



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:58 am BST

PDB ID : 6CIN  
Title : Crystal structure of pyruvate:ferredoxin oxidoreductase from *Moorella thermoacetica*  
Authors : Chen, P.Y.-T.; Drennan, C.L.  
Deposited on : 2018-02-24  
Resolution : 2.60 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

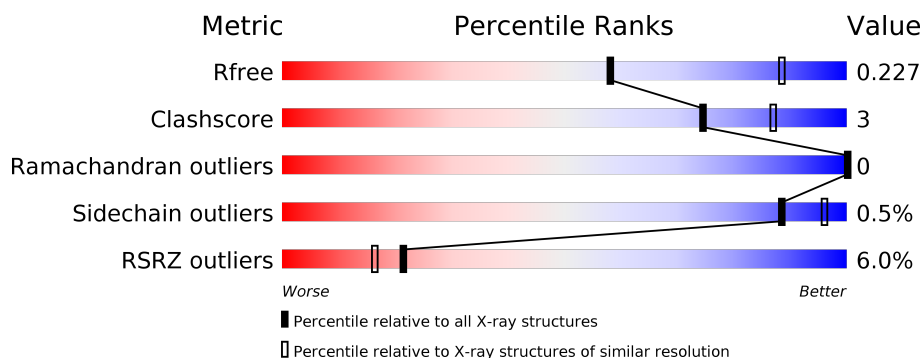
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	1171	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> </div>
1	B	1171	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div></div> </div> </div>
1	C	1171	<div> <div>8%</div> <div> <div></div> <div>92%</div> <div>8%</div> <div></div> </div> </div>
1	D	1171	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> </div>
1	E	1171	<div> <div>9%</div> <div> <div></div> <div>90%</div> <div>10%</div> <div></div> </div> </div>
1	F	1171	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	1207	-	-	X	-

## 2 Entry composition [i](#)

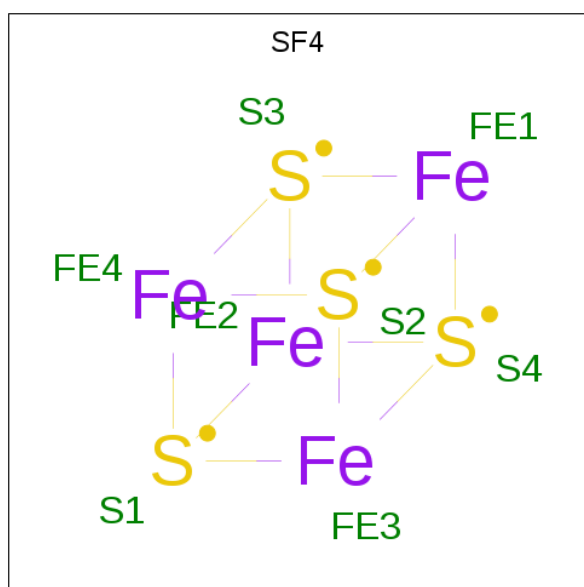
There are 6 unique types of molecules in this entry. The entry contains 53870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-FERREDOXIN OXIDOREDUCTASE.

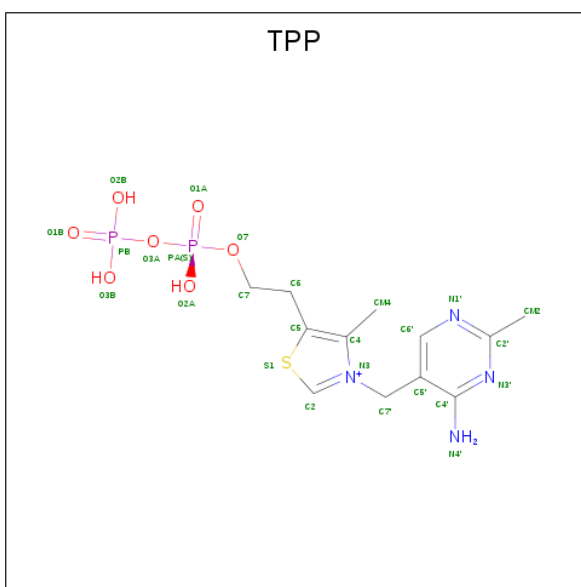
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1163	Total	C	N	O	S	0	0	0
			8871	5646	1509	1672	44			
1	B	1169	Total	C	N	O	S	0	0	0
			8905	5668	1515	1678	44			
1	C	1163	Total	C	N	O	S	0	0	0
			8862	5644	1506	1668	44			
1	D	1157	Total	C	N	O	S	0	0	0
			8788	5593	1494	1657	44			
1	E	1165	Total	C	N	O	S	0	0	0
			8875	5650	1511	1670	44			
1	F	1158	Total	C	N	O	S	0	0	0
			8789	5594	1495	1657	43			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).

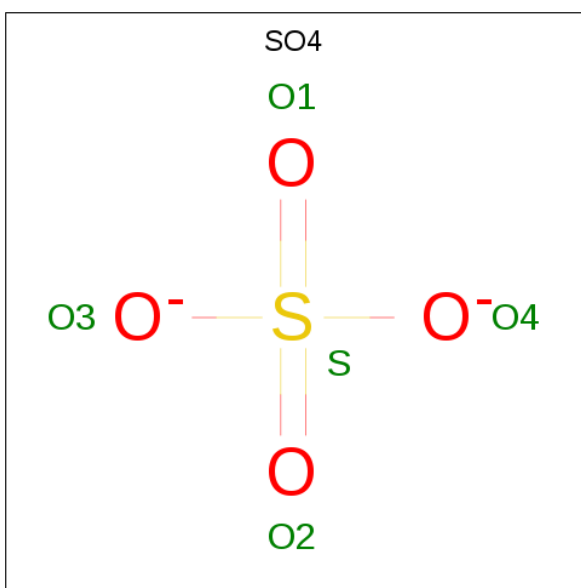


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	E	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	A	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		
6	B	88	Total	O	0	0
			88	88		
6	C	76	Total	O	0	0
			76	76		
6	D	83	Total	O	0	0
			83	83		

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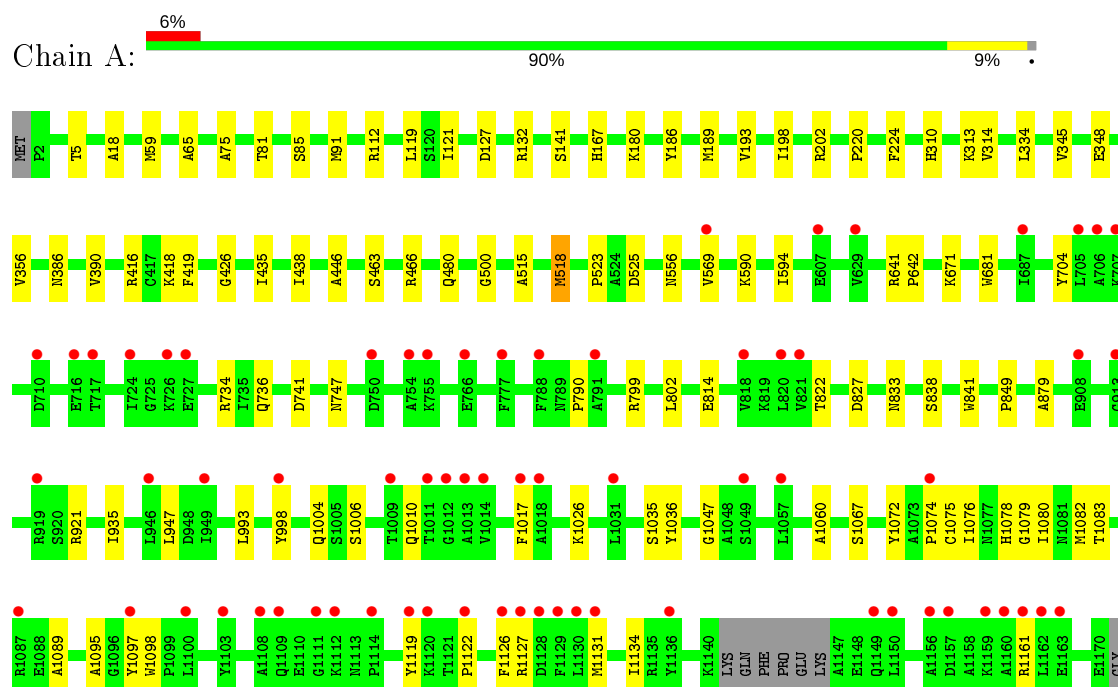
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	61	Total	O	0	0
			61	61		
6	F	58	Total	O	0	0
			58	58		



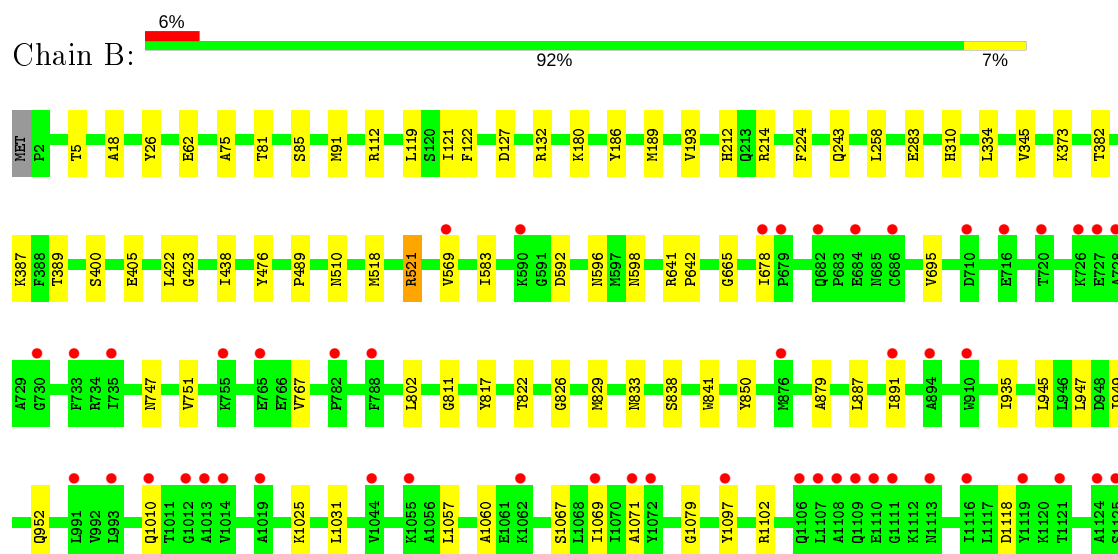
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-FERREDOXIN OXIDOREDUCTASE

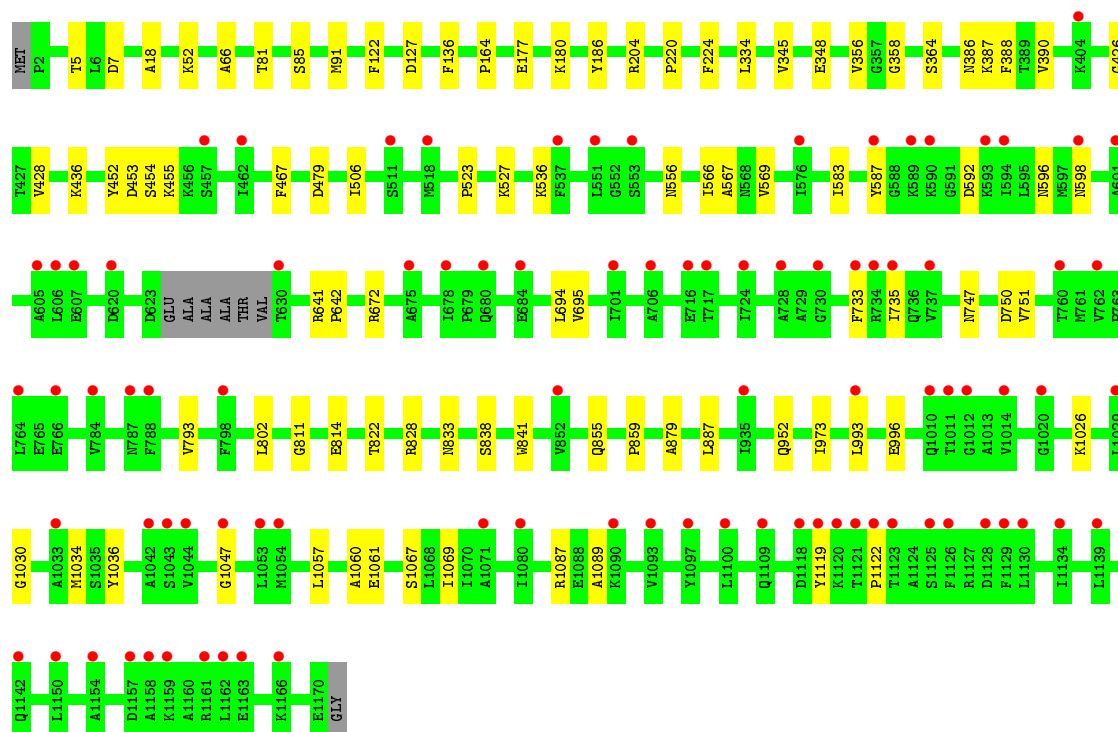
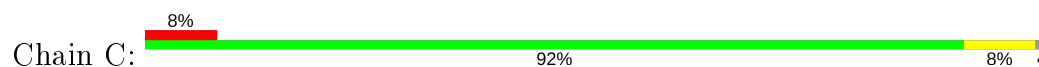


#### • Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

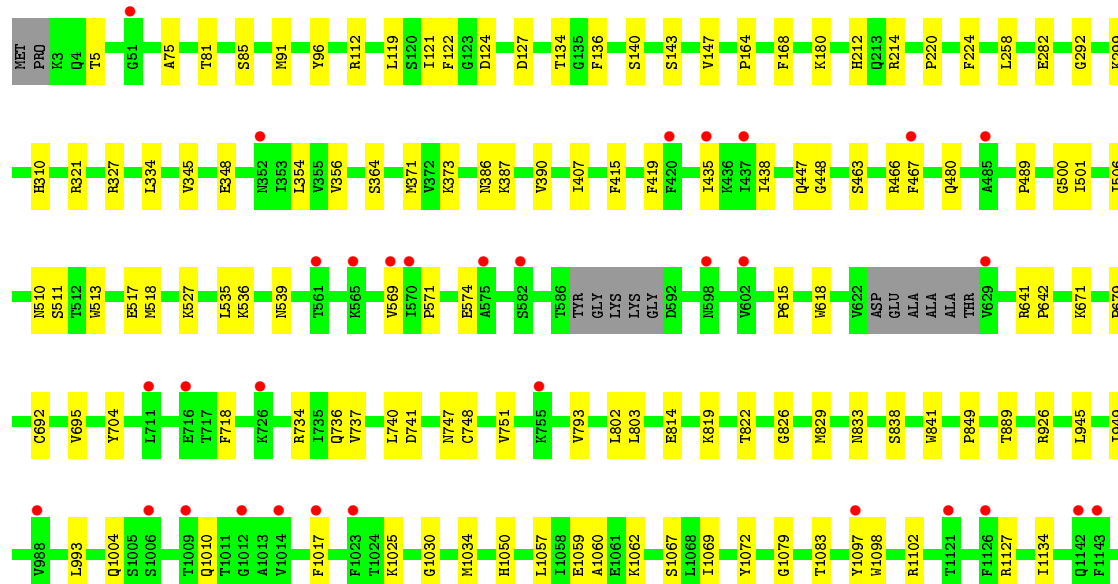
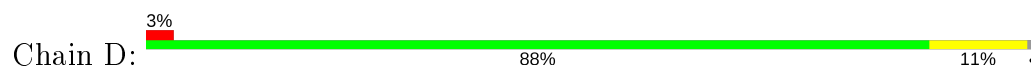


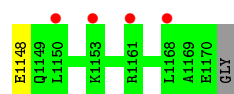


• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

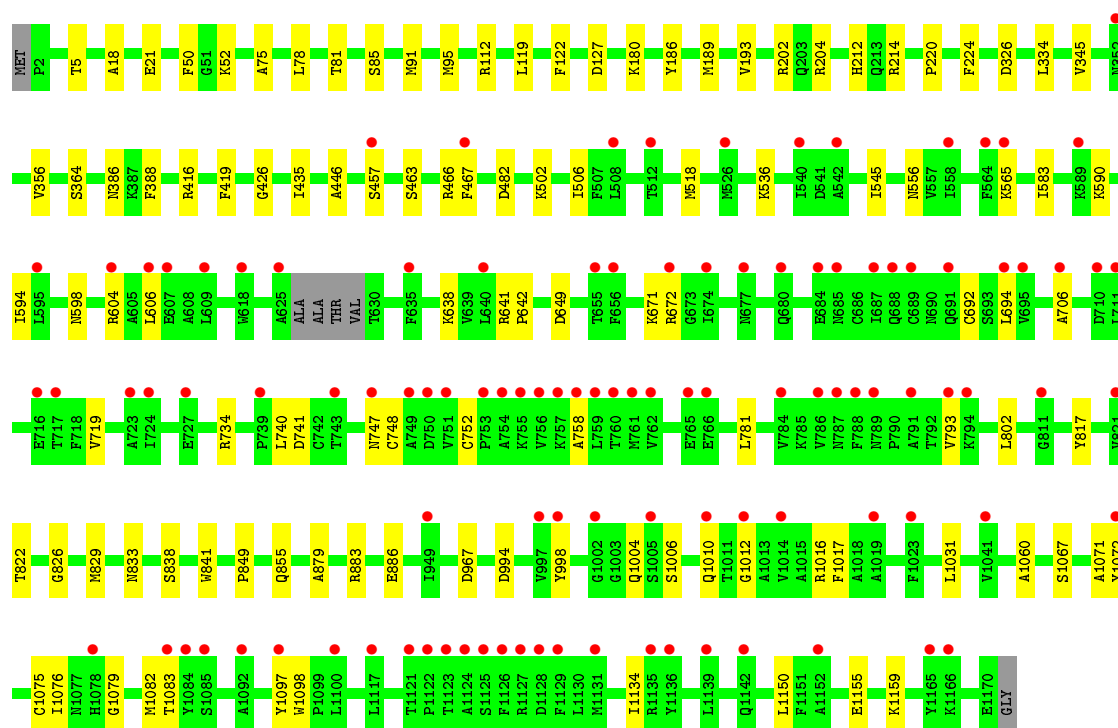
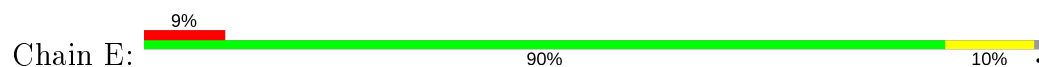


• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

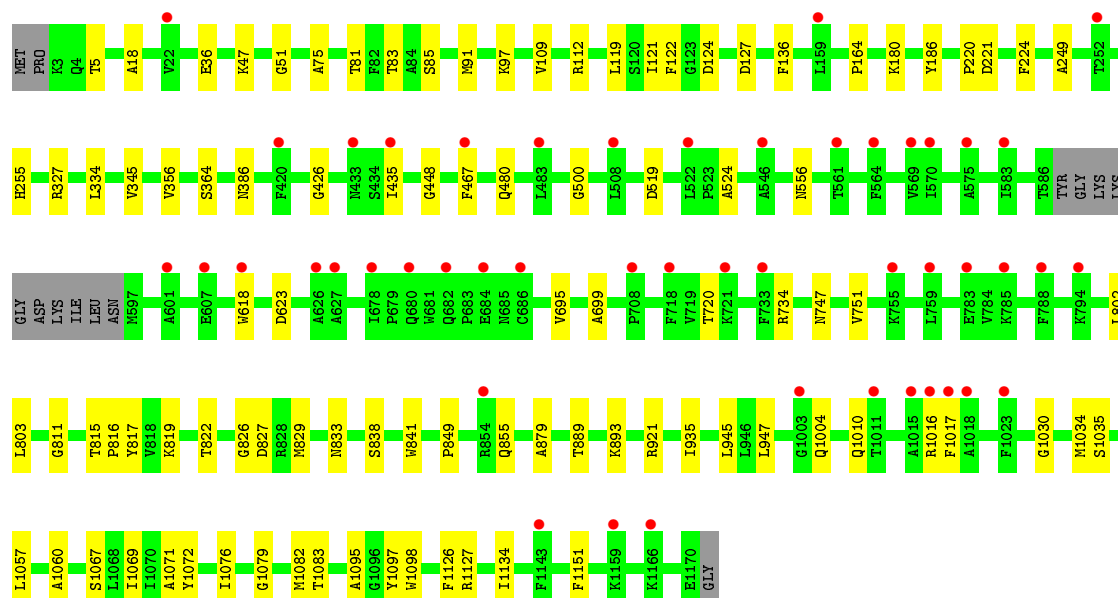
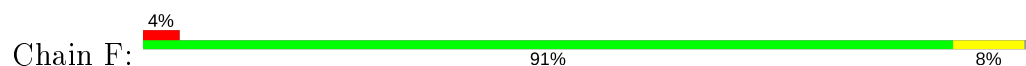




• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	340.61Å 106.63Å 239.08Å 90.00° 109.31° 90.00°	Depositor
Resolution (Å)	88.95 – 2.60 88.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (88.95-2.60) 98.4 (88.95-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.195 , 0.227 0.195 , 0.227	Depositor DCC
$R_{free}$ test set	12231 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	53870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1496e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MG, TPP, SF4, SO4

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	0.27	0/9063	0.44	0/12286
1	B	0.27	0/9099	0.45	0/12339
1	C	0.27	0/9055	0.44	0/12277
1	D	0.27	0/8978	0.44	0/12178
1	E	0.26	0/9068	0.44	0/12294
1	F	0.26	0/8980	0.43	0/12183
All	All	0.27	0/54243	0.44	0/73557

There are no bond length outliers.

There are no bond angle outliers.

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	8871	0	8796	62	0
1	B	8905	0	8821	53	0
1	C	8862	0	8779	54	0
1	D	8788	0	8658	75	0
1	E	8875	0	8788	66	0
1	F	8789	0	8666	59	0
2	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	0	0
2	E	24	0	0	0	0
2	F	24	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	0	0
3	C	26	0	16	2	0
3	D	26	0	16	0	0
3	E	26	0	16	0	0
3	F	26	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	0	0
5	B	10	0	0	3	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	A	73	0	0	1	0
6	B	88	0	0	1	0
6	C	76	0	0	2	0
6	D	83	0	0	5	0
6	E	61	0	0	1	0
6	F	58	0	0	0	0
All	All	53870	0	52604	344	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 3.

All (344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	5:B:1207:SO4:S	2.55	0.80
1:D:1057:LEU:HD23	1:D:1069:ILE:HD13	1.66	0.75
1:C:506:ILE:HG12	1:C:536:LYS:HE3	1.70	0.73
1:E:802:LEU:HB2	1:E:822:THR:HB	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:706:ALA:HB2	1:E:781:LEU:HD21	1.71	0.71
1:D:1059:GLU:OE1	6:D:1301:HOH:O	2.09	0.71
1:B:243:GLN:NE2	6:B:1302:HOH:O	2.29	0.64
1:F:1057:LEU:HD23	1:F:1069:ILE:HD13	1.78	0.64
1:A:112:ARG:HH21	1:A:119:LEU:HD11	1.63	0.63
1:C:345:VAL:HB	1:D:334:LEU:HD21	1.81	0.63
1:F:81:THR:HG21	1:F:91:MET:HE1	1.81	0.63
1:C:1057:LEU:HD23	1:C:1069:ILE:HD13	1.81	0.63
1:F:1127:ARG:HE	1:F:1151:PHE:HB3	1.63	0.63
1:E:204:ARG:NH2	6:E:1301:HOH:O	2.31	0.62
1:C:81:THR:HG21	1:C:91:MET:HE1	1.81	0.62
1:C:52:LYS:NZ	1:D:889:THR:OG1	2.32	0.62
1:A:671:LYS:NZ	1:A:741:ASP:OD2	2.26	0.61
1:C:204:ARG:NH2	6:C:1304:HOH:O	2.34	0.61
1:D:1079:GLY:HA3	1:D:1134:ILE:HB	1.83	0.61
1:B:521:ARG:NH2	5:B:1207:SO4:O3	2.32	0.61
1:C:5:THR:OG1	1:C:436:LYS:HG2	2.01	0.61
1:A:334:LEU:HD21	1:B:345:VAL:HB	1.82	0.61
1:B:438:ILE:HD13	1:B:569:VAL:HG11	1.82	0.60
1:F:838:SER:HA	1:F:841:TRP:CE2	2.36	0.60
1:F:5:THR:HG22	1:F:180:LYS:HB2	1.84	0.60
1:E:5:THR:HG22	1:E:180:LYS:HB2	1.84	0.59
1:E:52:LYS:NZ	1:F:889:THR:OG1	2.33	0.59
1:F:893:LYS:HB3	1:F:945:LEU:HD11	1.84	0.59
1:E:1079:GLY:HA3	1:E:1134:ILE:HB	1.84	0.59
1:C:750:ASP:OD1	1:C:1087:ARG:NH2	2.34	0.59
1:C:387:LYS:NZ	1:D:348:GLU:OE1	2.36	0.58
1:E:81:THR:HG21	1:E:91:MET:HE1	1.83	0.58
1:B:1057:LEU:HD23	1:B:1069:ILE:HD13	1.85	0.58
1:B:592:ASP:O	1:B:596:ASN:ND2	2.35	0.58
1:C:1036:TYR:O	1:D:1025:LYS:NZ	2.36	0.57
1:D:838:SER:HA	1:D:841:TRP:CE2	2.39	0.57
1:D:802:LEU:HB2	1:D:822:THR:HB	1.85	0.57
1:C:802:LEU:HB2	1:C:822:THR:HB	1.86	0.57
1:E:345:VAL:HB	1:F:334:LEU:HD21	1.87	0.57
1:A:802:LEU:HB2	1:A:822:THR:HB	1.86	0.56
1:E:671:LYS:NZ	1:E:741:ASP:OD2	2.32	0.56
1:C:828:ARG:NH2	1:C:1061:GLU:OE2	2.38	0.56
1:E:1004:GLN:HA	1:E:1016:ARG:HB2	1.89	0.55
1:A:1076:ILE:HA	1:A:1082:MET:HE3	1.89	0.55
1:B:838:SER:HA	1:B:841:TRP:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:PHE:HB2	1:E:463:SER:HB2	1.88	0.55
1:E:1072:TYR:HB2	1:E:1098:TRP:CE2	2.41	0.55
1:F:85:SER:HA	1:F:127:ASP:HB3	1.89	0.55
1:D:5:THR:HG22	1:D:180:LYS:HB2	1.88	0.55
1:D:292:GLY:HA3	1:E:638:LYS:HE2	1.89	0.54
1:C:5:THR:HG22	1:C:180:LYS:HB2	1.88	0.54
1:D:356:VAL:HG13	1:D:386:ASN:HA	1.88	0.54
1:E:506:ILE:HG12	1:E:536:LYS:HE3	1.89	0.54
1:A:1060:ALA:HB1	1:A:1067:SER:HB3	1.90	0.54
1:A:1095:ALA:HB1	1:A:1126:PHE:HA	1.90	0.54
1:A:1026:LYS:HZ3	1:A:1098:TRP:HZ3	1.54	0.53
1:A:345:VAL:HB	1:B:334:LEU:HD21	1.90	0.53
1:C:838:SER:HA	1:C:841:TRP:CE2	2.43	0.53
1:A:1079:GLY:HA3	1:A:1134:ILE:HB	1.91	0.53
1:B:81:THR:HG21	1:B:91:MET:HE1	1.90	0.53
1:E:416:ARG:HG2	1:E:466:ARG:HG2	1.91	0.53
1:E:112:ARG:HH21	1:E:119:LEU:HD11	1.74	0.52
1:E:671:LYS:HD2	1:E:740:LEU:HB2	1.90	0.52
1:A:5:THR:HG22	1:A:180:LYS:HB2	1.90	0.52
1:C:1060:ALA:HB1	1:C:1067:SER:HB3	1.92	0.52
1:E:545:ILE:HG23	1:E:604:ARG:HD2	1.91	0.52
1:F:1072:TYR:HB2	1:F:1098:TRP:CE2	2.45	0.52
1:F:519:ASP:OD1	1:F:618:TRP:NE1	2.39	0.52
1:C:122:PHE:CE2	1:D:220:PRO:HD3	2.45	0.52
1:E:1076:ILE:HG22	1:E:1082:MET:HG3	1.91	0.51
1:E:112:ARG:NH2	1:E:119:LEU:HD11	2.25	0.51
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	1.93	0.51
1:A:141:SER:OG	1:A:167:HIS:NE2	2.42	0.51
1:A:416:ARG:HG2	1:A:466:ARG:HG2	1.92	0.51
1:A:704:TYR:CE1	1:A:736:GLN:HB3	2.44	0.51
1:B:1060:ALA:HB1	1:B:1067:SER:HB3	1.93	0.51
1:D:793:VAL:HG21	1:D:1050:HIS:HB3	1.92	0.51
1:A:838:SER:HA	1:A:841:TRP:CE2	2.45	0.51
3:C:1204:TPP:HN42	3:C:1204:TPP:H2	1.75	0.51
1:E:1012:GLY:HA2	1:E:1150:LEU:HD13	1.92	0.51
1:C:85:SER:HA	1:C:127:ASP:HB3	1.93	0.50
1:F:1004:GLN:HG2	1:F:1017:PHE:CE2	2.45	0.50
1:F:1076:ILE:HG22	1:F:1082:MET:HG3	1.93	0.50
1:B:112:ARG:HH21	1:B:119:LEU:HD11	1.76	0.50
1:D:282:GLU:OE1	1:D:299:LYS:NZ	2.40	0.50
1:B:678:ILE:HD11	1:B:767:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:HG22	1:B:180:LYS:HB2	1.93	0.50
1:B:85:SER:HA	1:B:127:ASP:HB3	1.94	0.50
1:C:695:VAL:HG11	1:C:751:VAL:HG21	1.94	0.50
1:D:136:PHE:CE2	1:D:164:PRO:HB2	2.46	0.50
1:A:85:SER:HA	1:A:127:ASP:HB3	1.94	0.49
1:D:506:ILE:HG12	1:D:536:LYS:HE3	1.94	0.49
1:D:671:LYS:NZ	1:D:741:ASP:OD2	2.40	0.49
1:C:356:VAL:HG13	1:C:386:ASN:HA	1.93	0.49
1:C:583:ILE:HD13	1:C:598:ASN:HB3	1.94	0.49
1:D:81:THR:HG21	1:D:91:MET:HE1	1.93	0.49
1:F:435:ILE:HD13	1:F:448:GLY:HA3	1.94	0.49
1:A:814:GLU:HB3	1:A:993:LEU:HD13	1.95	0.49
1:B:112:ARG:NH2	1:B:119:LEU:HD11	2.28	0.49
1:E:1010:GLN:HG3	1:E:1097:TYR:OH	2.13	0.49
1:A:1036:TYR:O	1:B:1025:LYS:NZ	2.46	0.48
1:C:694:LEU:HD22	1:C:793:VAL:HG13	1.94	0.48
1:B:112:ARG:NE	1:B:121:ILE:HA	2.28	0.48
1:C:996:GLU:HG2	1:C:1026:LYS:HZ2	1.77	0.48
1:A:112:ARG:NE	1:A:121:ILE:HA	2.28	0.48
1:C:455:LYS:HD3	1:C:672:ARG:CZ	2.42	0.48
1:E:747:ASN:ND2	1:E:1083:THR:O	2.46	0.48
1:E:967:ASP:HB3	1:E:994:ASP:HA	1.95	0.48
1:D:679:PRO:HD2	1:D:737:VAL:HG21	1.96	0.48
1:A:220:PRO:HD3	1:B:122:PHE:CE2	2.48	0.48
1:B:695:VAL:HG11	1:B:751:VAL:HG21	1.96	0.48
1:E:1060:ALA:HB1	1:E:1067:SER:HB3	1.95	0.48
1:A:480:GLN:HA	1:A:500:GLY:O	2.13	0.48
1:F:747:ASN:ND2	1:F:1083:THR:O	2.46	0.47
1:F:356:VAL:HG13	1:F:386:ASN:HA	1.95	0.47
1:E:189:MET:O	1:E:193:VAL:HG23	2.14	0.47
1:E:457:SER:O	1:E:672:ARG:NH1	2.36	0.47
1:E:719:VAL:O	1:E:734:ARG:NH2	2.46	0.47
1:F:802:LEU:HB2	1:F:822:THR:HB	1.95	0.47
1:A:59:MET:HG3	1:A:65:ALA:HA	1.97	0.47
1:B:583:ILE:HD13	1:B:598:ASN:HB3	1.97	0.47
1:D:1072:TYR:HB2	1:D:1098:TRP:CE2	2.49	0.47
1:C:733:PHE:HE1	1:C:735:ILE:HG12	1.80	0.47
1:A:313:LYS:HG3	1:A:314:VAL:HG13	1.97	0.47
1:A:590:LYS:HB3	1:A:594:ILE:HD12	1.97	0.47
1:B:665:GLY:N	1:B:850:TYR:O	2.47	0.47
1:A:998:TYR:CE1	1:A:1006:SER:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1047:GLY:HA3	1:C:1089:ALA:HB3	1.97	0.47
1:C:523:PRO:O	1:C:527:LYS:HG3	2.15	0.47
1:E:855:GLN:N	1:E:855:GLN:OE1	2.48	0.46
1:F:1079:GLY:HA3	1:F:1134:ILE:HB	1.97	0.46
1:A:827:ASP:OD2	1:A:921:ARG:NH1	2.34	0.46
1:B:283:GLU:OE1	1:B:476:TYR:OH	2.24	0.46
1:F:136:PHE:CE2	1:F:164:PRO:HB2	2.51	0.46
1:C:358:GLY:HA3	1:C:388:PHE:CE1	2.51	0.46
1:D:85:SER:HA	1:D:127:ASP:HB3	1.98	0.46
1:B:826:GLY:HA2	1:B:829:MET:SD	2.56	0.46
1:D:1127:ARG:HH22	1:D:1148:GLU:CD	2.18	0.46
1:C:334:LEU:HD21	1:D:345:VAL:HB	1.98	0.46
1:E:334:LEU:HD21	1:F:345:VAL:HB	1.98	0.46
1:B:18:ALA:HB2	1:B:186:TYR:CZ	2.51	0.46
1:C:1030:GLY:O	1:C:1034:MET:HG3	2.16	0.46
1:D:1127:ARG:NH1	1:D:1148:GLU:OE2	2.47	0.46
3:F:1204:TPP:H2	3:F:1204:TPP:HN42	1.79	0.46
1:F:18:ALA:HB2	1:F:186:TYR:CE1	2.50	0.46
1:D:112:ARG:NE	1:D:121:ILE:HA	2.31	0.46
1:D:704:TYR:CE1	1:D:736:GLN:HB3	2.51	0.46
1:E:122:PHE:CE2	1:F:220:PRO:HD3	2.51	0.46
1:E:212:HIS:NE2	1:E:214:ARG:HD2	2.30	0.46
1:D:513:TRP:O	1:D:539:ASN:ND2	2.49	0.46
1:A:438:ILE:HD13	1:A:569:VAL:HG11	1.97	0.45
1:D:695:VAL:HG11	1:D:751:VAL:HG21	1.97	0.45
1:D:819:LYS:NZ	6:D:1320:HOH:O	2.48	0.45
1:A:790:PRO:HG3	1:A:799:ARG:NH2	2.31	0.45
1:C:1119:TYR:HE2	1:C:1122:PRO:HA	1.80	0.45
1:C:479:ASP:OD1	6:C:1301:HOH:O	2.20	0.45
1:F:18:ALA:HB2	1:F:186:TYR:CZ	2.51	0.45
1:F:935:ILE:HD13	1:F:947:LEU:HD23	1.97	0.45
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	1.98	0.45
1:B:747:ASN:OD1	1:B:811:GLY:HA2	2.15	0.45
1:D:419:PHE:HB2	1:D:463:SER:HB2	1.97	0.45
1:C:426:GLY:HA3	1:C:556:ASN:HB3	1.99	0.45
1:E:590:LYS:HB3	1:E:594:ILE:HD12	1.97	0.45
1:A:426:GLY:HA3	1:A:556:ASN:HB3	1.99	0.45
1:E:817:TYR:CZ	1:E:1071:ALA:HB1	2.51	0.45
1:F:122:PHE:HB3	1:F:364:SER:HB2	1.97	0.45
1:C:506:ILE:HG21	1:C:566:ILE:HD12	1.99	0.45
1:A:112:ARG:NH2	1:A:119:LEU:HD11	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:HIS:NE2	1:B:214:ARG:HD2	2.31	0.45
1:A:348:GLU:OE1	1:B:387:LYS:NZ	2.50	0.45
1:D:826:GLY:HA2	1:D:829:MET:SD	2.57	0.45
1:E:1004:GLN:HG2	1:E:1017:PHE:CE2	2.52	0.45
1:A:81:THR:HG21	1:A:91:MET:HE1	1.98	0.45
1:B:887:LEU:HD13	1:B:952:GLN:HB2	1.99	0.45
1:C:18:ALA:HB2	1:C:186:TYR:CE1	2.52	0.45
1:D:513:TRP:HE3	1:D:517:GLU:HG2	1.82	0.45
1:F:1127:ARG:HH21	1:F:1151:PHE:HB3	1.81	0.45
1:B:935:ILE:HD13	1:B:947:LEU:HD23	1.99	0.44
1:D:1060:ALA:HB1	1:D:1067:SER:HB3	1.98	0.44
1:E:85:SER:HA	1:E:127:ASP:HB3	1.99	0.44
1:B:521:ARG:NH2	5:B:1207:SO4:O1	2.45	0.44
1:A:681:TRP:CH2	1:A:734:ARG:HA	2.52	0.44
1:C:879:ALA:HB3	1:D:75:ALA:HB3	2.00	0.44
1:D:814:GLU:HB3	1:D:993:LEU:HD13	1.99	0.44
1:A:1119:TYR:HE2	1:A:1122:PRO:HA	1.83	0.44
1:B:802:LEU:HB2	1:B:822:THR:HB	1.99	0.44
1:D:480:GLN:HA	1:D:500:GLY:O	2.17	0.44
1:B:18:ALA:HB2	1:B:186:TYR:CE1	2.53	0.44
1:F:124:ASP:HA	1:F:327:ARG:HD3	1.99	0.44
1:A:1004:GLN:HG2	1:A:1017:PHE:CE2	2.53	0.44
1:A:1072:TYR:HB2	1:A:1098:TRP:CE2	2.52	0.44
3:A:1204:TPP:H2	3:A:1204:TPP:HN42	1.83	0.44
1:A:838:SER:O	6:A:1301:HOH:O	2.21	0.44
1:B:1102:ARG:NH1	1:B:1118:ASP:OD1	2.48	0.44
1:F:1010:GLN:HG3	1:F:1097:TYR:OH	2.18	0.44
1:D:122:PHE:HB3	1:D:364:SER:HB2	2.00	0.44
1:E:583:ILE:HD13	1:E:598:ASN:HB3	2.00	0.44
1:C:887:LEU:HD13	1:C:952:GLN:HB2	1.99	0.43
1:B:258:LEU:HD22	1:B:310:HIS:CG	2.53	0.43
1:C:814:GLU:HB3	1:C:993:LEU:HD13	2.00	0.43
1:D:1030:GLY:O	1:D:1034:MET:HG3	2.18	0.43
1:E:18:ALA:HB2	1:E:186:TYR:CE1	2.52	0.43
1:A:1047:GLY:HA3	1:A:1089:ALA:HB3	1.99	0.43
1:A:419:PHE:HB2	1:A:463:SER:HB2	2.00	0.43
1:B:817:TYR:CZ	1:B:1071:ALA:HB1	2.53	0.43
1:D:527:LYS:HD2	1:D:618:TRP:CE2	2.52	0.43
1:D:671:LYS:HD2	1:D:740:LEU:HB2	1.99	0.43
1:E:122:PHE:HB3	1:E:364:SER:HB2	1.99	0.43
1:C:747:ASN:OD1	1:C:811:GLY:HA2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1102:ARG:HD2	6:D:1301:HOH:O	2.19	0.43
1:D:571:PRO:HB2	1:D:574:GLU:HG3	2.00	0.43
1:D:718:PHE:CZ	1:D:734:ARG:HD3	2.53	0.43
1:E:75:ALA:HB3	1:F:879:ALA:HB3	2.01	0.43
1:A:310:HIS:HA	1:A:313:LYS:CD	2.48	0.43
1:B:1010:GLN:HG3	1:B:1097:TYR:OH	2.19	0.43
1:C:583:ILE:HG23	1:C:587:TYR:HD2	1.84	0.43
1:D:489:PRO:HG3	1:D:510:ASN:O	2.19	0.43
1:E:356:VAL:HG13	1:E:386:ASN:HA	2.00	0.43
1:F:426:GLY:HA3	1:F:556:ASN:HB3	2.01	0.43
1:F:720:THR:HG22	1:F:734:ARG:HB2	2.01	0.43
1:F:695:VAL:HG11	1:F:751:VAL:HG21	2.00	0.43
1:B:891:ILE:HG12	1:B:949:ILE:HD12	2.01	0.43
1:D:501:ILE:HD13	1:D:535:LEU:HD13	2.01	0.43
1:E:356:VAL:HG12	1:E:388:PHE:HE1	1.83	0.43
1:A:189:MET:O	1:A:193:VAL:HG23	2.19	0.43
1:A:198:ILE:O	1:A:202:ARG:HG2	2.19	0.43
1:D:1004:GLN:HG2	1:D:1017:PHE:CE2	2.54	0.43
1:D:435:ILE:HD13	1:D:448:GLY:HA3	2.00	0.43
1:D:438:ILE:HD13	1:D:569:VAL:HG11	2.01	0.43
1:D:945:LEU:O	1:D:949:ILE:HG12	2.19	0.42
1:F:817:TYR:CZ	1:F:1071:ALA:HB1	2.53	0.42
1:F:83:THR:O	1:F:109:VAL:HA	2.19	0.42
1:A:1010:GLN:HG3	1:A:1097:TYR:CZ	2.53	0.42
1:B:489:PRO:HG3	1:B:510:ASN:O	2.19	0.42
1:D:124:ASP:HA	1:D:327:ARG:HD3	2.00	0.42
1:B:1031:LEU:HD21	1:B:1164:GLN:HE22	1.83	0.42
1:C:802:LEU:HD13	1:C:859:PRO:HD3	2.00	0.42
1:D:321:ARG:HG2	1:D:354:LEU:HB3	2.01	0.42
1:D:511:SER:HB2	1:D:513:TRP:CD1	2.54	0.42
1:F:97:LYS:HE3	1:F:97:LYS:HB3	1.86	0.42
1:A:515:ALA:O	1:A:518:MET:HB2	2.19	0.42
1:D:112:ARG:NH2	1:D:119:LEU:HD11	2.34	0.42
1:A:1127:ARG:O	1:A:1131:MET:HG2	2.20	0.42
1:B:389:THR:O	1:B:400:SER:HA	2.20	0.42
1:D:1062:LYS:HG3	6:D:1310:HOH:O	2.19	0.42
1:D:96:TYR:CE1	1:D:134:THR:HA	2.55	0.42
1:D:258:LEU:HD22	1:D:310:HIS:CG	2.54	0.42
1:D:371:MET:HB3	1:D:390:VAL:CG1	2.49	0.42
1:F:480:GLN:HA	1:F:500:GLY:O	2.18	0.42
1:C:7:ASP:HA	1:C:177:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:PRO:HG2	1:D:618:TRP:CD1	2.54	0.42
1:F:699:ALA:HB2	1:F:819:LYS:HD2	2.00	0.42
1:F:855:GLN:OE1	1:F:855:GLN:N	2.52	0.42
1:A:18:ALA:HB2	1:A:186:TYR:CE1	2.55	0.42
1:B:422:LEU:HD22	1:B:423:GLY:H	1.85	0.42
1:E:752:CYS:SG	1:E:758:ALA:HB3	2.59	0.42
1:F:827:ASP:OD2	1:F:921:ARG:NH1	2.29	0.42
1:A:1074:PRO:HA	1:A:1078:HIS:CE1	2.54	0.42
1:A:1010:GLN:HE22	1:A:1161:ARG:HH12	1.68	0.42
1:A:75:ALA:HB3	1:B:879:ALA:HB3	2.02	0.42
1:C:18:ALA:HB2	1:C:186:TYR:CZ	2.54	0.42
1:C:220:PRO:HD3	1:D:122:PHE:CE2	2.55	0.42
1:D:140:SER:HB2	1:D:168:PHE:CZ	2.54	0.42
1:E:998:TYR:CE1	1:E:1006:SER:HB2	2.54	0.42
1:F:112:ARG:NE	1:F:121:ILE:HA	2.35	0.42
1:F:112:ARG:NH2	1:F:119:LEU:HD11	2.34	0.42
1:F:841:TRP:O	1:F:849:PRO:HG3	2.20	0.42
1:A:356:VAL:HG13	1:A:386:ASN:HA	2.02	0.42
1:F:747:ASN:OD1	1:F:811:GLY:HA2	2.20	0.42
1:D:641:ARG:HB2	1:D:642:PRO:HD3	2.02	0.42
1:E:1155:GLU:HG2	1:E:1159:LYS:HE3	2.01	0.42
1:F:47:LYS:HD2	1:F:51:GLY:C	2.40	0.42
1:A:879:ALA:HB3	1:B:75:ALA:HB3	2.02	0.41
1:D:671:LYS:NZ	6:D:1314:HOH:O	2.42	0.41
1:F:826:GLY:HA2	1:F:829:MET:SD	2.60	0.41
1:D:373:LYS:HD2	1:D:407:ILE:HD13	2.02	0.41
1:D:803:LEU:HD12	1:D:849:PRO:HB2	2.02	0.41
1:F:1127:ARG:HH21	1:F:1151:PHE:CB	2.33	0.41
1:B:189:MET:O	1:B:193:VAL:HG23	2.21	0.41
1:E:1010:GLN:HG3	1:E:1097:TYR:CZ	2.55	0.41
1:E:565:LYS:HD3	1:E:606:LEU:HD22	2.02	0.41
1:C:567:ALA:HB1	1:C:569:VAL:HG23	2.03	0.41
1:D:447:GLN:OE1	1:D:466:ARG:NH2	2.42	0.41
1:E:482:ASP:OD1	1:E:502:LYS:HD2	2.21	0.41
1:E:641:ARG:HB2	1:E:642:PRO:HD3	2.02	0.41
1:E:220:PRO:HD3	1:F:122:PHE:CE2	2.56	0.41
1:A:1075:CYS:SG	1:A:1076:ILE:N	2.93	0.41
1:E:694:LEU:HD22	1:E:793:VAL:HG13	2.03	0.41
1:C:592:ASP:O	1:C:596:ASN:ND2	2.52	0.41
1:D:415:PHE:O	1:D:466:ARG:HA	2.21	0.41
1:E:826:GLY:HA2	1:E:829:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:841:TRP:O	1:E:849:PRO:HG3	2.20	0.41
1:F:1095:ALA:HB1	1:F:1126:PHE:HA	2.02	0.41
1:A:1035:SER:HB2	1:B:1031:LEU:HD23	2.03	0.41
1:A:841:TRP:O	1:A:849:PRO:HG3	2.21	0.41
1:B:26:TYR:HB3	1:B:62:GLU:HG3	2.03	0.41
1:B:945:LEU:O	1:B:949:ILE:HG12	2.21	0.41
1:D:747:ASN:ND2	1:D:1083:THR:O	2.52	0.41
1:E:692:CYS:HB2	1:E:748:CYS:HB2	2.02	0.41
1:C:136:PHE:CE2	1:C:164:PRO:HB2	2.55	0.41
1:E:426:GLY:HA3	1:E:556:ASN:HB3	2.03	0.41
1:A:435:ILE:HG23	1:A:446:ALA:HB1	2.03	0.41
1:A:641:ARG:HB2	1:A:642:PRO:HD3	2.01	0.41
1:E:21:GLU:OE2	1:E:202:ARG:NH1	2.42	0.41
1:E:50:PHE:CZ	1:E:78:LEU:HD12	2.55	0.41
1:A:747:ASN:ND2	1:A:1083:THR:O	2.53	0.41
1:A:523:PRO:HB2	1:A:525:ASP:OD1	2.21	0.41
1:C:641:ARG:HB2	1:C:642:PRO:HD3	2.03	0.41
1:D:1010:GLN:HG3	1:D:1097:TYR:CZ	2.56	0.41
1:D:692:CYS:HB2	1:D:748:CYS:HB2	2.03	0.41
1:E:1031:LEU:HD23	1:F:1035:SER:HB2	2.02	0.41
1:E:649:ASP:OD1	1:F:221:ASP:HA	2.21	0.41
1:A:935:ILE:HD13	1:A:947:LEU:HD23	2.03	0.41
1:B:521:ARG:HD2	1:B:521:ARG:HA	1.81	0.41
1:C:453:ASP:OD1	1:C:454:SER:N	2.52	0.41
1:C:855:GLN:OE1	1:C:855:GLN:N	2.54	0.41
1:D:85:SER:HB2	1:D:112:ARG:HB3	2.03	0.41
1:E:1075:CYS:SG	1:E:1076:ILE:N	2.94	0.41
1:E:435:ILE:HG23	1:E:446:ALA:HB1	2.03	0.41
1:F:815:THR:OG1	1:F:816:PRO:HD3	2.21	0.41
1:B:373:LYS:HE2	1:B:405:GLU:OE2	2.20	0.40
1:B:641:ARG:HB2	1:B:642:PRO:HD3	2.02	0.40
1:C:973:ILE:HD11	3:C:1204:TPP:HM23	2.02	0.40
1:D:212:HIS:NE2	1:D:214:ARG:HD2	2.37	0.40
1:A:132:ARG:HH11	1:B:132:ARG:HH11	1.69	0.40
1:C:348:GLU:OE1	1:D:387:LYS:NZ	2.54	0.40
1:D:143:SER:O	1:D:147:VAL:HG23	2.21	0.40
1:E:18:ALA:HB2	1:E:186:TYR:CZ	2.56	0.40
1:F:36:GLU:CD	1:F:1016:ARG:HD3	2.41	0.40
1:F:122:PHE:HB3	1:F:364:SER:CB	2.51	0.40
1:C:66:ALA:HB2	1:C:91:MET:HE2	2.02	0.40
1:E:838:SER:HA	1:E:841:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1060:ALA:HB1	1:F:1067:SER:HB3	2.02	0.40
1:C:122:PHE:HB3	1:C:364:SER:HB2	2.04	0.40
1:C:428:VAL:HG11	1:C:452:TYR:OH	2.22	0.40
1:E:883:ARG:NH2	1:E:886:GLU:OE1	2.41	0.40
1:F:1030:GLY:O	1:F:1034:MET:HG3	2.22	0.40
1:F:249:ALA:HB1	1:F:255:HIS:CD2	2.56	0.40
1:E:879:ALA:HB3	1:F:75:ALA:HB3	2.03	0.40
1:A:418:LYS:HA	1:A:463:SER:O	2.22	0.40
1:D:1010:GLN:HG3	1:D:1097:TYR:OH	2.21	0.40
1:E:91:MET:O	1:E:95:MET:HG3	2.22	0.40
1:F:524:ALA:HB3	1:F:623:ASP:HA	2.02	0.40
1:F:803:LEU:HD12	1:F:849:PRO:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1159/1171 (99%)	1142 (98%)	17 (2%)	0	100	100
1	B	1167/1171 (100%)	1148 (98%)	19 (2%)	0	100	100
1	C	1159/1171 (99%)	1143 (99%)	16 (1%)	0	100	100
1	D	1151/1171 (98%)	1132 (98%)	19 (2%)	0	100	100
1	E	1161/1171 (99%)	1143 (98%)	18 (2%)	0	100	100
1	F	1154/1171 (98%)	1135 (98%)	19 (2%)	0	100	100
All	All	6951/7026 (99%)	6843 (98%)	108 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	918/932 (98%)	914 (100%)	4 (0%)	91	97
1	B	920/932 (99%)	915 (100%)	5 (0%)	88	96
1	C	916/932 (98%)	912 (100%)	4 (0%)	91	97
1	D	903/932 (97%)	898 (99%)	5 (1%)	86	95
1	E	916/932 (98%)	911 (100%)	5 (0%)	88	96
1	F	902/932 (97%)	899 (100%)	3 (0%)	92	98
All	All	5475/5592 (98%)	5449 (100%)	26 (0%)	88	96

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	PHE
1	A	390	VAL
1	A	518	MET
1	A	833	ASN
1	B	224	PHE
1	B	382	THR
1	B	518	MET
1	B	521	ARG
1	B	833	ASN
1	C	224	PHE
1	C	390	VAL
1	C	467	PHE
1	C	833	ASN
1	D	224	PHE
1	D	467	PHE
1	D	518	MET
1	D	833	ASN
1	D	926	ARG
1	E	224	PHE
1	E	326	ASP
1	E	467	PHE
1	E	518	MET

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Mol	Chain	Res	Type
1	E	833	ASN
1	F	224	PHE
1	F	467	PHE
1	F	833	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	1164	GLN
1	D	547	GLN
1	F	255	HIS
1	F	433	ASN
1	F	560	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SF4	C	1201	1	0,12,12	0.00	-	-		
2	SF4	E	1203	1	0,12,12	0.00	-	-		
3	TPP	E	1204	4	22,27,27	2.00	6 (27%)	29,40,40	1.61	8 (27%)
2	SF4	A	1203	1	0,12,12	0.00	-	-		
3	TPP	B	1204	4	22,27,27	2.04	6 (27%)	29,40,40	1.60	7 (24%)
2	SF4	C	1202	1	0,12,12	0.00	-	-		
5	SO4	B	1207	-	4,4,4	0.13	0	6,6,6	0.12	0
5	SO4	C	1206	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	D	1206	-	4,4,4	0.15	0	6,6,6	0.14	0
3	TPP	A	1204	4	22,27,27	1.94	6 (27%)	29,40,40	1.59	7 (24%)
3	TPP	D	1204	4	22,27,27	1.98	6 (27%)	29,40,40	1.67	8 (27%)
2	SF4	B	1201	1	0,12,12	0.00	-	-		
2	SF4	F	1201	1	0,12,12	0.00	-	-		
2	SF4	D	1201	1	0,12,12	0.00	-	-		
2	SF4	B	1202	1	0,12,12	0.00	-	-		
2	SF4	F	1202	1	0,12,12	0.00	-	-		
2	SF4	A	1201	1	0,12,12	0.00	-	-		
2	SF4	B	1203	1	0,12,12	0.00	-	-		
2	SF4	D	1203	1	0,12,12	0.00	-	-		
5	SO4	B	1206	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	E	1206	-	4,4,4	0.14	0	6,6,6	0.13	0
5	SO4	F	1206	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SF4	D	1202	1	0,12,12	0.00	-	-		
2	SF4	E	1202	1	0,12,12	0.00	-	-		
2	SF4	E	1201	1	0,12,12	0.00	-	-		
2	SF4	F	1203	1	0,12,12	0.00	-	-		
3	TPP	C	1204	4	22,27,27	1.96	6 (27%)	29,40,40	1.58	5 (17%)
5	SO4	A	1206	-	4,4,4	0.16	0	6,6,6	0.04	0
3	TPP	F	1204	4	22,27,27	1.98	6 (27%)	29,40,40	1.78	7 (24%)
2	SF4	C	1203	1	0,12,12	0.00	-	-		
2	SF4	A	1202	1	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	1201	1	-	-	0/6/5/5
2	SF4	E	1203	1	-	-	0/6/5/5
3	TPP	E	1204	4	-	3/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	1203	1	-	-	0/6/5/5
3	TPP	B	1204	4	-	2/16/17/17	0/2/2/2
2	SF4	C	1202	1	-	-	0/6/5/5
3	TPP	A	1204	4	-	5/16/17/17	0/2/2/2
3	TPP	D	1204	4	-	5/16/17/17	0/2/2/2
2	SF4	B	1201	1	-	-	0/6/5/5
2	SF4	F	1201	1	-	-	0/6/5/5
2	SF4	D	1201	1	-	-	0/6/5/5
2	SF4	B	1202	1	-	-	0/6/5/5
2	SF4	F	1202	1	-	-	0/6/5/5
2	SF4	A	1201	1	-	-	0/6/5/5
2	SF4	B	1203	1	-	-	0/6/5/5
2	SF4	D	1203	1	-	-	0/6/5/5
2	SF4	D	1202	1	-	-	0/6/5/5
2	SF4	E	1202	1	-	-	0/6/5/5
2	SF4	E	1201	1	-	-	0/6/5/5
2	SF4	F	1203	1	-	-	0/6/5/5
3	TPP	C	1204	4	-	5/16/17/17	0/2/2/2
3	TPP	F	1204	4	-	4/16/17/17	0/2/2/2
2	SF4	C	1203	1	-	-	0/6/5/5
2	SF4	A	1202	1	-	-	0/6/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	TPP	C4-N3	-4.85	1.35	1.39
3	F	1204	TPP	C4-N3	-4.55	1.35	1.39
3	E	1204	TPP	C4-N3	-4.46	1.35	1.39
3	C	1204	TPP	C4-N3	-4.46	1.35	1.39
3	A	1204	TPP	C4-N3	-4.26	1.36	1.39
3	E	1204	TPP	C4'-N4'	3.91	1.43	1.34
3	D	1204	TPP	C4-N3	-3.83	1.36	1.39
3	D	1204	TPP	C6-C5	3.83	1.52	1.50
3	C	1204	TPP	C4'-N4'	3.82	1.43	1.34
3	F	1204	TPP	C4'-N4'	3.82	1.43	1.34
3	B	1204	TPP	C4'-N4'	3.82	1.43	1.34
3	A	1204	TPP	C4'-N4'	3.72	1.43	1.34
3	D	1204	TPP	C4'-N4'	3.69	1.43	1.34
3	A	1204	TPP	C7'-N3	-3.46	1.42	1.48
3	F	1204	TPP	C7'-N3	-3.45	1.42	1.48
3	C	1204	TPP	C7'-N3	-3.44	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	TPP	C7'-N3	-3.34	1.42	1.48
3	E	1204	TPP	C7'-N3	-3.30	1.42	1.48
3	D	1204	TPP	C7'-N3	-3.30	1.42	1.48
3	E	1204	TPP	C6-C5	3.29	1.52	1.50
3	C	1204	TPP	C7'-C5'	3.26	1.58	1.51
3	E	1204	TPP	C7'-C5'	3.24	1.58	1.51
3	B	1204	TPP	C6-C5	3.22	1.52	1.50
3	D	1204	TPP	C7'-C5'	3.21	1.57	1.51
3	A	1204	TPP	C7'-C5'	3.18	1.57	1.51
3	B	1204	TPP	C7'-C5'	3.17	1.57	1.51
3	F	1204	TPP	C7'-C5'	3.09	1.57	1.51
3	F	1204	TPP	C6-C5	3.08	1.52	1.50
3	A	1204	TPP	C6-C5	2.83	1.52	1.50
3	C	1204	TPP	C6-C5	2.39	1.52	1.50
3	A	1204	TPP	C6'-C5'	2.36	1.42	1.37
3	B	1204	TPP	C6'-C5'	2.31	1.42	1.37
3	C	1204	TPP	C6'-C5'	2.26	1.42	1.37
3	D	1204	TPP	C6'-C5'	2.25	1.42	1.37
3	F	1204	TPP	C6'-C5'	2.25	1.42	1.37
3	E	1204	TPP	C6'-C5'	2.24	1.42	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1204	TPP	C6-C5-C4	-4.90	123.50	127.43
3	D	1204	TPP	C6-C5-C4	-4.35	123.94	127.43
3	B	1204	TPP	C6-C5-C4	-4.18	124.08	127.43
3	C	1204	TPP	C6-C5-C4	-3.90	124.30	127.43
3	E	1204	TPP	C6-C5-C4	-3.79	124.39	127.43
3	A	1204	TPP	C6-C5-C4	-3.35	124.75	127.43
3	C	1204	TPP	C6'-N1'-C2'	3.33	121.63	115.96
3	F	1204	TPP	C6'-N1'-C2'	3.32	121.61	115.96
3	B	1204	TPP	C6'-N1'-C2'	3.17	121.36	115.96
3	D	1204	TPP	C6'-N1'-C2'	3.16	121.34	115.96
3	E	1204	TPP	C6'-N1'-C2'	3.15	121.33	115.96
3	A	1204	TPP	C6'-N1'-C2'	3.12	121.27	115.96
3	C	1204	TPP	C5'-C6'-N1'	-3.10	118.65	123.82
3	F	1204	TPP	C5'-C6'-N1'	-2.96	118.89	123.82
3	B	1204	TPP	C5'-C6'-N1'	-2.84	119.09	123.82
3	D	1204	TPP	C5'-C6'-N1'	-2.81	119.15	123.82
3	A	1204	TPP	C5'-C6'-N1'	-2.78	119.19	123.82
3	E	1204	TPP	C5'-C6'-N1'	-2.72	119.29	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1204	TPP	CM4-C4-N3	2.69	125.95	122.53
3	E	1204	TPP	N4'-C4'-N3'	2.53	120.61	117.03
3	D	1204	TPP	CM4-C4-N3	2.44	125.64	122.53
3	F	1204	TPP	PA-O3A-PB	-2.37	124.69	132.83
3	A	1204	TPP	PA-O3A-PB	-2.31	124.89	132.83
3	C	1204	TPP	CM4-C4-N3	2.31	125.47	122.53
3	F	1204	TPP	CM4-C4-N3	2.30	125.47	122.53
3	F	1204	TPP	N1'-C2'-N3'	-2.29	121.60	125.54
3	E	1204	TPP	PA-O3A-PB	-2.26	125.06	132.83
3	B	1204	TPP	PA-O3A-PB	-2.23	125.18	132.83
3	D	1204	TPP	N1'-C2'-N3'	-2.21	121.73	125.54
3	D	1204	TPP	PA-O3A-PB	-2.20	125.27	132.83
3	E	1204	TPP	CM4-C4-N3	2.18	125.31	122.53
3	F	1204	TPP	N4'-C4'-N3'	2.16	120.09	117.03
3	D	1204	TPP	CM2-C2'-N1'	2.16	119.51	117.14
3	B	1204	TPP	N1'-C2'-N3'	-2.16	121.83	125.54
3	A	1204	TPP	N4'-C4'-N3'	2.10	120.00	117.03
3	E	1204	TPP	N1'-C2'-N3'	-2.07	121.97	125.54
3	B	1204	TPP	N4'-C4'-N3'	2.07	119.96	117.03
3	D	1204	TPP	C2'-N3'-C4'	2.07	121.31	118.08
3	A	1204	TPP	N1'-C2'-N3'	-2.07	121.98	125.54
3	C	1204	TPP	N1'-C2'-N3'	-2.05	122.01	125.54
3	E	1204	TPP	CM2-C2'-N3'	2.05	120.35	117.15
3	B	1204	TPP	C2'-N3'-C4'	2.01	121.22	118.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	TPP	PA-O3A-PB-O1B
3	F	1204	TPP	PA-O3A-PB-O1B
3	E	1204	TPP	C5-C6-C7-O7
3	A	1204	TPP	C5-C6-C7-O7
3	D	1204	TPP	C5-C6-C7-O7
3	C	1204	TPP	C5-C6-C7-O7
3	C	1204	TPP	PA-O3A-PB-O3B
3	F	1204	TPP	PA-O3A-PB-O3B
3	E	1204	TPP	C4-C5-C6-C7
3	B	1204	TPP	C4-C5-C6-C7
3	C	1204	TPP	C4-C5-C6-C7
3	F	1204	TPP	C5-C6-C7-O7
3	E	1204	TPP	PA-O3A-PB-O3B

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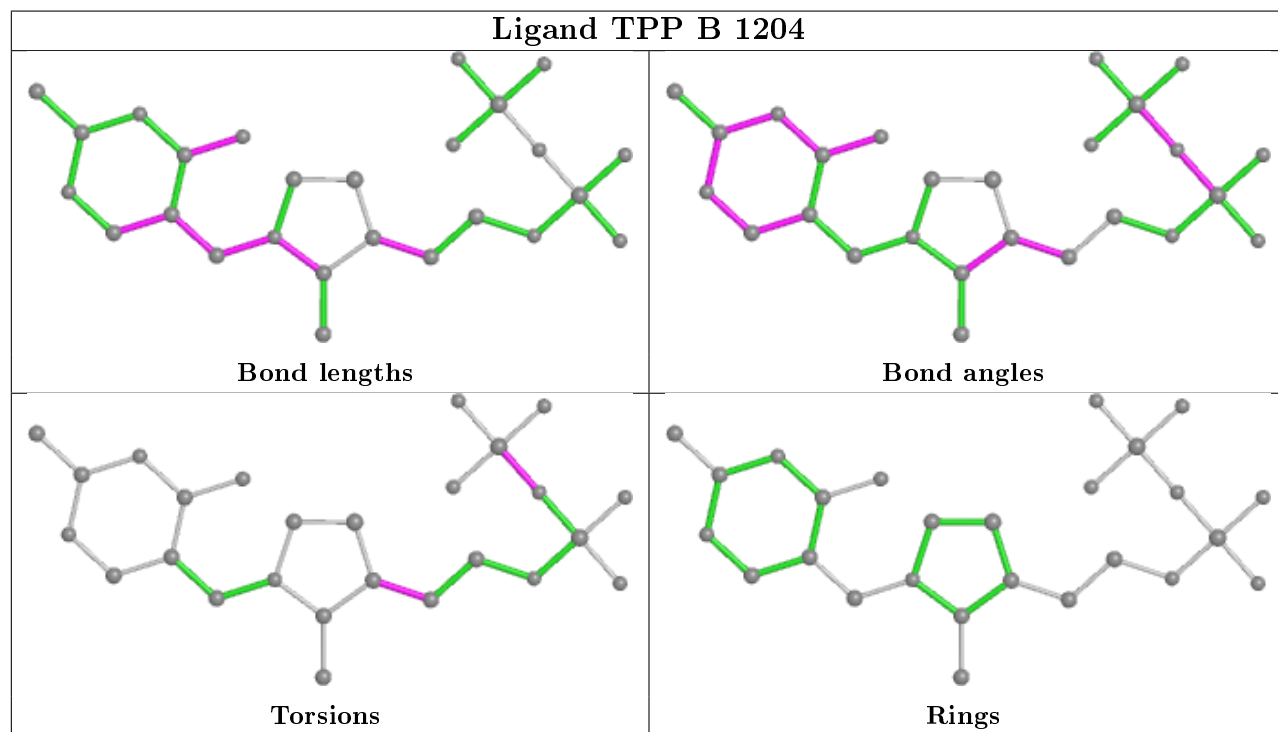
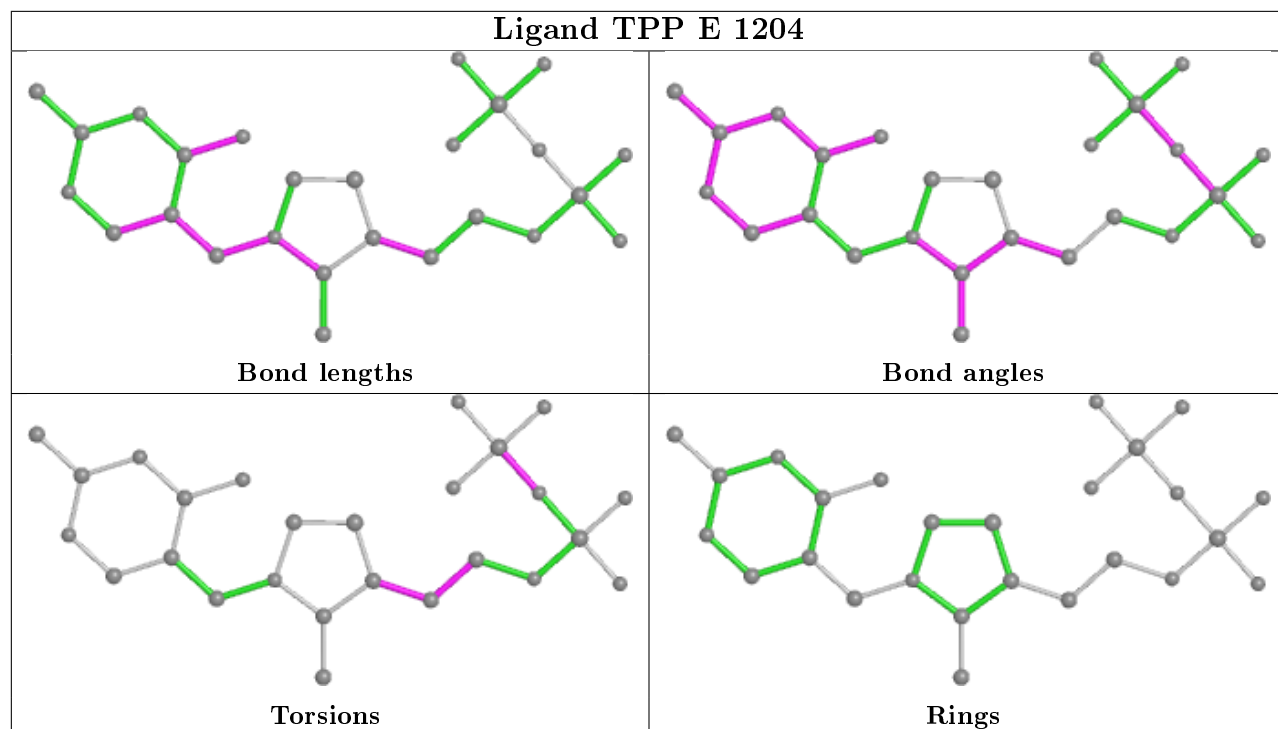
Mol	Chain	Res	Type	Atoms
3	B	1204	TPP	PA-O3A-PB-O3B
3	A	1204	TPP	PA-O3A-PB-O3B
3	D	1204	TPP	PA-O3A-PB-O2B
3	D	1204	TPP	PA-O3A-PB-O3B
3	C	1204	TPP	PA-O3A-PB-O2B
3	A	1204	TPP	C7-O7-PA-O1A
3	D	1204	TPP	C7-O7-PA-O1A
3	C	1204	TPP	C7-O7-PA-O1A
3	A	1204	TPP	C4-C5-C6-C7
3	D	1204	TPP	C4-C5-C6-C7
3	F	1204	TPP	C4-C5-C6-C7

There are no ring outliers.

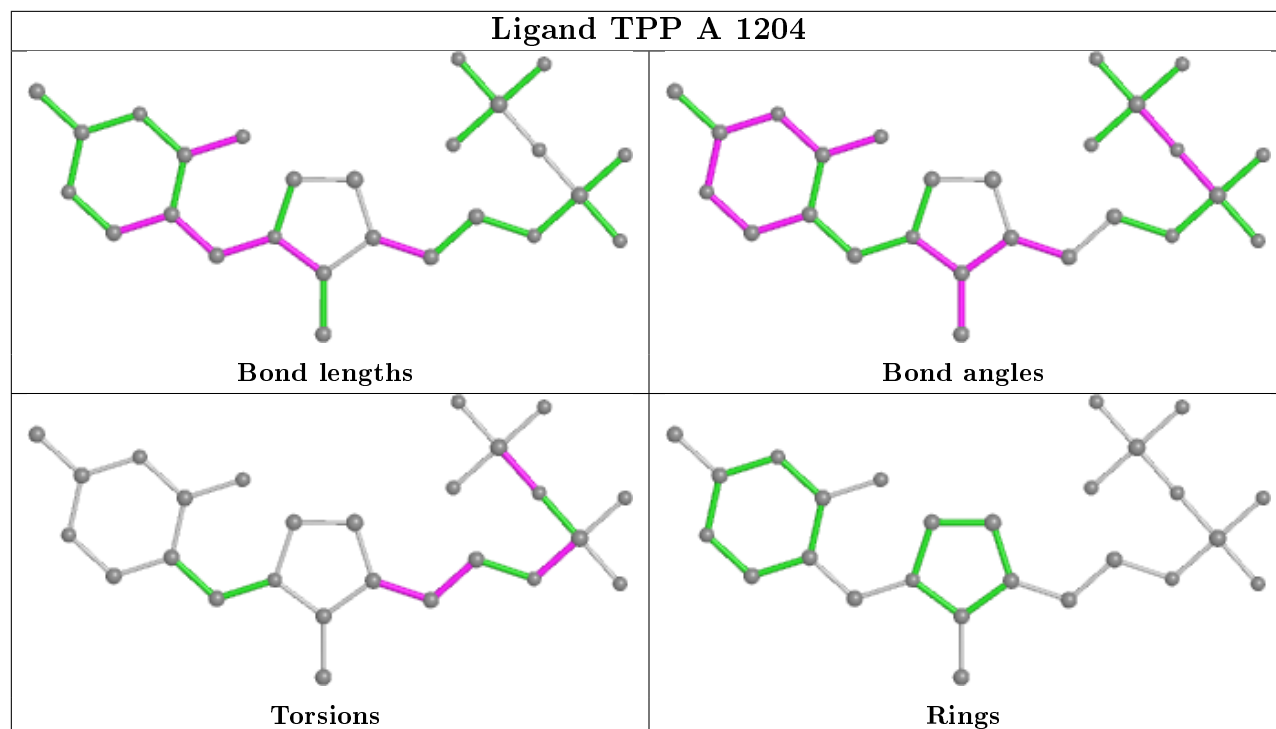
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1207	SO4	3	0
3	A	1204	TPP	1	0
3	C	1204	TPP	2	0
3	F	1204	TPP	1	0

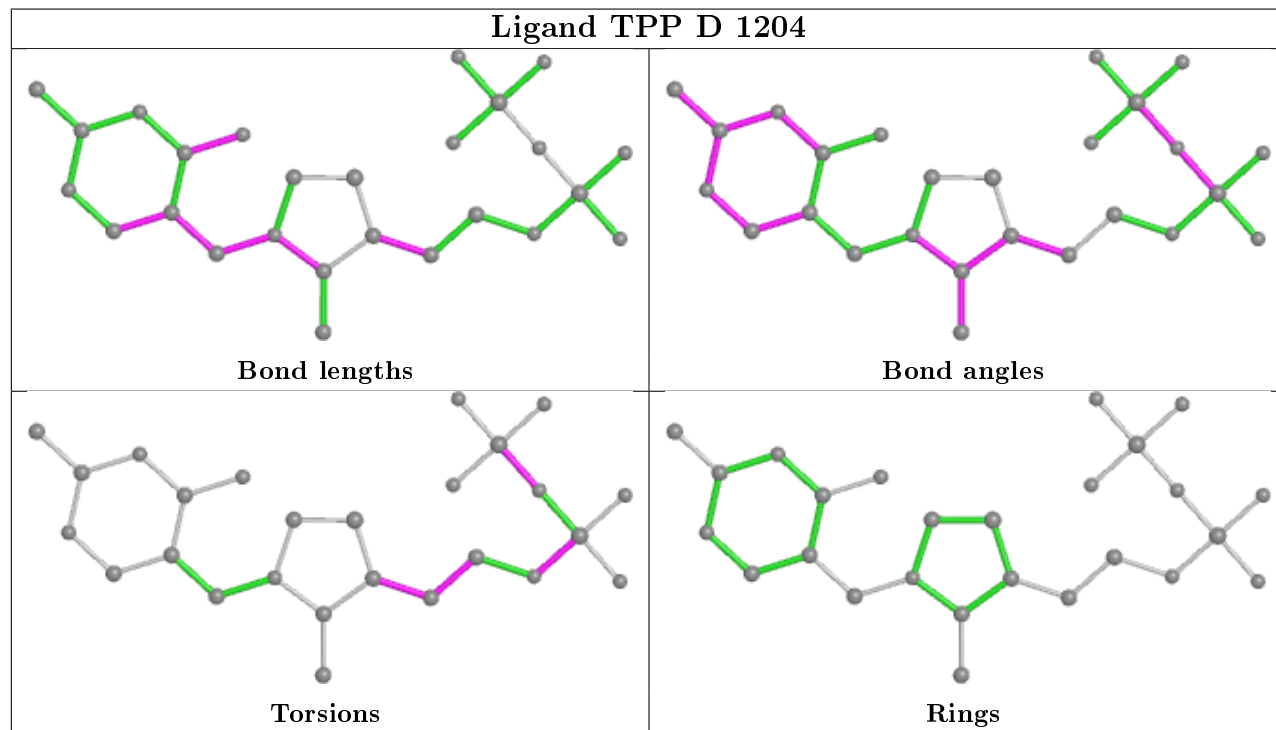
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



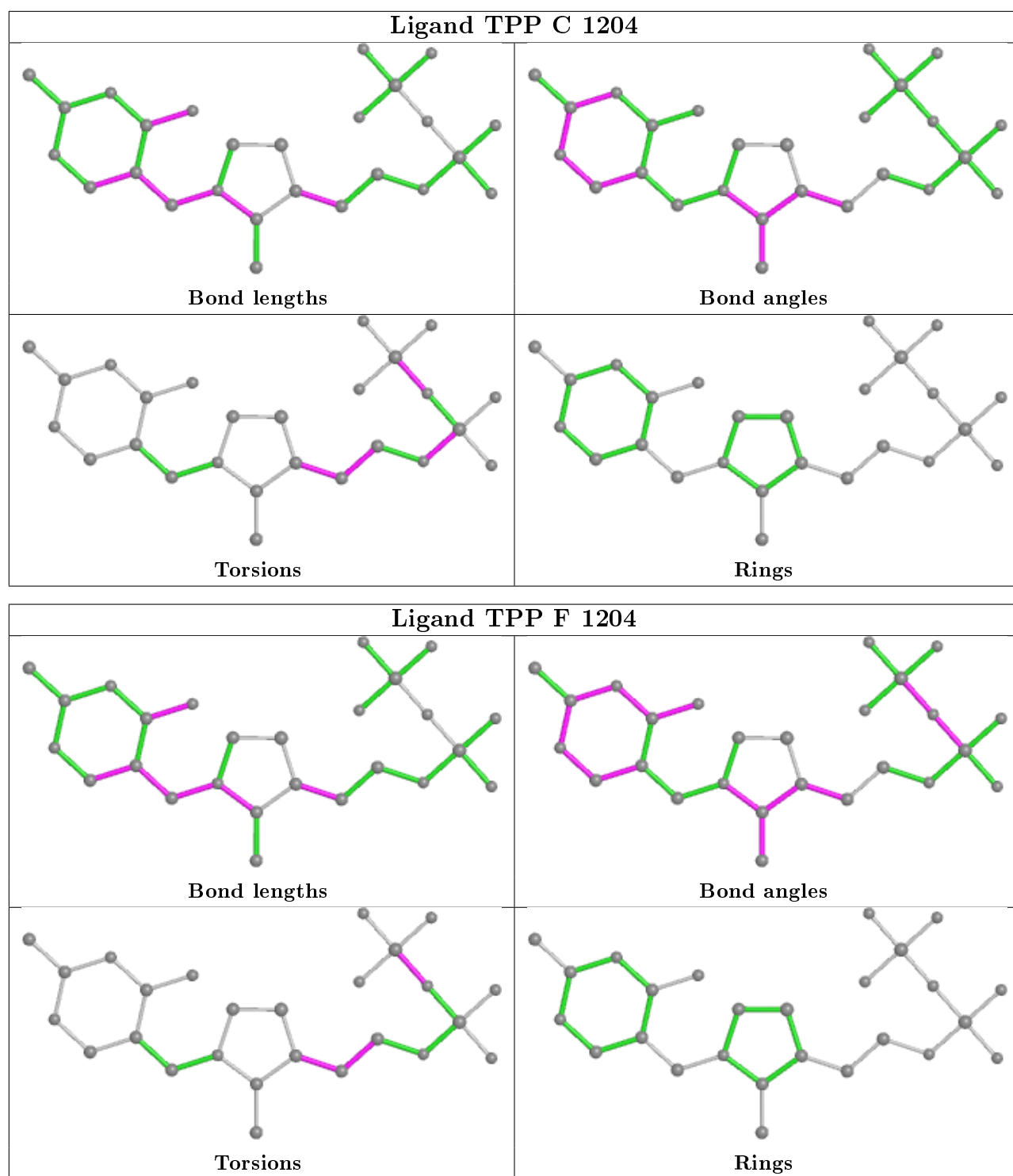
## Ligand TPP A 1204



## Ligand TPP D 1204







## 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

### 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, 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	1163/1171 (99%)	0.31	68 (5%)	23 17	36, 66, 125, 151	0
1	B	1169/1171 (99%)	0.26	68 (5%)	23 17	34, 66, 117, 171	0
1	C	1163/1171 (99%)	0.40	90 (7%)	13 10	36, 74, 130, 165	0
1	D	1157/1171 (98%)	0.22	36 (3%)	49 42	45, 77, 130, 170	0
1	E	1165/1171 (99%)	0.46	108 (9%)	8 6	29, 77, 128, 161	0
1	F	1158/1171 (98%)	0.22	48 (4%)	37 30	37, 78, 132, 188	0
All	All	6975/7026 (99%)	0.31	418 (5%)	21 16	29, 73, 128, 188	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1131	MET	7.8
1	E	754	ALA	7.6
1	E	788	PHE	7.3
1	B	1150	LEU	6.9
1	F	1018	ALA	6.1
1	E	757	LYS	5.7
1	A	629	VAL	5.7
1	C	678	ILE	5.5
1	E	755	LYS	5.4
1	C	1044	VAL	5.4
1	C	594	ILE	5.2
1	E	607	GLU	5.1
1	A	1122	PRO	4.9
1	C	598	ASN	4.9
1	E	687	ILE	4.8
1	A	1012	GLY	4.8
1	A	818	VAL	4.7
1	A	788	PHE	4.7
1	E	766	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	1109	GLN	4.7
1	A	1136	TYR	4.6
1	E	1136	TYR	4.6
1	E	1123	THR	4.6
1	E	1166	LYS	4.5
1	B	1139	LEU	4.5
1	C	788	PHE	4.5
1	C	706	ALA	4.5
1	A	1128	ASP	4.5
1	D	435	ILE	4.4
1	C	1126	PHE	4.4
1	E	794	LYS	4.4
1	A	687	ILE	4.3
1	C	1123	THR	4.3
1	E	1005	SER	4.2
1	A	716	GLU	4.2
1	F	522	LEU	4.2
1	B	1107	LEU	4.1
1	B	1128	ASP	4.1
1	C	605	ALA	4.1
1	B	1119	TYR	4.1
1	A	1129	PHE	4.1
1	E	791	ALA	4.1
1	F	561	THR	4.1
1	E	1019	ALA	4.1
1	E	724	ILE	4.0
1	F	607	GLU	4.0
1	E	635	PHE	4.0
1	E	716	GLU	4.0
1	E	759	LEU	3.9
1	A	821	VAL	3.9
1	C	716	GLU	3.9
1	C	735	ILE	3.9
1	E	787	ASN	3.9
1	E	1131	MET	3.9
1	B	1106	GLN	3.8
1	A	1127	ARG	3.8
1	C	1097	TYR	3.8
1	B	728	ALA	3.8
1	A	727	GLU	3.8
1	E	761	MET	3.8
1	E	688	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	1097	TYR	3.7
1	C	728	ALA	3.7
1	A	1161	ARG	3.7
1	E	997	VAL	3.7
1	A	1126	PHE	3.7
1	E	674	ILE	3.7
1	E	1002	GLY	3.7
1	B	733	PHE	3.6
1	C	798	PHE	3.6
1	E	765	GLU	3.6
1	E	758	ALA	3.6
1	C	1093	VAL	3.6
1	B	894	ALA	3.6
1	B	1113	ASN	3.6
1	E	747	ASN	3.6
1	A	1009	THR	3.5
1	D	598	ASN	3.5
1	E	1125	SER	3.5
1	A	1163	GLU	3.5
1	E	691	GLN	3.5
1	B	710	ASP	3.5
1	C	762	VAL	3.5
1	E	756	VAL	3.5
1	E	821	VAL	3.4
1	B	1069	ILE	3.4
1	D	1153	LYS	3.4
1	E	784	VAL	3.4
1	E	606	LEU	3.4
1	B	1142	GLN	3.4
1	B	1151	PHE	3.4
1	C	1109	GLN	3.4
1	A	706	ALA	3.4
1	E	751	VAL	3.4
1	C	1158	ALA	3.3
1	F	783	GLU	3.3
1	A	1109	GLN	3.3
1	A	1057	LEU	3.3
1	C	1150	LEU	3.3
1	E	760	THR	3.3
1	E	467	PHE	3.3
1	F	1159	LYS	3.3
1	C	551	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	629	VAL	3.3
1	C	404	LYS	3.3
1	E	1072	TYR	3.3
1	C	1012	GLY	3.2
1	F	1017	PHE	3.2
1	B	1164	GLN	3.2
1	E	1078	HIS	3.2
1	C	784	VAL	3.2
1	B	1127	ARG	3.2
1	B	1014	VAL	3.2
1	A	1159	LYS	3.2
1	C	1154	ALA	3.2
1	E	540	ILE	3.2
1	C	1042	ALA	3.2
1	A	705	LEU	3.2
1	A	1031	LEU	3.2
1	C	1122	PRO	3.2
1	D	420	PHE	3.2
1	E	1041	VAL	3.2
1	C	1119	TYR	3.2
1	A	1130	LEU	3.2
1	B	1121	THR	3.1
1	F	435	ILE	3.1
1	C	993	LEU	3.1
1	C	1121	THR	3.1
1	E	739	PRO	3.1
1	A	777	PHE	3.1
1	B	1110	GLU	3.1
1	B	726	LYS	3.1
1	A	1103	TYR	3.1
1	C	1120	LYS	3.1
1	C	1157	ASP	3.1
1	F	1143	PHE	3.1
1	E	542	ALA	3.1
1	E	526	MET	3.0
1	F	718	PHE	3.0
1	E	685	ASN	3.0
1	A	755	LYS	3.0
1	B	1108	ALA	3.0
1	B	686	CYS	3.0
1	F	433	ASN	3.0
1	B	788	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	910	TRP	3.0
1	B	1071	ALA	3.0
1	D	1017	PHE	3.0
1	A	1162	LEU	3.0
1	A	1156	ALA	3.0
1	B	730	GLY	3.0
1	E	680	GLN	3.0
1	C	553	SER	3.0
1	B	1163	GLU	3.0
1	E	711	LEU	2.9
1	E	786	VAL	2.9
1	D	1097	TYR	2.9
1	C	590	LYS	2.9
1	F	626	ALA	2.9
1	F	627	ALA	2.9
1	B	1125	SER	2.9
1	B	1019	ALA	2.9
1	C	1071	ALA	2.9
1	F	854	ARG	2.9
1	E	1100	LEU	2.9
1	D	565	LYS	2.9
1	E	656	PHE	2.9
1	D	352	ASN	2.9
1	E	762	VAL	2.8
1	E	1014	VAL	2.8
1	A	1087	ARG	2.8
1	A	1149	GLN	2.8
1	C	1128	ASP	2.8
1	D	726	LYS	2.8
1	C	601	ALA	2.8
1	A	1049	SER	2.8
1	A	791	ALA	2.8
1	F	788	PHE	2.8
1	E	717	THR	2.8
1	F	601	ALA	2.8
1	E	1142	GLN	2.8
1	A	820	LEU	2.8
1	F	570	ILE	2.8
1	A	1097	TYR	2.8
1	E	1126	PHE	2.8
1	F	420	PHE	2.8
1	C	1166	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	1127	ARG	2.8
1	C	1142	GLN	2.7
1	E	1122	PRO	2.7
1	E	998	TYR	2.7
1	D	1161	ARG	2.7
1	A	1011	THR	2.7
1	C	1047	GLY	2.7
1	C	717	THR	2.7
1	E	609	LEU	2.7
1	D	1150	LEU	2.7
1	F	1011	THR	2.7
1	A	919	ARG	2.7
1	A	1150	LEU	2.7
1	E	1129	PHE	2.7
1	B	1044	VAL	2.7
1	C	1020	GLY	2.7
1	A	1119	TYR	2.7
1	E	564	PHE	2.7
1	C	684	GLU	2.7
1	F	686	CYS	2.7
1	C	935	ILE	2.7
1	E	1083	THR	2.7
1	A	1013	ALA	2.6
1	E	508	LEU	2.6
1	E	595	LEU	2.6
1	C	1134	ILE	2.6
1	E	949	ILE	2.6
1	D	1126	PHE	2.6
1	B	1111	GLY	2.6
1	B	1161	ARG	2.6
1	C	1080	ILE	2.6
1	C	787	ASN	2.6
1	A	1157	ASP	2.6
1	D	582	SER	2.6
1	E	1012	GLY	2.6
1	F	684	GLU	2.6
1	E	695	VAL	2.6
1	A	949	ILE	2.6
1	D	561	THR	2.6
1	E	677	ASN	2.6
1	C	852	VAL	2.6
1	E	793	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	569	VAL	2.6
1	F	682	GLN	2.6
1	B	1062	LYS	2.6
1	E	753	PRO	2.6
1	F	678	ILE	2.6
1	C	589	LYS	2.6
1	B	1147	ALA	2.5
1	F	575	ALA	2.5
1	C	1139	LEU	2.5
1	C	1159	LYS	2.5
1	E	689	CYS	2.5
1	D	51	GLY	2.5
1	C	1161	ARG	2.5
1	B	1126	PHE	2.5
1	E	789	ASN	2.5
1	E	1152	ALA	2.5
1	A	1100	LEU	2.5
1	E	1135	ARG	2.5
1	C	1125	SER	2.5
1	D	1012	GLY	2.5
1	F	1003	GLY	2.5
1	A	1017	PHE	2.5
1	A	710	ASP	2.5
1	C	701	ILE	2.5
1	D	437	ILE	2.5
1	E	1010	GLN	2.5
1	C	457	SER	2.5
1	C	764	LEU	2.5
1	B	1097	TYR	2.5
1	B	782	PRO	2.5
1	C	766	GLU	2.5
1	A	724	ILE	2.5
1	A	754	ALA	2.5
1	B	1165	TYR	2.5
1	E	1165	TYR	2.5
1	C	630	THR	2.4
1	F	618	TRP	2.4
1	B	1055	LYS	2.4
1	B	1124	ALA	2.4
1	E	1121	THR	2.4
1	C	1130	LEU	2.4
1	E	1139	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	620	ASP	2.4
1	D	716	GLU	2.4
1	B	590	LYS	2.4
1	D	485	ALA	2.4
1	A	946	LEU	2.4
1	B	1162	LEU	2.4
1	C	606	LEU	2.4
1	B	682	GLN	2.4
1	C	537	PHE	2.4
1	D	1023	PHE	2.4
1	B	876	MET	2.4
1	D	1009	THR	2.4
1	F	755	LYS	2.4
1	A	998	TYR	2.4
1	A	1018	ALA	2.4
1	C	1100	LEU	2.4
1	E	694	LEU	2.4
1	B	679	PRO	2.4
1	C	1011	THR	2.4
1	C	1014	VAL	2.4
1	F	733	PHE	2.4
1	B	727	GLU	2.4
1	C	680	GLN	2.4
1	A	726	LYS	2.4
1	C	593	LYS	2.4
1	E	565	LYS	2.4
1	F	1166	LYS	2.4
1	D	602	VAL	2.4
1	F	1023	PHE	2.4
1	C	1029	LEU	2.3
1	B	684	GLU	2.3
1	B	1116	ILE	2.3
1	C	1163	GLU	2.3
1	E	1117	LEU	2.3
1	E	558	ILE	2.3
1	F	583	ILE	2.3
1	A	1014	VAL	2.3
1	B	765	GLU	2.3
1	B	993	LEU	2.3
1	E	684	GLU	2.3
1	E	655	THR	2.3
1	C	576	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	707	LYS	2.3
1	E	1023	PHE	2.3
1	B	716	GLU	2.3
1	A	717	THR	2.3
1	B	678	ILE	2.3
1	D	1006	SER	2.3
1	B	1159	LYS	2.3
1	D	1014	VAL	2.3
1	E	672	ARG	2.3
1	D	1168	LEU	2.3
1	E	640	LEU	2.3
1	C	760	THR	2.3
1	C	734	ARG	2.3
1	B	755	LYS	2.3
1	E	589	LYS	2.3
1	D	988	VAL	2.3
1	C	511	SER	2.2
1	C	1010	GLN	2.2
1	B	1131	MET	2.2
1	B	1129	PHE	2.2
1	C	733	PHE	2.2
1	E	1128	ASP	2.2
1	A	913	GLY	2.2
1	A	1108	ALA	2.2
1	D	575	ALA	2.2
1	A	607	GLU	2.2
1	E	352	ASN	2.2
1	E	618	TRP	2.2
1	C	1054	MET	2.2
1	C	1129	PHE	2.2
1	B	569	VAL	2.2
1	C	724	ILE	2.2
1	C	1053	LEU	2.2
1	E	512	THR	2.2
1	E	710	ASP	2.2
1	B	1010	GLN	2.2
1	D	1142	GLN	2.2
1	B	1072	TYR	2.2
1	F	467	PHE	2.2
1	F	564	PHE	2.2
1	F	508	LEU	2.2
1	A	766	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1157	ASP	2.2
1	C	730	GLY	2.2
1	F	1015	ALA	2.2
1	D	467	PHE	2.2
1	E	604	ARG	2.2
1	B	735	ILE	2.2
1	D	569	VAL	2.2
1	A	908	GLU	2.2
1	A	1112	LYS	2.2
1	B	991	LEU	2.2
1	F	794	LYS	2.2
1	E	811	GLY	2.2
1	C	518	MET	2.2
1	E	1092	ALA	2.2
1	F	546	ALA	2.2
1	F	1016	ARG	2.2
1	C	587	TYR	2.1
1	C	737	VAL	2.1
1	A	1074	PRO	2.1
1	F	759	LEU	2.1
1	E	706	ALA	2.1
1	C	607	GLU	2.1
1	E	1085	SER	2.1
1	F	22	VAL	2.1
1	E	625	ALA	2.1
1	E	743	THR	2.1
1	A	569	VAL	2.1
1	C	462	ILE	2.1
1	D	711	LEU	2.1
1	F	785	LYS	2.1
1	C	675	ALA	2.1
1	A	1120	LYS	2.1
1	B	891	ILE	2.1
1	C	1118	ASP	2.1
1	A	1114	PRO	2.1
1	E	723	ALA	2.1
1	D	1121	THR	2.1
1	A	1111	GLY	2.1
1	E	727	GLU	2.1
1	C	1043	SER	2.1
1	E	457	SER	2.1
1	F	159	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1084	TYR	2.1
1	F	708	PRO	2.1
1	F	721	LYS	2.1
1	B	1012	GLY	2.1
1	D	570	ILE	2.1
1	B	1169	ALA	2.1
1	E	1124	ALA	2.1
1	A	750	ASP	2.1
1	D	1143	PHE	2.1
1	C	1090	LYS	2.0
1	C	1162	LEU	2.0
1	F	483	LEU	2.0
1	E	750	ASP	2.0
1	F	680	GLN	2.0
1	A	1160	ALA	2.0
1	B	1013	ALA	2.0
1	C	1033	ALA	2.0
1	D	755	LYS	2.0
1	E	749	ALA	2.0
1	B	720	THR	2.0
1	F	252	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	D	1206	5/5	0.94	0.15	87,89,90,92	0
5	SO4	E	1206	5/5	0.94	0.13	79,80,82,83	0

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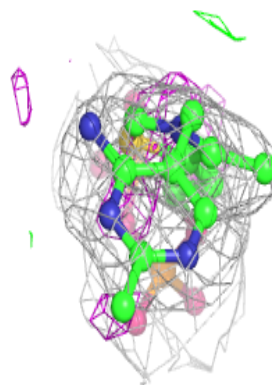
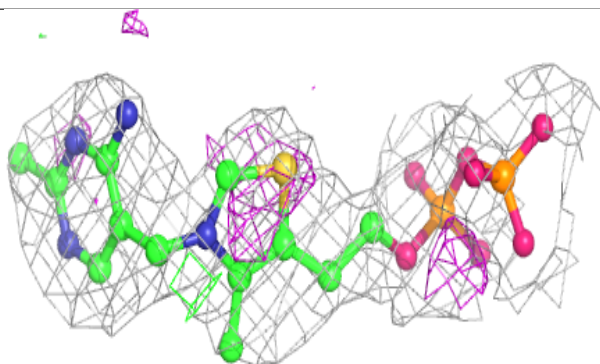
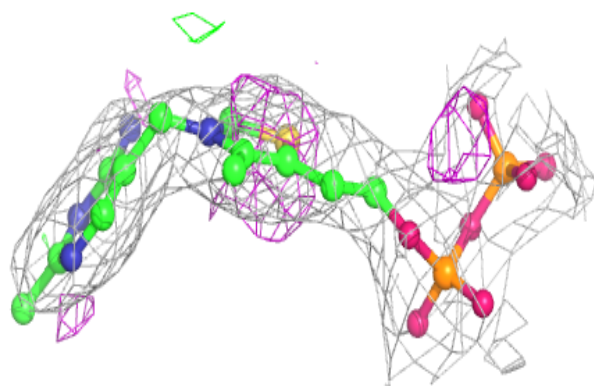
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	F	1205	1/1	0.94	0.13	35,35,35,35	0
5	SO4	F	1206	5/5	0.95	0.10	101,101,103,103	0
5	SO4	B	1207	5/5	0.95	0.15	87,87,88,89	0
3	TPP	C	1204	26/26	0.95	0.18	57,70,80,87	0
2	SF4	C	1203	8/8	0.95	0.10	73,87,107,124	0
3	TPP	A	1204	26/26	0.96	0.17	52,75,86,95	0
5	SO4	B	1206	5/5	0.96	0.17	93,95,95,96	0
3	TPP	B	1204	26/26	0.96	0.16	59,70,83,87	0
4	MG	A	1205	1/1	0.96	0.07	44,44,44,44	0
3	TPP	E	1204	26/26	0.96	0.15	44,70,77,82	0
4	MG	C	1205	1/1	0.96	0.06	31,31,31,31	0
5	SO4	A	1206	5/5	0.96	0.14	88,89,89,89	0
2	SF4	A	1203	8/8	0.96	0.13	70,85,115,169	0
2	SF4	E	1203	8/8	0.97	0.11	63,95,138,162	0
3	TPP	D	1204	26/26	0.97	0.15	58,64,73,82	0
2	SF4	D	1202	8/8	0.97	0.25	73,82,95,121	0
2	SF4	F	1201	8/8	0.97	0.16	88,92,105,106	0
2	SF4	B	1203	8/8	0.97	0.12	60,79,85,96	0
2	SF4	D	1203	8/8	0.97	0.14	59,67,72,78	0
4	MG	E	1205	1/1	0.97	0.08	44,44,44,44	0
5	SO4	C	1206	5/5	0.98	0.12	75,75,78,78	0
2	SF4	D	1201	8/8	0.98	0.16	73,76,81,84	0
2	SF4	E	1202	8/8	0.98	0.11	80,88,105,113	0
2	SF4	F	1203	8/8	0.98	0.15	61,66,85,103	0
2	SF4	B	1202	8/8	0.98	0.13	68,71,72,73	0
2	SF4	A	1201	8/8	0.98	0.11	95,103,122,123	0
3	TPP	F	1204	26/26	0.98	0.14	48,68,71,77	0
4	MG	D	1205	1/1	0.98	0.14	32,32,32,32	0
2	SF4	A	1202	8/8	0.98	0.16	75,81,86,88	0
2	SF4	C	1202	8/8	0.99	0.10	72,76,81,82	0
2	SF4	C	1201	8/8	0.99	0.09	96,100,109,122	0
2	SF4	B	1201	8/8	0.99	0.10	83,88,93,104	0
2	SF4	F	1202	8/8	0.99	0.19	75,79,85,88	0
4	MG	B	1205	1/1	0.99	0.09	32,32,32,32	0
2	SF4	E	1201	8/8	0.99	0.09	95,97,110,115	0

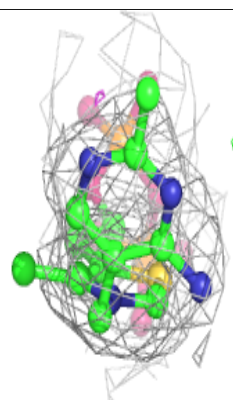
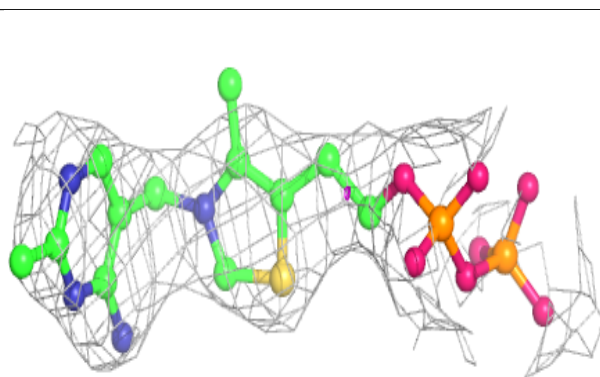
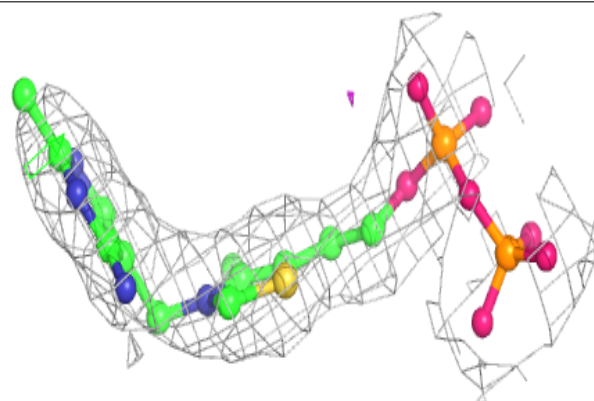
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP C 1204:**

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

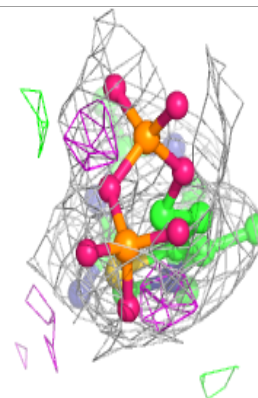
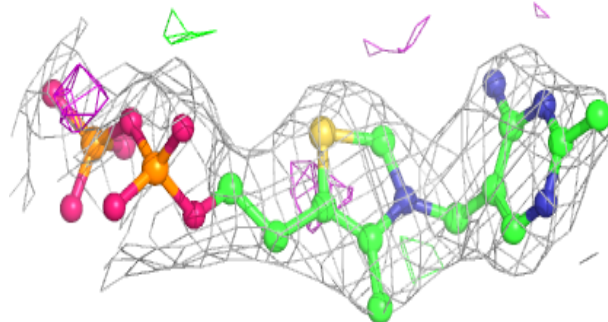
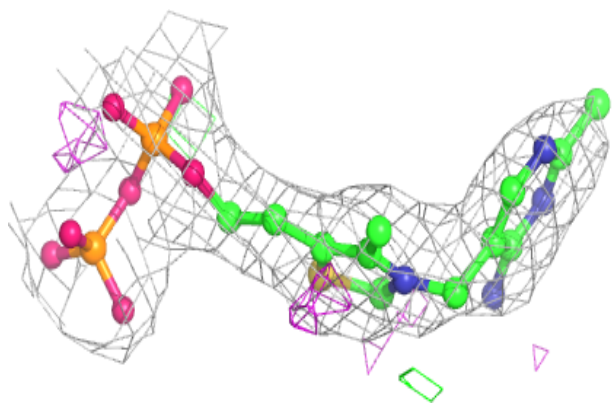
**Electron density around TPP A 1204:**

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

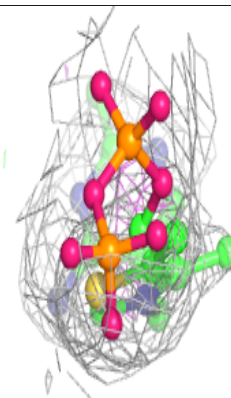
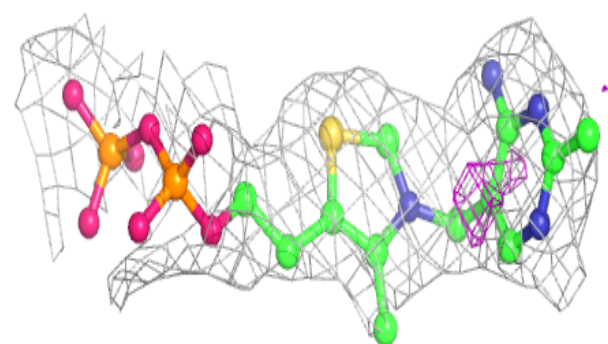
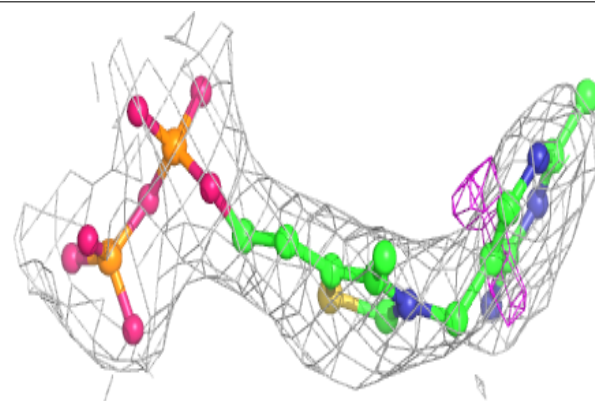


**Electron density around TPP B 1204:**

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

**Electron density around TPP E 1204:**

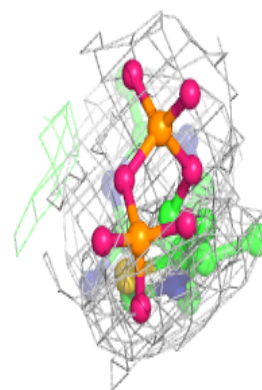
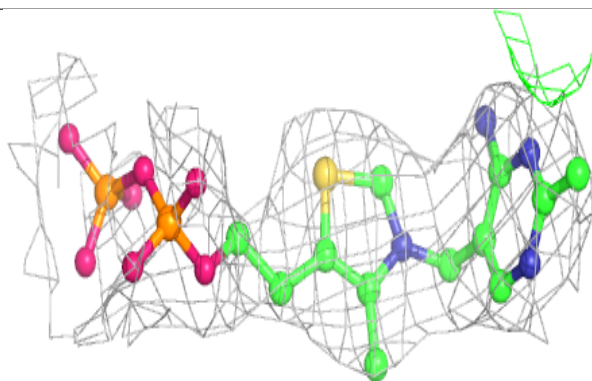
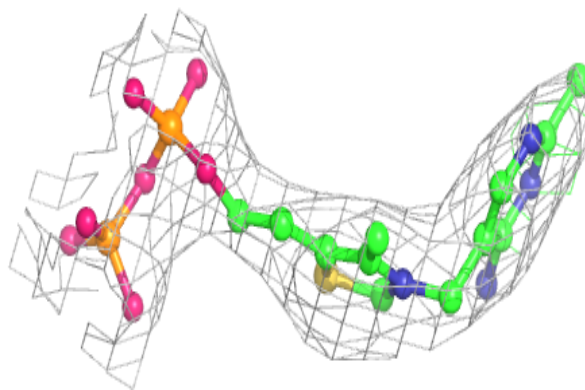
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



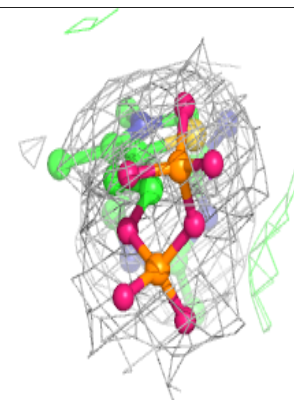
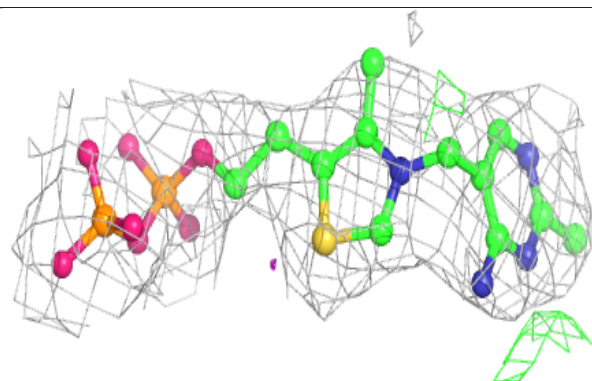
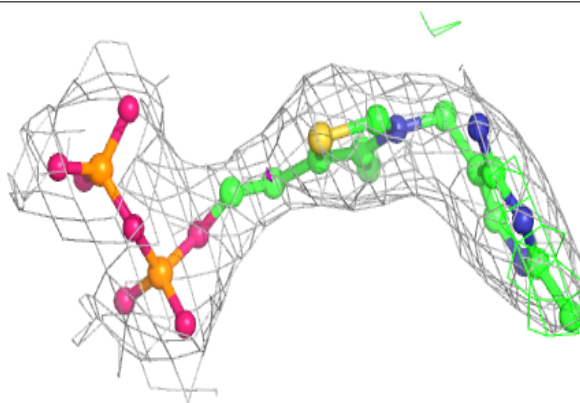


**Electron density around TPP D 1204:**

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

**Electron density around TPP F 1204:**

$2mF_o-DF_c$  (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.