327	GLU
2	D	100	ILE
2	D	233	VAL
2	D	277	ASN
1	E	33	VAL
1	E	52	ARG
1	E	93	GLU
1	E	144	ILE
1	E	164	LYS
1	E	173	ASP
1	E	231	ILE
1	E	254	ASN
1	E	267	ARG
1	E	313	GLU
1	E	329	ILE
1	E	330	LYS
1	E	339	LYS
1	E	365	LYS
2	F	100	ILE
2	F	176	TYR
2	F	281	ILE
2	F	282	LEU
2	F	320	LYS
1	G	5	PHE
1	G	18	GLU

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Mol	Chain	Res	Type
1	G	52	ARG
1	G	111	HIS
1	G	173	ASP
1	G	206	ILE
1	G	210	VAL
1	G	211	GLU
1	G	274	SER
1	G	329	ILE
1	G	368	LYS
2	H	18	LYS
2	H	40	THR
3	I	148	LEU
3	I	158	VAL
3	J	144	VAL
3	J	145	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	136	ASN
1	A	178	GLN
1	A	202	ASN
1	A	271	HIS
2	B	33	ASN
2	B	44	GLN
2	B	72	GLN
2	B	81	GLN
2	B	139	GLN
2	B	265	GLN
2	B	302	GLN
2	B	323	ASN
1	C	271	HIS
2	D	19	ASN
2	D	123	HIS
2	D	139	GLN
1	E	61	GLN
2	F	139	GLN
2	F	271	ASN
2	F	277	ASN
1	G	271	HIS
2	H	72	GLN

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Mol	Chain	Res	Type
2	H	139	GLN
2	H	265	GLN
2	H	271	ASN
2	H	323	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	$\# Z > 2$
6	TPP	C	1370	4	26,27,27	1.82	6 (23%)	38,40,40	1.52	5 (13%)
6	TPP	A	1370	4	26,27,27	1.71	6 (23%)	38,40,40	1.68	11 (28%)
5	PEG	G	1369	-	6,6,6	0.48	0	5,5,5	0.22	0
5	PEG	C	1369	-	6,6,6	0.51	0	5,5,5	0.24	0
5	PEG	A	1369	-	6,6,6	0.49	0	5,5,5	0.20	0
6	TPP	G	1370	4	26,27,27	1.83	6 (23%)	38,40,40	1.61	7 (18%)
6	TPP	E	1370	4	26,27,27	1.71	6 (23%)	38,40,40	1.96	11 (28%)

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
6	TPP	C	1370	4	-	3/17/17/17	0/2/2/2
6	TPP	A	1370	4	-	7/17/17/17	0/2/2/2
5	PEG	G	1369	-	-	3/4/4/4	-
5	PEG	C	1369	-	-	1/4/4/4	-
5	PEG	A	1369	-	-	3/4/4/4	-
6	TPP	G	1370	4	-	1/17/17/17	0/2/2/2
6	TPP	E	1370	4	-	6/17/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1370	TPP	C5'-C4'	5.50	1.51	1.42
6	G	1370	TPP	C5'-C4'	5.14	1.51	1.42
6	A	1370	TPP	C5'-C4'	4.54	1.50	1.42
6	E	1370	TPP	C5'-C4'	4.51	1.50	1.42
6	C	1370	TPP	PA-O3A	3.49	1.63	1.59
6	E	1370	TPP	C4-N3	-3.32	1.33	1.39
6	G	1370	TPP	C4-N3	-3.05	1.33	1.39
6	G	1370	TPP	C4'-N3'	3.04	1.39	1.35
6	C	1370	TPP	C4-N3	-2.97	1.33	1.39
6	A	1370	TPP	PA-O3A	2.96	1.62	1.59
6	A	1370	TPP	C4-N3	-2.92	1.33	1.39
6	G	1370	TPP	PA-O3A	2.88	1.62	1.59
6	E	1370	TPP	PB-O1B	2.84	1.59	1.50
6	A	1370	TPP	C2-N3	-2.52	1.26	1.32
6	A	1370	TPP	PA-O1A	2.44	1.59	1.50
6	E	1370	TPP	PA-O3A	2.41	1.62	1.59
6	E	1370	TPP	PA-O1A	2.41	1.59	1.50
6	C	1370	TPP	C7'-N3	-2.39	1.43	1.48
6	G	1370	TPP	PA-O1A	2.32	1.58	1.50
6	E	1370	TPP	C4'-N3'	2.22	1.38	1.35
6	C	1370	TPP	PA-O1A	2.15	1.58	1.50
6	C	1370	TPP	C4'-N3'	2.15	1.37	1.35
6	A	1370	TPP	C7'-N3	-2.12	1.44	1.48
6	G	1370	TPP	C5-S1	-2.06	1.67	1.72

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1370	TPP	C2-S1-C5	-7.49	86.25	91.22
6	G	1370	TPP	C2-S1-C5	-4.97	87.92	91.22
6	A	1370	TPP	C2-S1-C5	-4.49	88.24	91.22
6	G	1370	TPP	C6'-N1'-C2'	3.77	122.26	116.07
6	A	1370	TPP	C6'-N1'-C2'	3.68	122.12	116.07
6	C	1370	TPP	C2-S1-C5	-3.56	88.85	91.22
6	E	1370	TPP	C6'-N1'-C2'	3.52	121.85	116.07
6	C	1370	TPP	C6'-N1'-C2'	3.13	121.21	116.07
6	E	1370	TPP	N4'-C4'-N3'	3.10	121.21	117.03
6	C	1370	TPP	C5'-C4'-N3'	-3.09	116.78	121.31
6	E	1370	TPP	O3B-PB-O2B	3.07	119.30	107.80
6	G	1370	TPP	N4'-C4'-N3'	3.03	121.11	117.03
6	A	1370	TPP	N4'-C4'-N3'	3.00	121.07	117.03
6	A	1370	TPP	C5'-C4'-N3'	-2.99	116.92	121.31
6	E	1370	TPP	S1-C2-N3	2.57	115.56	112.30
6	A	1370	TPP	C5'-C6'-N1'	-2.46	119.83	123.83
6	E	1370	TPP	C5'-C4'-N3'	-2.45	117.72	121.31
6	E	1370	TPP	C4-C5-S1	2.45	114.38	110.56
6	E	1370	TPP	N1'-C2'-N3'	-2.33	121.66	125.53
6	A	1370	TPP	N1'-C2'-N3'	-2.27	121.76	125.53
6	C	1370	TPP	C7'-N3-C2	-2.27	118.75	123.48
6	A	1370	TPP	C6-C5-C4	-2.26	122.51	128.17
6	C	1370	TPP	N4'-C4'-N3'	2.24	120.05	117.03
6	G	1370	TPP	N1'-C2'-N3'	-2.22	121.83	125.53
6	E	1370	TPP	C5'-C6'-N1'	-2.20	120.25	123.83
6	A	1370	TPP	CM2-C2'-N3'	2.20	120.42	117.13
6	G	1370	TPP	C5'-C6'-N1'	-2.15	120.34	123.83
6	G	1370	TPP	C5'-C4'-N3'	-2.14	118.17	121.31
6	E	1370	TPP	C6-C5-C4	-2.14	122.81	128.17
6	A	1370	TPP	C7'-N3-C2	-2.14	119.03	123.48
6	G	1370	TPP	CM2-C2'-N3'	2.12	120.31	117.13
6	A	1370	TPP	C6'-C5'-C4'	2.11	118.15	115.55
6	E	1370	TPP	C7-C6-C5	-2.11	106.11	112.73
6	A	1370	TPP	C2'-N3'-C4'	2.03	121.22	118.10

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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

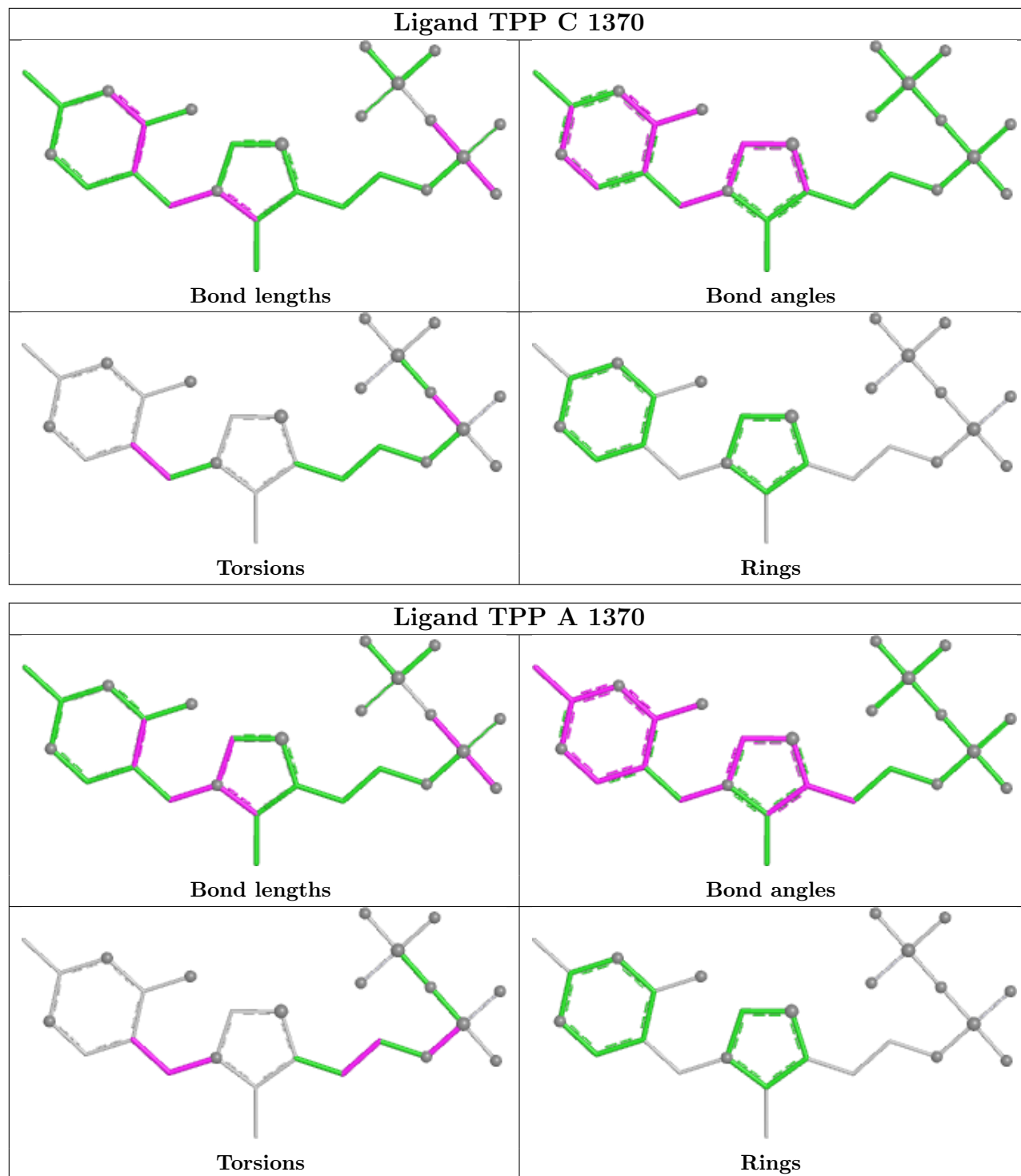
There are no ring outliers.

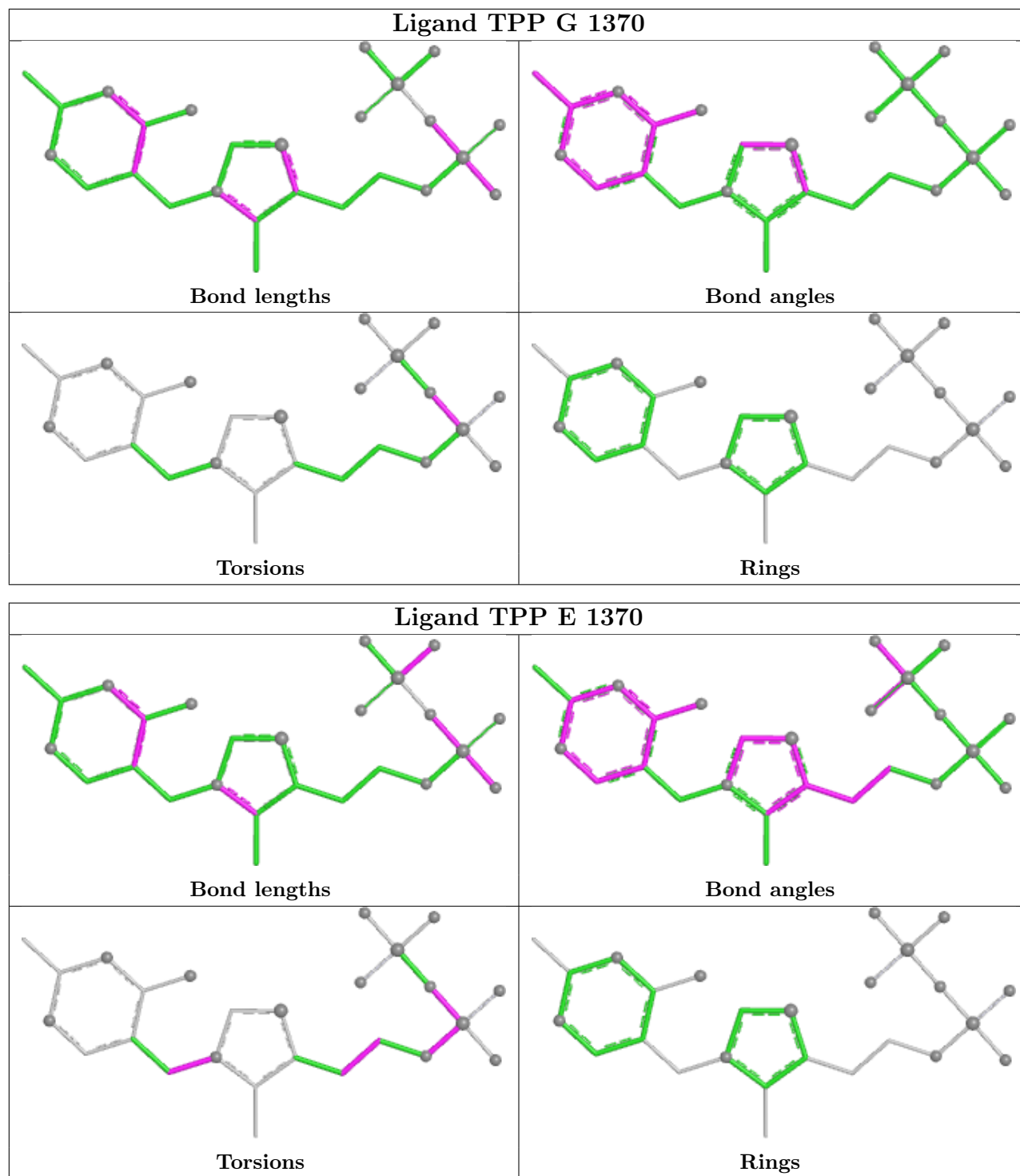
5 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1370	TPP	12	0
6	A	1370	TPP	19	0
5	C	1369	PEG	1	0
6	G	1370	TPP	12	0
6	E	1370	TPP	10	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 ⓘ

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(Å ²)	Q<0.9
1	A	359/368 (97%)	-0.27	5 (1%) 73 73	11, 19, 34, 47	2 (0%)
1	C	365/368 (99%)	-0.45	0 100 100	8, 17, 29, 37	2 (0%)
1	E	350/368 (95%)	-0.01	5 (1%) 73 73	18, 27, 42, 48	1 (0%)
1	G	364/368 (98%)	-0.28	1 (0%) 90 89	14, 21, 31, 43	1 (0%)
2	B	324/324 (100%)	-0.50	0 100 100	11, 17, 26, 31	0
2	D	324/324 (100%)	-0.60	0 100 100	10, 15, 22, 25	0
2	F	324/324 (100%)	-0.29	0 100 100	15, 22, 32, 36	0
2	H	324/324 (100%)	-0.46	0 100 100	13, 18, 25, 28	0
3	I	42/49 (85%)	1.25	8 (19%) 3 3	34, 49, 55, 57	0
3	J	35/49 (71%)	1.89	12 (34%) 1 1	43, 56, 63, 63	0
All	All	2811/2866 (98%)	-0.30	31 (1%) 78 77	8, 20, 38, 63	6 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	158	VAL	4.6
1	E	290	TRP	3.9
3	J	139	ALA	3.8
1	A	286	LEU	3.8
3	J	163	ILE	3.7
1	E	287	GLU	3.5
1	A	287	GLU	3.4
3	I	158	VAL	3.4
1	A	290	TRP	3.3
3	J	159	LEU	3.1
3	J	144	VAL	3.1
3	J	135	VAL	2.9
3	I	148	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	J	146	ILE	2.9
3	J	130	ILE	2.8
1	A	204	PHE	2.7
3	J	156	GLY	2.5
3	I	167	LEU	2.5
1	E	233	VAL	2.5
3	I	150	GLN	2.4
3	I	159	LEU	2.3
1	E	32	VAL	2.3
3	I	139	ALA	2.3
3	J	138	TYR	2.3
3	I	163	ILE	2.2
1	A	210	VAL	2.2
1	G	233	VAL	2.2
1	E	288	ASN	2.2
3	J	166	PHE	2.1
3	I	146	ILE	2.0
3	J	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 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.

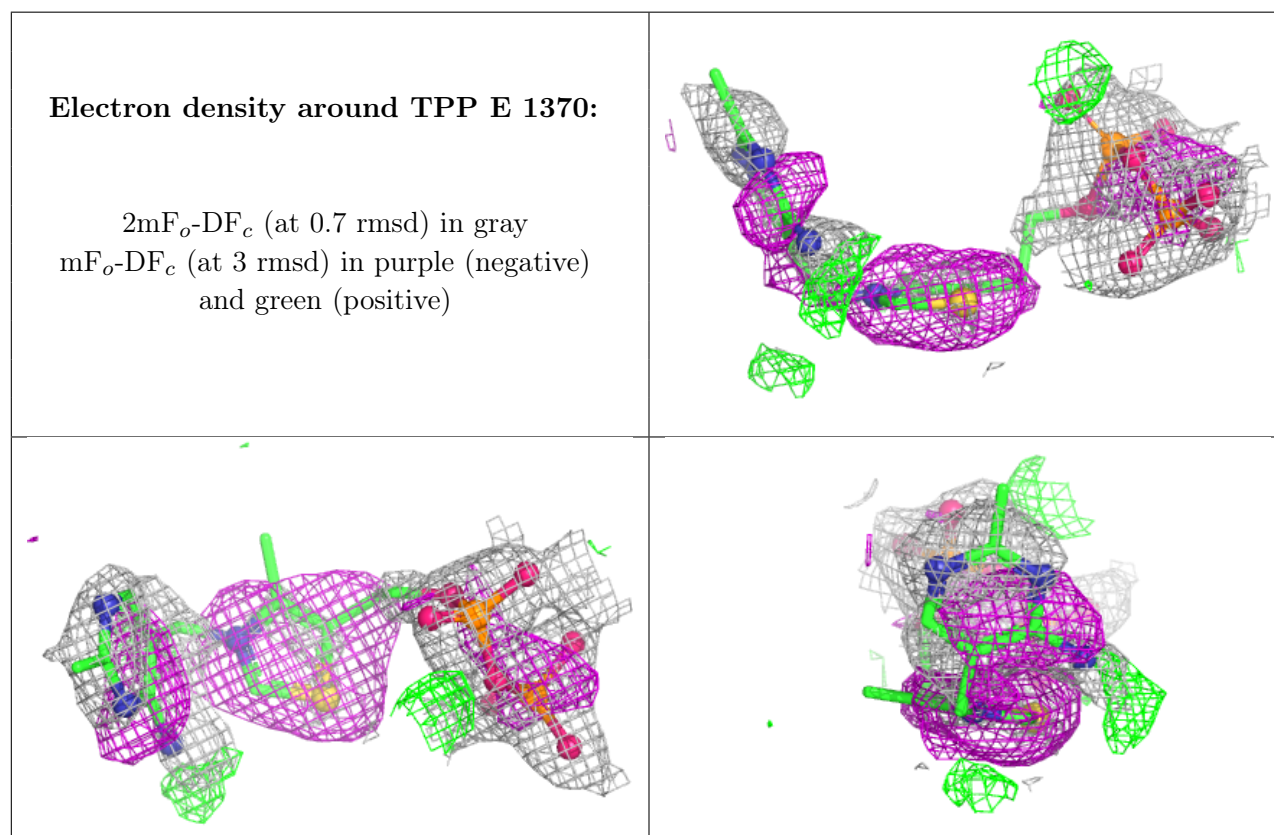
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	C	1369	7/7	0.75	0.15	53,53,54,54	0
6	TPP	E	1370	26/26	0.76	0.17	42,44,45,45	0
6	TPP	A	1370	26/26	0.79	0.15	34,38,38,39	0
5	PEG	G	1369	7/7	0.82	0.11	42,42,42,42	0
6	TPP	G	1370	26/26	0.85	0.17	25,33,34,34	0

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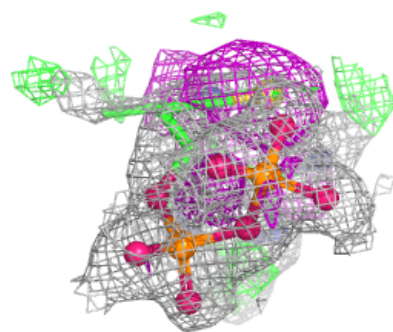
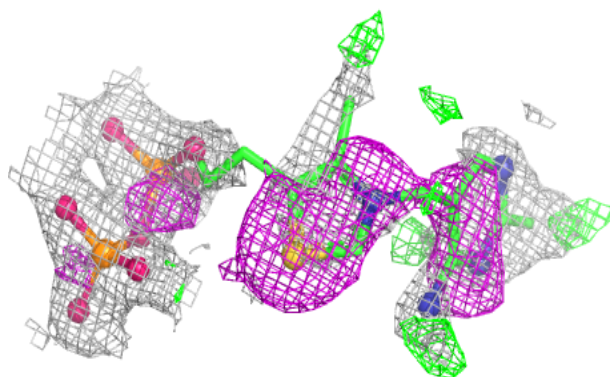
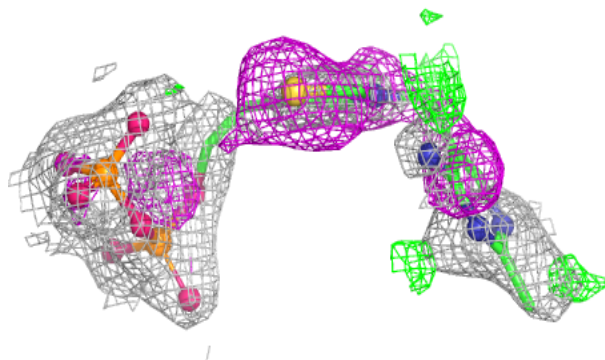
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	TPP	C	1370	26/26	0.87	0.15	20,30,31,31	0
5	PEG	A	1369	7/7	0.89	0.12	51,51,51,51	0
4	MG	E	1368	1/1	0.97	0.03	24,24,24,24	0
4	MG	F	1326	1/1	0.98	0.02	14,14,14,14	0
4	MG	A	1368	1/1	0.98	0.03	20,20,20,20	0
7	K	F	1325	1/1	0.98	0.05	28,28,28,28	0
4	MG	G	1368	1/1	0.99	0.06	9,9,9,9	0
4	MG	B	1326	1/1	0.99	0.02	15,15,15,15	0
7	K	B	1325	1/1	0.99	0.05	18,18,18,18	0
7	K	D	1325	1/1	0.99	0.05	19,19,19,19	0
4	MG	C	1368	1/1	0.99	0.08	7,7,7,7	0
7	K	H	1325	1/1	0.99	0.04	21,21,21,21	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.

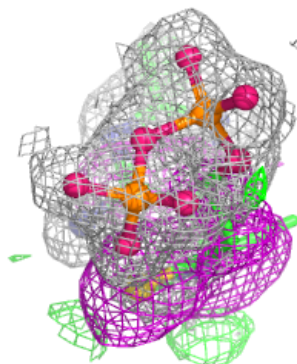
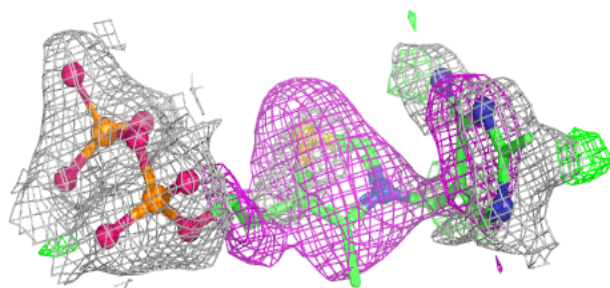
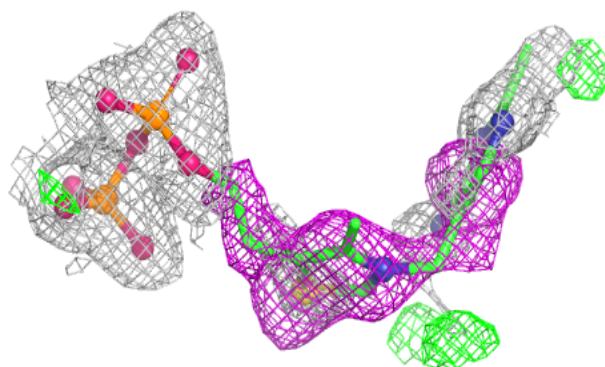


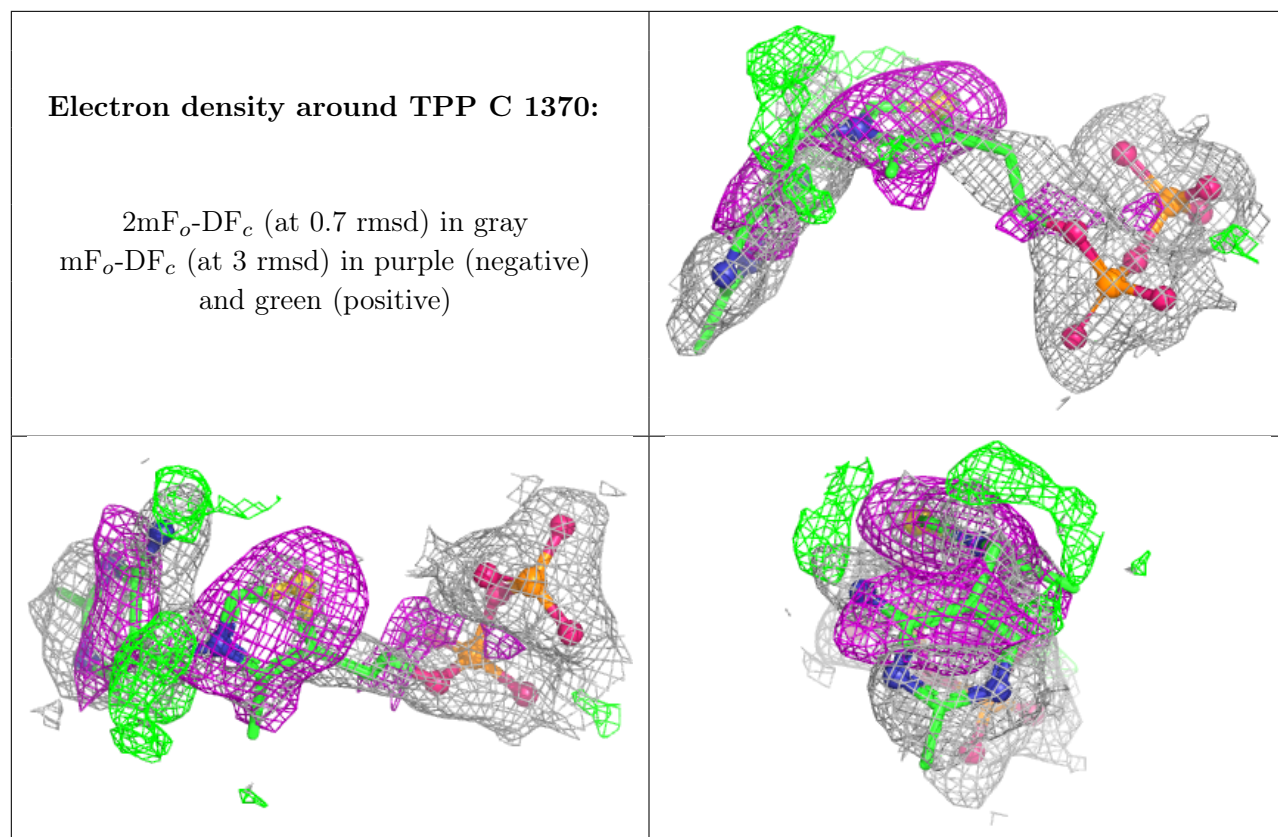
Electron density around TPP A 1370:

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

**Electron density around TPP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.