



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:15 PM UTC

PDB ID : 6CIN / pdb\_00006cin  
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.

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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

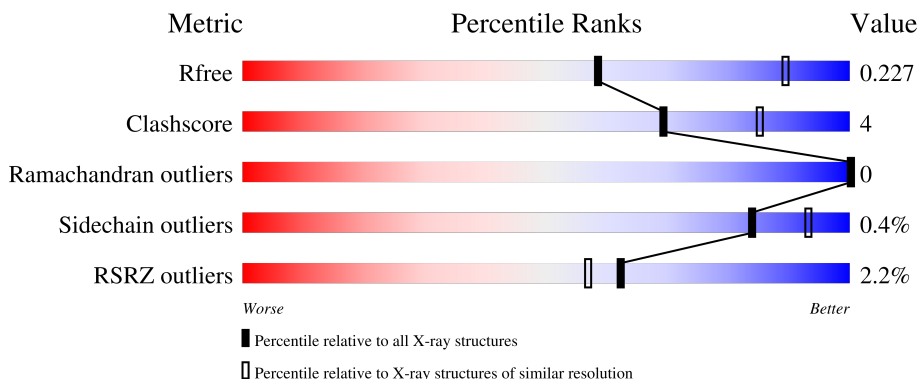
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


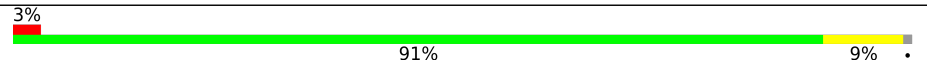
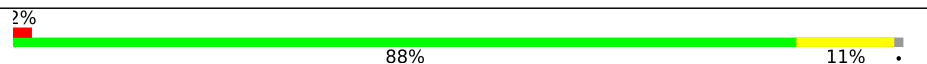
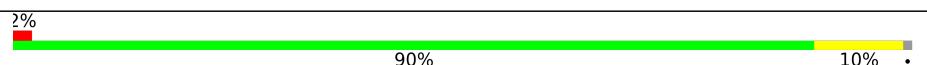
The reported resolution of this entry is 2.60 Å.

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))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1171	 2% 90% 10%
1	B	1171	 2% 92% 8%
1	C	1171	 3% 91% 9%
1	D	1171	 2% 88% 11%
1	E	1171	 2% 90% 10%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	1171	

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](#)

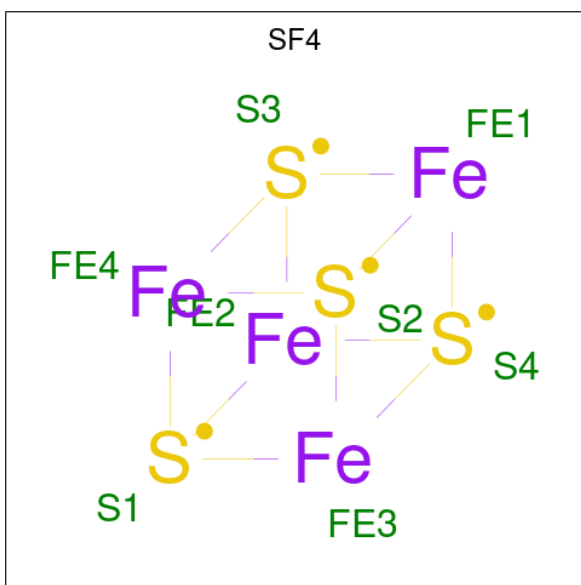
There are 6 unique types of molecules in this entry. The entry contains 53870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

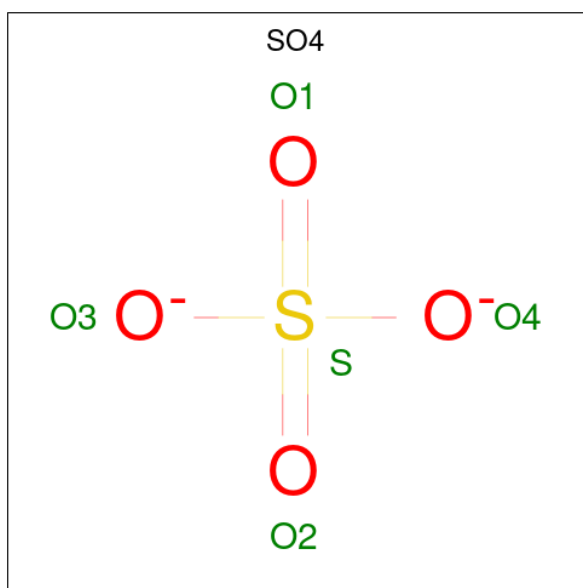


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 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 (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



- Molecule 5 is SULFATE ION (CCD ID: 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		

*Continued on next page...*

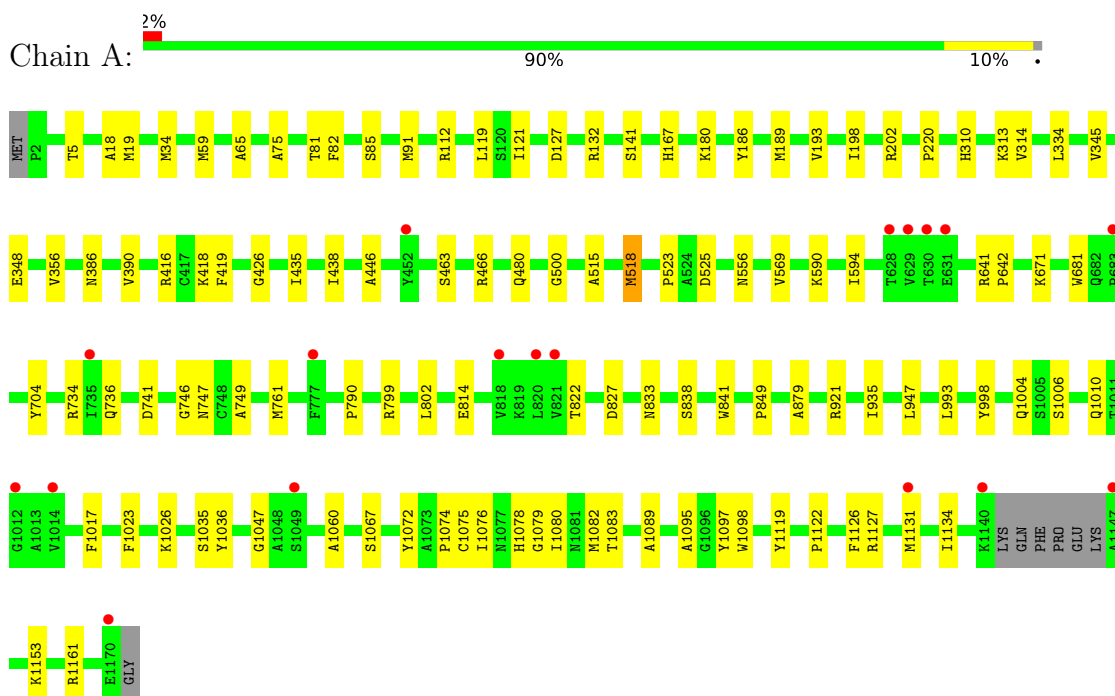
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	E	61	Total O 61 61	0	0
6	F	58	Total O 58 58	0	0

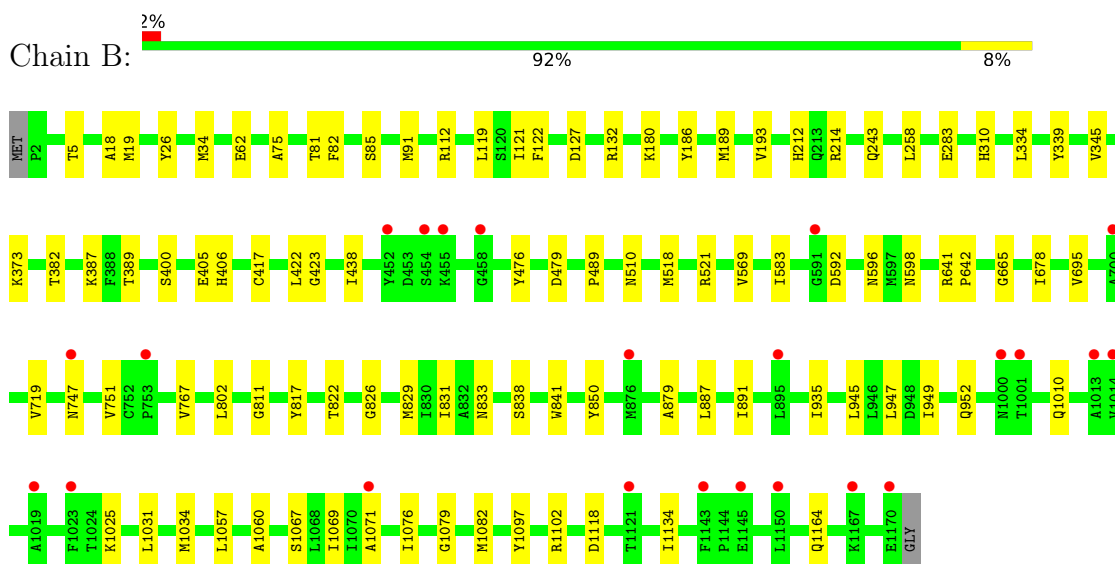
### 3 Residue-property plots i

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

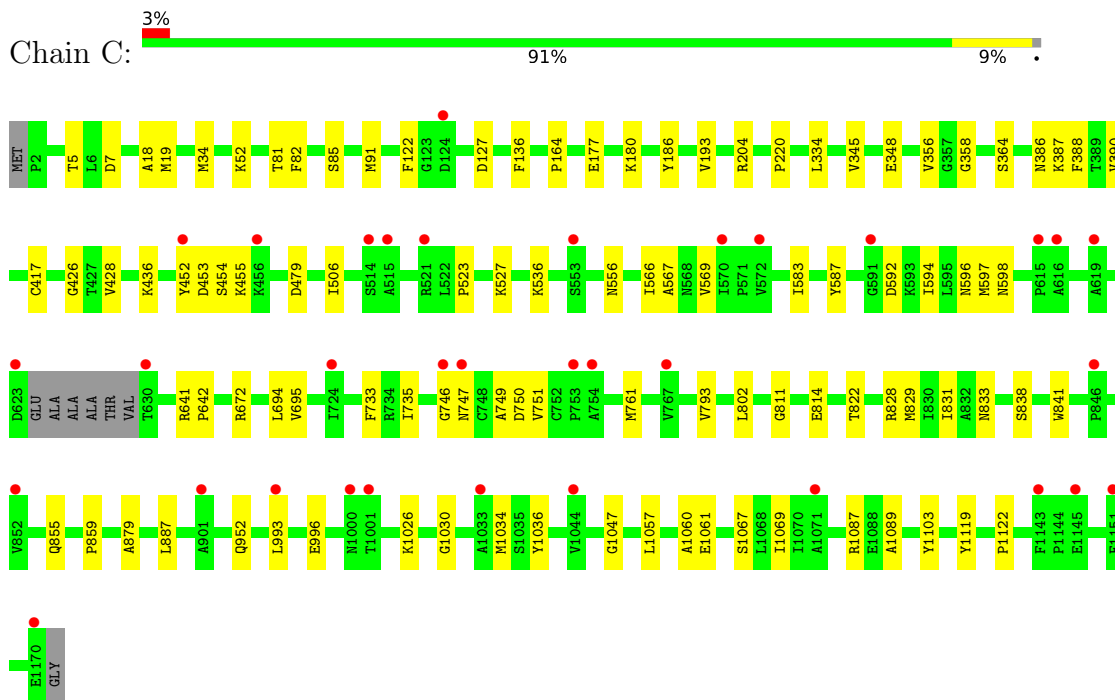
#### • Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



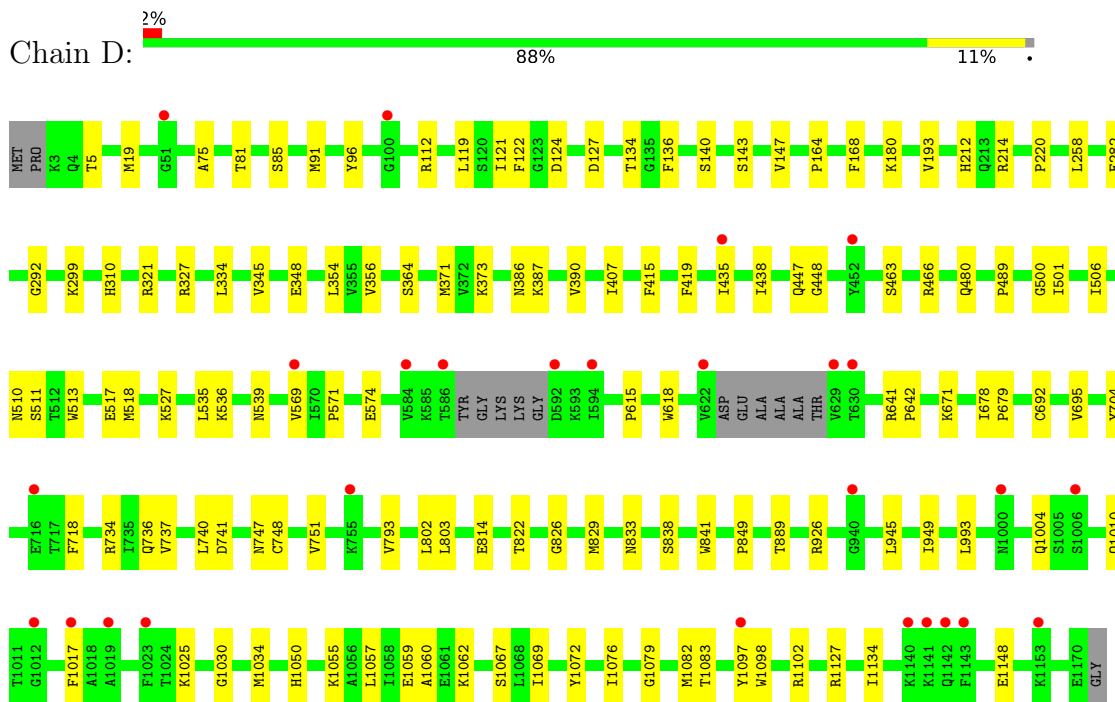
#### • Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



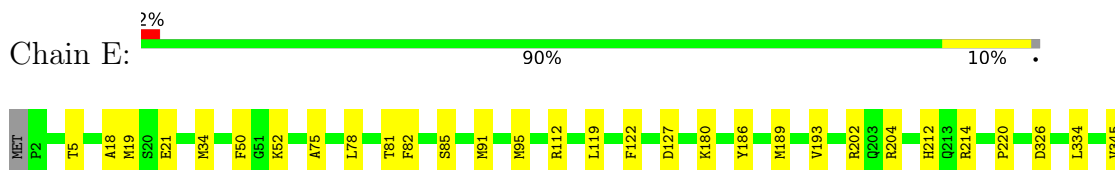
- Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

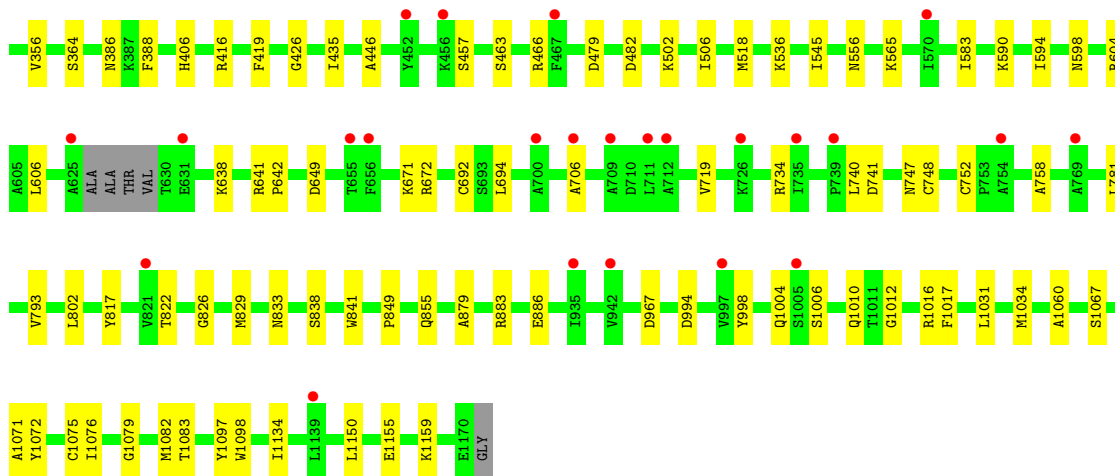


- Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

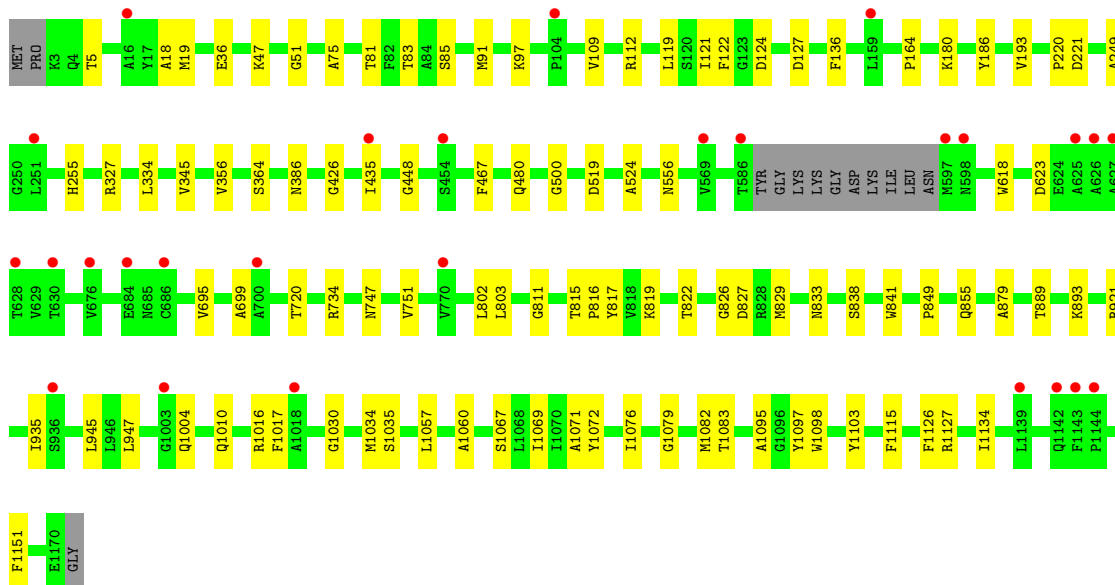
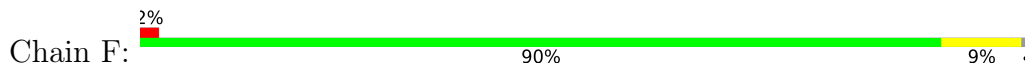


- Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





● 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)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.195 , 0.227 0.196 , 0.227	Depositor DCC
$R_{free}$ test set	12392 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtrriage
Anisotropy	0.564	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage'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: TPP, SO4, MG, SF4

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	0.14	0/9063	0.33	0/12286
1	B	0.14	0/9099	0.33	0/12339
1	C	0.14	0/9055	0.33	0/12277
1	D	0.14	0/8978	0.33	0/12178
1	E	0.13	0/9068	0.32	0/12294
1	F	0.13	0/8980	0.32	0/12183
All	All	0.14	0/54243	0.33	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	68	0
1	B	8905	0	8821	60	0
1	C	8862	0	8779	59	0
1	D	8788	0	8658	77	0
1	E	8875	0	8788	70	0
1	F	8789	0	8666	63	0
2	A	24	0	0	0	0

*Continued on next page...*

Continued from previous page...

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	1	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	4	0
6	E	61	0	0	1	0
6	F	58	0	0	0	0
All	All	53870	0	52604	371	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 4.

All (371) 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:C:81:THR:HG21	1:C:91:MET:HE1	1.57	0.87
1:B:81:THR:HG21	1:B:91:MET:HE1	1.62	0.81
1:B:521:ARG:NH2	5:B:1207:SO4:S	2.55	0.80
1:E:81:THR:HG21	1:E:91:MET:HE1	1.62	0.80

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:THR:HG21	1:F:91:MET:HE1	1.62	0.79
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:D:81:THR:HG21	1:D:91:MET:HE1	1.68	0.73
1:E:802:LEU:HB2	1:E:822:THR:HB	1.71	0.73
1:E:706:ALA:HB2	1:E:781:LEU:HD21	1.71	0.71
1:A:81:THR:HG21	1:A:91:MET:HE1	1.72	0.71
1:D:1059:GLU:OE1	6:D:1301:HOH:O	2.09	0.71
1:A:746:GLY:HA2	1:A:761:MET:HE3	1.72	0.71
1:C:1034:MET:HE2	1:C:1103:TYR:HB2	1.72	0.71
1:C:746:GLY:HA2	1:C:761:MET:HE3	1.75	0.69
1:F:1034:MET:HE2	1:F:1103:TYR:HB2	1.75	0.67
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: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:C:19:MET:HE1	1:C:193:VAL:HG22	1.81	0.62
1:E:204:ARG:NH2	6:E:1301:HOH:O	2.31	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:E:671:LYS:NZ	1:E:741:ASP:OD2	2.32	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: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:A:1076:ILE:HA	1:A:1082:MET:HE3	1.86	0.57
1:C:1036:TYR:O	1:D:1025:LYS:NZ	2.36	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:838:SER:HA	1:B:841:TRP:CE2	2.42	0.55
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: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: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:E:1031:LEU:HA	1:E:1034:MET:HE3	1.91	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:519:ASP:OD1	1:F:618:TRP:NE1	2.39	0.52
1:F:1072:TYR:HB2	1:F:1098:TRP:CE2	2.45	0.52
1:C:122:PHE:CE2	1:D:220:PRO:HD3	2.45	0.52
1:E:112:ARG:NH2	1:E:119:LEU:HD11	2.25	0.51
1:E:1076:ILE:HG22	1:E:1082:MET:HG3	1.91	0.51
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	1.93	0.51
1:C:594:ILE:HA	1:C:597:MET:HE2	1.92	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:E:19:MET:HE1	1:E:193:VAL:HG22	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:SER:HA	1:A:841:TRP:CE2	2.45	0.51
3:C:1204:TPP:H2	3:C:1204:TPP:HN42	1.75	0.51
1:E:1012:GLY:HA2	1:E:1150:LEU:HD13	1.92	0.51
1:D:1127:ARG:HH22	1:D:1148:GLU:CD	2.18	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
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:F:19:MET:HE1	1:F:193:VAL:HG22	1.94	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:C:34:MET:HE3	1:C:82:PHE:HB3	1.95	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:A:112:ARG:NE	1:A:121:ILE:HA	2.28	0.48
1:B:829:MET:HE2	1:B:831:ILE:HD11	1.96	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:B:19:MET:HE1	1:B:193:VAL:HG22	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:A:749:ALA:HB2	1:A:761:MET:HE2	1.96	0.48
1:F:747:ASN:ND2	1:F:1083:THR:O	2.46	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:733:PHE:HE1	1:C:735:ILE:HG12	1.80	0.47
1:A:998:TYR:CE1	1:A:1006:SER:HB2	2.50	0.47
1:A:1026:LYS:HZ3	1:A:1098:TRP:HZ3	1.63	0.47
1:D:19:MET:HE1	1:D:193:VAL:HG22	1.96	0.47
1:C:523:PRO:O	1:C:527:LYS:HG3	2.15	0.47
1:C:1047:GLY:HA3	1:C:1089:ALA:HB3	1.97	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:47:LYS:HD2	1:F:51:GLY:C	2.40	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: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
1:F:18:ALA:HB2	1:F:186:TYR:CE1	2.50	0.46
3:F:1204:TPP:H2	3:F:1204:TPP:HN42	1.79	0.46
1:B:1031:LEU:HA	1:B:1034:MET:HE3	1.98	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PRO:HG3	1:A:799:ARG:NH2	2.31	0.45
1:C:479:ASP:OD1	6:C:1301:HOH:O	2.20	0.45
1:C:1119:TYR:HE2	1:C:1122:PRO:HA	1.80	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: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:F:36:GLU:CD	1:F:1016:ARG:HD3	2.41	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
1:B:212:HIS:NE2	1:B:214:ARG:HD2	2.31	0.45
1:C:829:MET:HE2	1:C:831:ILE:HD11	1.98	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: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:34:MET:HE3	1:A:82:PHE:HB3	1.99	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:838:SER:O	6:A:1301:HOH:O	2.21	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1034:MET:HE1	1:F:1115:PHE:CE1	2.53	0.43
1:B:258:LEU:HD22	1:B:310:HIS:CG	2.53	0.43
1:C:749:ALA:HB2	1:C:761:MET:HE2	2.00	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:419:PHE:HB2	1:A:463:SER:HB2	2.00	0.43
1:A:1047:GLY:HA3	1:A:1089:ALA:HB3	1.99	0.43
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	2.01	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:A:19:MET:HE1	1:A:193:VAL:HG22	2.01	0.43
1:C:747:ASN:OD1	1:C:811:GLY:HA2	2.17	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:D:1102:ARG:HD2	6:D:1301:HOH:O	2.19	0.43
1:E:34:MET:HE3	1:E:82:PHE:HB3	2.01	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:695:VAL:HG11	1:F:751:VAL:HG21	2.00	0.43
1:F:720:THR:HG22	1:F:734:ARG:HB2	2.01	0.43
1:B:891:ILE:HG12	1:B:949:ILE:HD12	2.01	0.43
1:B:1076:ILE:HG23	1:B:1082:MET:HE2	1.99	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1004:GLN:HG2	1:D:1017:PHE:CE2	2.54	0.43
1:D:945:LEU:O	1:D:949:ILE:HG12	2.19	0.42
1:F:83:THR:O	1:F:109:VAL:HA	2.19	0.42
1:F:817:TYR:CZ	1:F:1071:ALA:HB1	2.53	0.42
1:A:1010:GLN:HG3	1:A:1097:TYR:CZ	2.53	0.42
1:A:1023:PHE:O	1:A:1153:LYS:NZ	2.46	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: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:D:1062:LYS:HG3	6:D:1310:HOH:O	2.19	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
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:N	1:F:855:GLN:OE1	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:75:ALA:HB3	1:B:879:ALA:HB3	2.02	0.42
1:A:1010:GLN:HE22	1:A:1161:ARG:HH12	1.68	0.42
1:A:1074:PRO:HA	1:A:1078:HIS:CE1	2.54	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:996:GLU:HG2	1:C:1026:LYS:HZ1	1.84	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:D:1055:LYS:HE3	1:D:1059:GLU:CD	2.45	0.42
1:E:1155:GLU:HG2	1:E:1159:LYS:HE3	2.01	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:1034:MET:HE1	1:F:1115:PHE:HE1	1.84	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:565:LYS:HD3	1:E:606:LEU:HD22	2.02	0.41
1:E:1010:GLN:HG3	1:E:1097:TYR:CZ	2.55	0.41
1:B:34:MET:HE3	1:B:82:PHE:HB3	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:220:PRO:HD3	1:F:122:PHE:CE2	2.56	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:A:348:GLU:OE1	1:B:339:TYR:OH	2.31	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:D:1076:ILE:HG23	1:D:1082:MET:HE2	2.02	0.41
1:E:826:GLY:HA2	1:E:829:MET:SD	2.61	0.41
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:841:TRP:O	1:A:849:PRO:HG3	2.21	0.41
1:A:1035:SER:HB2	1:B:1031:LEU:HD23	2.03	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:406:HIS:HE2	1:E:479:ASP:CG	2.29	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:523:PRO:HB2	1:A:525:ASP:OD1	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ARG:HB2	1:A:642:PRO:HD3	2.01	0.41
1:A:747:ASN:ND2	1:A:1083:THR:O	2.53	0.41
1:C:641:ARG:HB2	1:C:642:PRO:HD3	2.03	0.41
1:D:692:CYS:HB2	1:D:748:CYS:HB2	2.03	0.41
1:D:1010:GLN:HG3	1:D:1097:TYR:CZ	2.56	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:E:649:ASP:OD1	1:F:221:ASP:HA	2.21	0.41
1:E:1031:LEU:HD23	1:F:1035:SER:HB2	2.02	0.41
1:A:935:ILE:HD13	1:A:947:LEU:HD23	2.03	0.41
1:B:521:ARG:HA	1:B:521:ARG:HD2	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:435:ILE:HG23	1:E:446:ALA:HB1	2.03	0.41
1:E:1075:CYS:SG	1:E:1076:ILE:N	2.94	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:406:HIS:HE2	1:B:479:ASP:CG	2.29	0.40
1:B:641:ARG:HB2	1:B:642:PRO:HD3	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:122:PHE:HB3	1:F:364:SER:CB	2.51	0.40
1:E:838:SER:HA	1:E:841:TRP:CE2	2.56	0.40
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:879:ALA:HB3	1:F:75:ALA:HB3	2.03	0.40
1:E:883:ARG:NH2	1:E:886:GLU:OE1	2.41	0.40
1:F:249:ALA:HB1	1:F:255:HIS:CD2	2.56	0.40
1:F:1030:GLY:O	1:F:1034:MET:HG3	2.22	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%)	915 (100%)	3 (0%)	86	94
1	B	920/932 (99%)	915 (100%)	5 (0%)	81	92
1	C	916/932 (98%)	913 (100%)	3 (0%)	86	94
1	D	903/932 (97%)	899 (100%)	4 (0%)	84	93
1	E	916/932 (98%)	913 (100%)	3 (0%)	86	94
1	F	902/932 (97%)	900 (100%)	2 (0%)	87	95
All	All	5475/5592 (98%)	5455 (100%)	20 (0%)	84	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	VAL
1	A	518	MET
1	A	833	ASN
1	B	382	THR
1	B	417	CYS
1	B	518	MET
1	B	719	VAL
1	B	833	ASN
1	C	390	VAL
1	C	417	CYS
1	C	833	ASN
1	D	518	MET
1	D	678	ILE
1	D	833	ASN
1	D	926	ARG
1	E	326	ASP
1	E	518	MET
1	E	833	ASN
1	F	467	PHE
1	F	833	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	433	ASN
1	A	539	ASN
1	A	547	GLN
1	A	560	GLN
1	A	682	GLN
1	A	1000	ASN
1	A	1010	GLN
1	B	94	ASN
1	B	343	GLN
1	B	433	ASN
1	B	539	ASN
1	B	547	GLN
1	B	560	GLN
1	B	637	GLN
1	B	680	GLN
1	B	682	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	691	GLN
1	B	1000	ASN
1	B	1164	GLN
1	C	94	ASN
1	C	406	HIS
1	C	431	ASN
1	C	547	GLN
1	C	682	GLN
1	C	690	ASN
1	C	1000	ASN
1	D	94	ASN
1	D	255	HIS
1	D	431	ASN
1	D	547	GLN
1	D	682	GLN
1	D	833	ASN
1	D	1010	GLN
1	D	1077	ASN
1	E	55	GLN
1	E	94	ASN
1	E	243	GLN
1	E	255	HIS
1	E	398	HIS
1	E	433	ASN
1	E	539	ASN
1	E	547	GLN
1	E	560	GLN
1	E	682	GLN
1	E	1000	ASN
1	E	1010	GLN
1	F	94	ASN
1	F	255	HIS
1	F	406	HIS
1	F	431	ASN
1	F	433	ASN
1	F	547	GLN
1	F	560	GLN
1	F	682	GLN
1	F	1000	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	$\# Z  > 2$
5	SO4	E	1206	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SF4	B	1201	1	0,12,12	-	-	-	-	-
3	TPP	E	1204	4	26,27,27	1.88	7 (26%)	38,40,40	1.77	10 (26%)
3	TPP	A	1204	4	26,27,27	1.87	7 (26%)	38,40,40	1.79	9 (23%)
5	SO4	D	1206	-	4,4,4	0.24	0	6,6,6	0.17	0
5	SO4	F	1206	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SF4	E	1201	1	0,12,12	-	-	-	-	-
2	SF4	D	1203	1	0,12,12	-	-	-	-	-
3	TPP	F	1204	4	26,27,27	1.85	8 (30%)	38,40,40	1.85	9 (23%)
2	SF4	C	1202	1	0,12,12	-	-	-	-	-
5	SO4	A	1206	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SF4	C	1201	1	0,12,12	-	-	-	-	-
2	SF4	C	1203	1	0,12,12	-	-	-	-	-
5	SO4	B	1207	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SF4	F	1201	1	0,12,12	-	-	-	-	-
2	SF4	F	1202	1	0,12,12	-	-	-	-	-
2	SF4	A	1203	1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TPP	D	1204	4	26,27,27	1.86	7 (26%)	38,40,40	1.74	10 (26%)
3	TPP	C	1204	4	26,27,27	1.87	7 (26%)	38,40,40	1.81	9 (23%)
2	SF4	D	1201	1	0,12,12	-	-	-	-	-
3	TPP	B	1204	4	26,27,27	1.87	8 (30%)	38,40,40	1.83	9 (23%)
5	SO4	B	1206	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	C	1206	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SF4	D	1202	1	0,12,12	-	-	-	-	-
2	SF4	A	1201	1	0,12,12	-	-	-	-	-
2	SF4	B	1202	1	0,12,12	-	-	-	-	-
2	SF4	E	1202	1	0,12,12	-	-	-	-	-
2	SF4	E	1203	1	0,12,12	-	-	-	-	-
2	SF4	A	1202	1	0,12,12	-	-	-	-	-
2	SF4	B	1203	1	0,12,12	-	-	-	-	-
2	SF4	F	1203	1	0,12,12	-	-	-	-	-

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	B	1201	1	-	-	0/6/5/5
3	TPP	E	1204	4	-	6/17/17/17	0/2/2/2
3	TPP	A	1204	4	-	8/17/17/17	0/2/2/2
2	SF4	E	1201	1	-	-	0/6/5/5
2	SF4	D	1203	1	-	-	0/6/5/5
3	TPP	F	1204	4	-	7/17/17/17	0/2/2/2
2	SF4	C	1202	1	-	-	0/6/5/5
2	SF4	C	1201	1	-	-	0/6/5/5
2	SF4	C	1203	1	-	-	0/6/5/5
2	SF4	F	1201	1	-	-	0/6/5/5
2	SF4	F	1202	1	-	-	0/6/5/5
2	SF4	A	1203	1	-	-	0/6/5/5
3	TPP	D	1204	4	-	8/17/17/17	0/2/2/2
3	TPP	C	1204	4	-	8/17/17/17	0/2/2/2
2	SF4	D	1201	1	-	-	0/6/5/5
3	TPP	B	1204	4	-	6/17/17/17	0/2/2/2
2	SF4	D	1202	1	-	-	0/6/5/5
2	SF4	A	1201	1	-	-	0/6/5/5
2	SF4	B	1202	1	-	-	0/6/5/5
2	SF4	E	1202	1	-	-	0/6/5/5

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	E	1203	1	-	-	0/6/5/5
2	SF4	A	1202	1	-	-	0/6/5/5
2	SF4	B	1203	1	-	-	0/6/5/5
2	SF4	F	1203	1	-	-	0/6/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1204	TPP	C4'-N4'	3.81	1.43	1.34
3	A	1204	TPP	C5-S1	-3.77	1.62	1.72
3	C	1204	TPP	C7'-C5'	3.73	1.58	1.51
3	C	1204	TPP	C4'-N4'	3.72	1.43	1.34
3	F	1204	TPP	C4'-N4'	3.72	1.43	1.34
3	B	1204	TPP	C4'-N4'	3.72	1.43	1.34
3	E	1204	TPP	C7'-C5'	3.71	1.58	1.51
3	E	1204	TPP	C5-S1	-3.69	1.63	1.72
3	D	1204	TPP	C7'-C5'	3.68	1.57	1.51
3	A	1204	TPP	C7'-C5'	3.64	1.57	1.51
3	B	1204	TPP	C7'-C5'	3.63	1.57	1.51
3	D	1204	TPP	C5-S1	-3.63	1.63	1.72
3	A	1204	TPP	C4'-N4'	3.63	1.43	1.34
3	D	1204	TPP	C4'-N4'	3.59	1.43	1.34
3	F	1204	TPP	C5-S1	-3.56	1.63	1.72
3	C	1204	TPP	C5-S1	-3.56	1.63	1.72
3	F	1204	TPP	C7'-C5'	3.55	1.57	1.51
3	B	1204	TPP	C5-S1	-3.52	1.63	1.72
3	B	1204	TPP	C2-N3	3.14	1.40	1.32
3	E	1204	TPP	C2-N3	3.00	1.39	1.32
3	D	1204	TPP	C2-N3	2.98	1.39	1.32
3	C	1204	TPP	C2-N3	2.97	1.39	1.32
3	F	1204	TPP	C2-N3	2.93	1.39	1.32
3	A	1204	TPP	C2-N3	2.91	1.39	1.32
3	A	1204	TPP	C7'-N3	-2.90	1.42	1.48
3	F	1204	TPP	C7'-N3	-2.89	1.42	1.48
3	C	1204	TPP	C7'-N3	-2.89	1.42	1.48
3	B	1204	TPP	C7'-N3	-2.80	1.42	1.48
3	E	1204	TPP	C7'-N3	-2.77	1.42	1.48
3	D	1204	TPP	C7'-N3	-2.77	1.42	1.48
3	A	1204	TPP	C6'-C5'	2.49	1.42	1.37
3	B	1204	TPP	C6'-C5'	2.44	1.42	1.37
3	C	1204	TPP	C6'-C5'	2.38	1.42	1.37
3	B	1204	TPP	C5-C4	2.38	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1204	TPP	C6'-C5'	2.37	1.42	1.37
3	F	1204	TPP	C6'-C5'	2.37	1.42	1.37
3	E	1204	TPP	C5-C4	2.36	1.40	1.35
3	E	1204	TPP	C6'-C5'	2.36	1.42	1.37
3	D	1204	TPP	C5-C4	2.33	1.40	1.35
3	A	1204	TPP	C5-C4	2.30	1.40	1.35
3	F	1204	TPP	C5-C4	2.27	1.40	1.35
3	C	1204	TPP	C5-C4	2.24	1.39	1.35
3	B	1204	TPP	C4-N3	-2.14	1.35	1.39
3	F	1204	TPP	C4-N3	-2.01	1.35	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	TPP	C2-S1-C5	-4.70	88.10	91.22
3	C	1204	TPP	C2-S1-C5	-4.35	88.34	91.22
3	D	1204	TPP	C2-N3-C4	-4.27	108.30	114.06
3	F	1204	TPP	C2-S1-C5	-4.24	88.40	91.22
3	B	1204	TPP	C2-N3-C4	-4.18	108.41	114.06
3	E	1204	TPP	C2-N3-C4	-4.09	108.54	114.06
3	A	1204	TPP	C2-N3-C4	-4.08	108.54	114.06
3	F	1204	TPP	C2-N3-C4	-4.08	108.55	114.06
3	A	1204	TPP	C2-S1-C5	-3.93	88.61	91.22
3	C	1204	TPP	C2-N3-C4	-3.91	108.77	114.06
3	B	1204	TPP	S1-C2-N3	3.86	117.19	112.30
3	E	1204	TPP	C2-S1-C5	-3.85	88.66	91.22
3	F	1204	TPP	S1-C2-N3	3.77	117.08	112.30
3	C	1204	TPP	S1-C2-N3	3.70	116.98	112.30
3	A	1204	TPP	S1-C2-N3	3.68	116.96	112.30
3	C	1204	TPP	C4-C5-S1	3.65	116.25	110.56
3	B	1204	TPP	C4-C5-S1	3.63	116.23	110.56
3	E	1204	TPP	S1-C2-N3	3.60	116.86	112.30
3	D	1204	TPP	S1-C2-N3	3.54	116.78	112.30
3	A	1204	TPP	C4-C5-S1	3.49	116.01	110.56
3	F	1204	TPP	C4-C5-S1	3.46	115.96	110.56
3	C	1204	TPP	C6'-N1'-C2'	3.38	121.63	116.07
3	E	1204	TPP	C4-C5-S1	3.38	115.84	110.56
3	F	1204	TPP	C6'-N1'-C2'	3.37	121.61	116.07
3	D	1204	TPP	C2-S1-C5	-3.36	88.99	91.22
3	B	1204	TPP	C6'-N1'-C2'	3.22	121.36	116.07
3	D	1204	TPP	C6'-N1'-C2'	3.21	121.34	116.07
3	E	1204	TPP	C6'-N1'-C2'	3.20	121.33	116.07

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1204	TPP	C5'-C6'-N1'	-3.18	118.65	123.83
3	A	1204	TPP	C6'-N1'-C2'	3.17	121.27	116.07
3	D	1204	TPP	C4-C5-S1	3.10	115.39	110.56
3	F	1204	TPP	C5'-C6'-N1'	-3.04	118.89	123.83
3	B	1204	TPP	C5'-C6'-N1'	-2.91	119.09	123.83
3	D	1204	TPP	C5'-C6'-N1'	-2.88	119.15	123.83
3	A	1204	TPP	C5'-C6'-N1'	-2.86	119.19	123.83
3	E	1204	TPP	C5'-C6'-N1'	-2.79	119.29	123.83
3	E	1204	TPP	N4'-C4'-N3'	2.65	120.61	117.03
3	F	1204	TPP	N1'-C2'-N3'	-2.36	121.60	125.53
3	A	1204	TPP	CM4-C4-N3	2.33	125.95	120.57
3	D	1204	TPP	N1'-C2'-N3'	-2.28	121.73	125.53
3	F	1204	TPP	N4'-C4'-N3'	2.27	120.09	117.03
3	B	1204	TPP	N1'-C2'-N3'	-2.23	121.83	125.53
3	A	1204	TPP	N4'-C4'-N3'	2.20	120.00	117.03
3	D	1204	TPP	CM4-C4-N3	2.20	125.64	120.57
3	B	1204	TPP	N4'-C4'-N3'	2.17	119.96	117.03
3	D	1204	TPP	CM2-C2'-N1'	2.17	119.51	117.20
3	E	1204	TPP	CM2-C2'-N3'	2.15	120.35	117.13
3	E	1204	TPP	N1'-C2'-N3'	-2.14	121.97	125.53
3	A	1204	TPP	N1'-C2'-N3'	-2.14	121.98	125.53
3	C	1204	TPP	CM4-C4-N3	2.12	125.47	120.57
3	F	1204	TPP	CM4-C4-N3	2.12	125.47	120.57
3	C	1204	TPP	N1'-C2'-N3'	-2.12	122.01	125.53
3	D	1204	TPP	C2'-N3'-C4'	2.09	121.31	118.10
3	E	1204	TPP	CM4-C4-N3	2.05	125.31	120.57
3	C	1204	TPP	N4'-C4'-N3'	2.05	119.79	117.03
3	B	1204	TPP	C2'-N3'-C4'	2.03	121.22	118.10

There are no chirality outliers.

All (43) 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	A	1204	TPP	C5'-C7'-N3-C2
3	B	1204	TPP	C5'-C7'-N3-C2
3	C	1204	TPP	C5'-C7'-N3-C2
3	D	1204	TPP	C5'-C7'-N3-C2
3	E	1204	TPP	C5'-C7'-N3-C2
3	F	1204	TPP	C5'-C7'-N3-C2
3	C	1204	TPP	PA-O3A-PB-O3B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	F	1204	TPP	PA-O3A-PB-O3B
3	A	1204	TPP	C5-C6-C7-O7
3	C	1204	TPP	C5-C6-C7-O7
3	D	1204	TPP	C5-C6-C7-O7
3	E	1204	TPP	C5-C6-C7-O7
3	F	1204	TPP	C5-C6-C7-O7
3	A	1204	TPP	S1-C5-C6-C7
3	B	1204	TPP	S1-C5-C6-C7
3	C	1204	TPP	S1-C5-C6-C7
3	D	1204	TPP	S1-C5-C6-C7
3	E	1204	TPP	S1-C5-C6-C7
3	C	1204	TPP	C5'-C7'-N3-C4
3	A	1204	TPP	C7-O7-PA-O1A
3	C	1204	TPP	C7-O7-PA-O1A
3	D	1204	TPP	C7-O7-PA-O1A
3	B	1204	TPP	C4-C5-C6-C7
3	D	1204	TPP	C5'-C7'-N3-C4
3	E	1204	TPP	C5'-C7'-N3-C4
3	F	1204	TPP	S1-C5-C6-C7
3	A	1204	TPP	C4-C5-C6-C7
3	C	1204	TPP	C4-C5-C6-C7
3	E	1204	TPP	C4-C5-C6-C7
3	A	1204	TPP	C5'-C7'-N3-C4
3	B	1204	TPP	C5'-C7'-N3-C4
3	F	1204	TPP	C5'-C7'-N3-C4
3	D	1204	TPP	C4-C5-C6-C7
3	A	1204	TPP	PA-O3A-PB-O3B
3	B	1204	TPP	PA-O3A-PB-O3B
3	C	1204	TPP	PA-O3A-PB-O2B
3	D	1204	TPP	PA-O3A-PB-O2B
3	D	1204	TPP	PA-O3A-PB-O3B
3	E	1204	TPP	PA-O3A-PB-O3B
3	B	1204	TPP	C5-C6-C7-O7
3	F	1204	TPP	C4-C5-C6-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

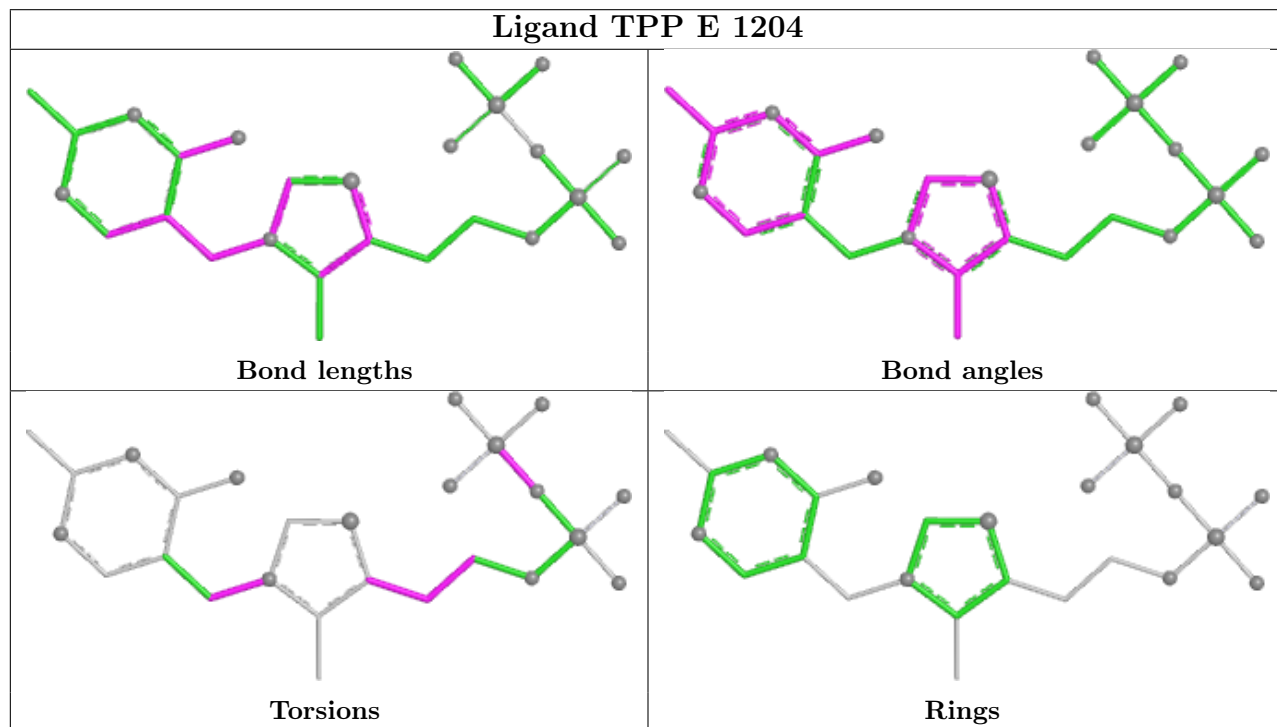
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	TPP	1	0
3	F	1204	TPP	1	0
5	B	1207	SO4	3	0

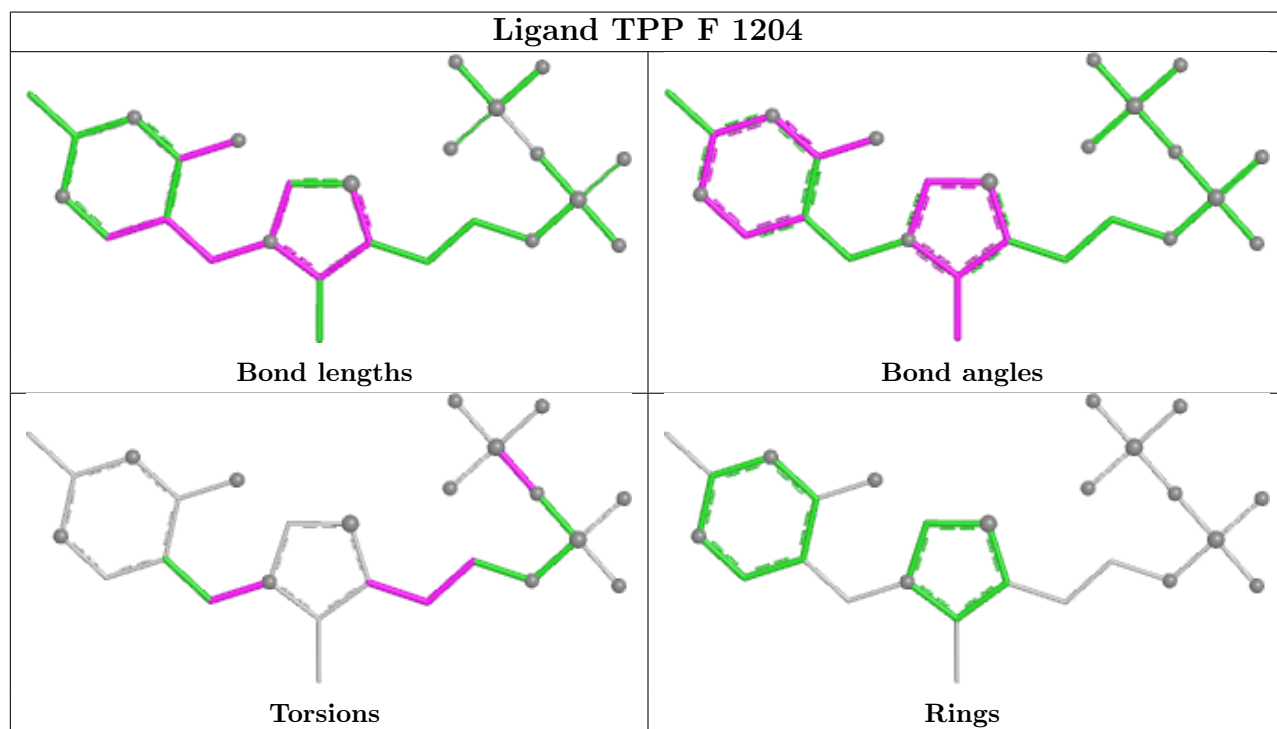
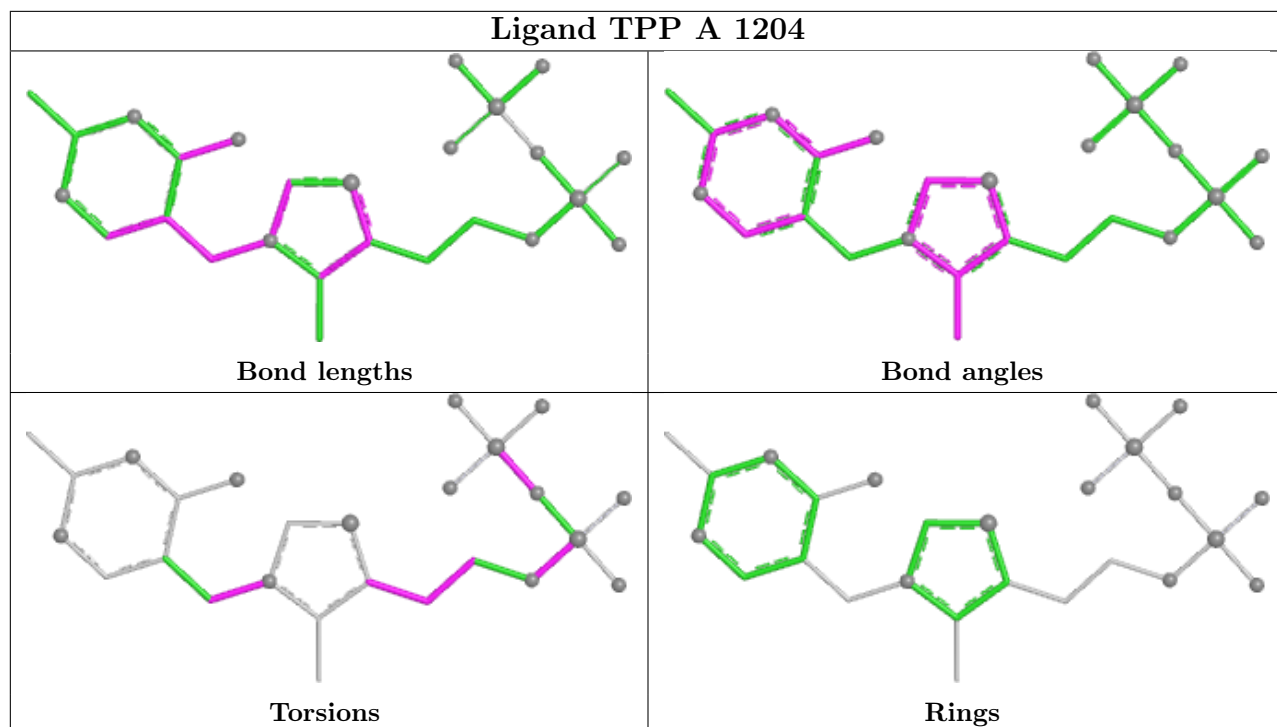
*Continued on next page...*

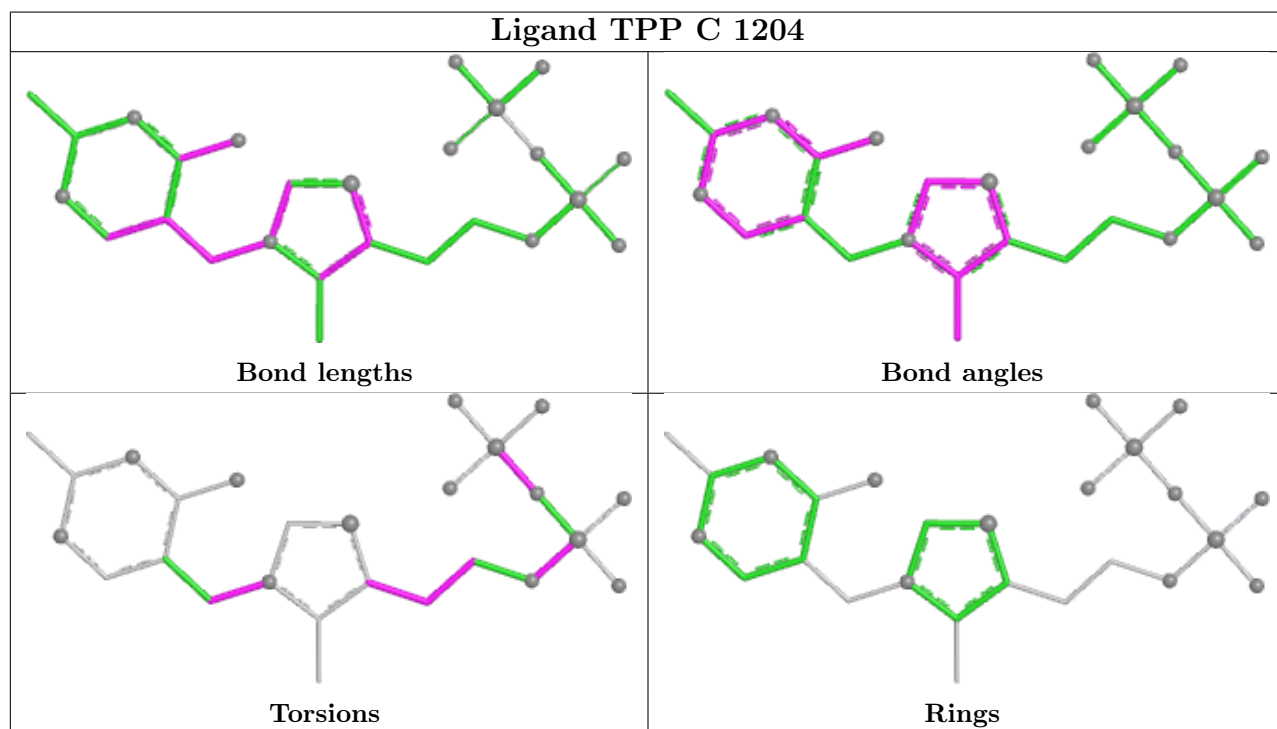
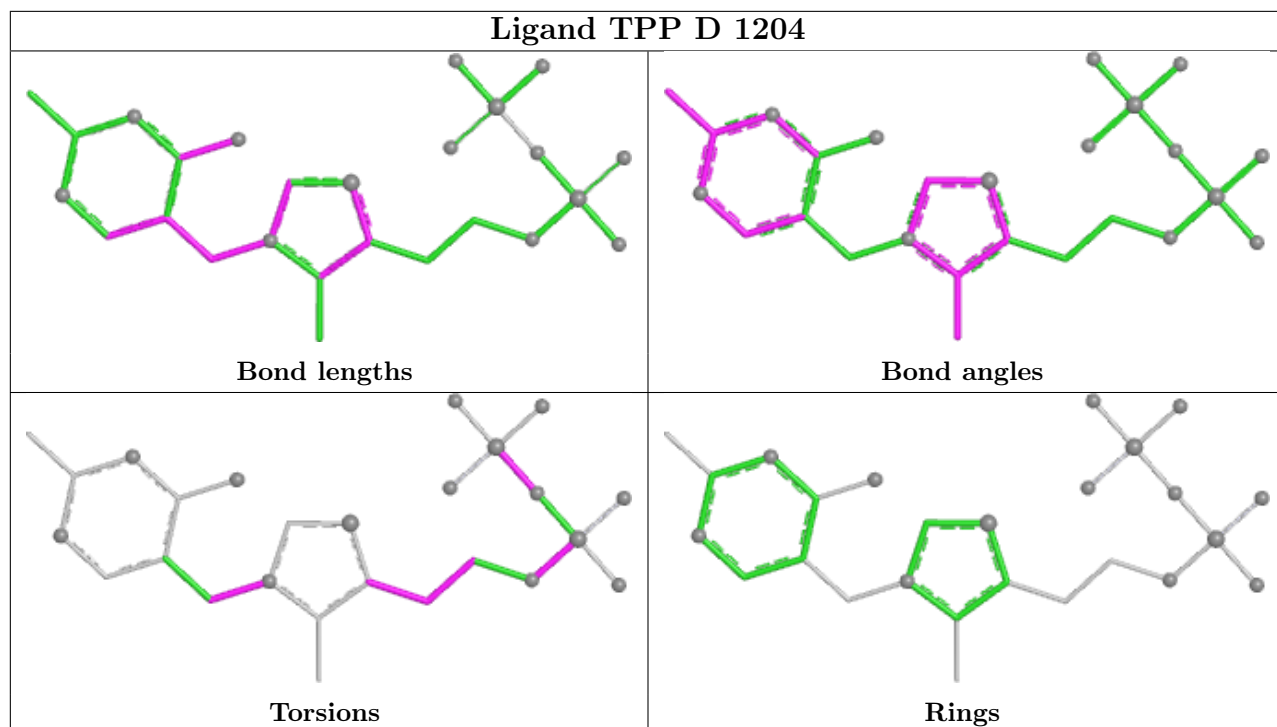
Continued from previous page...

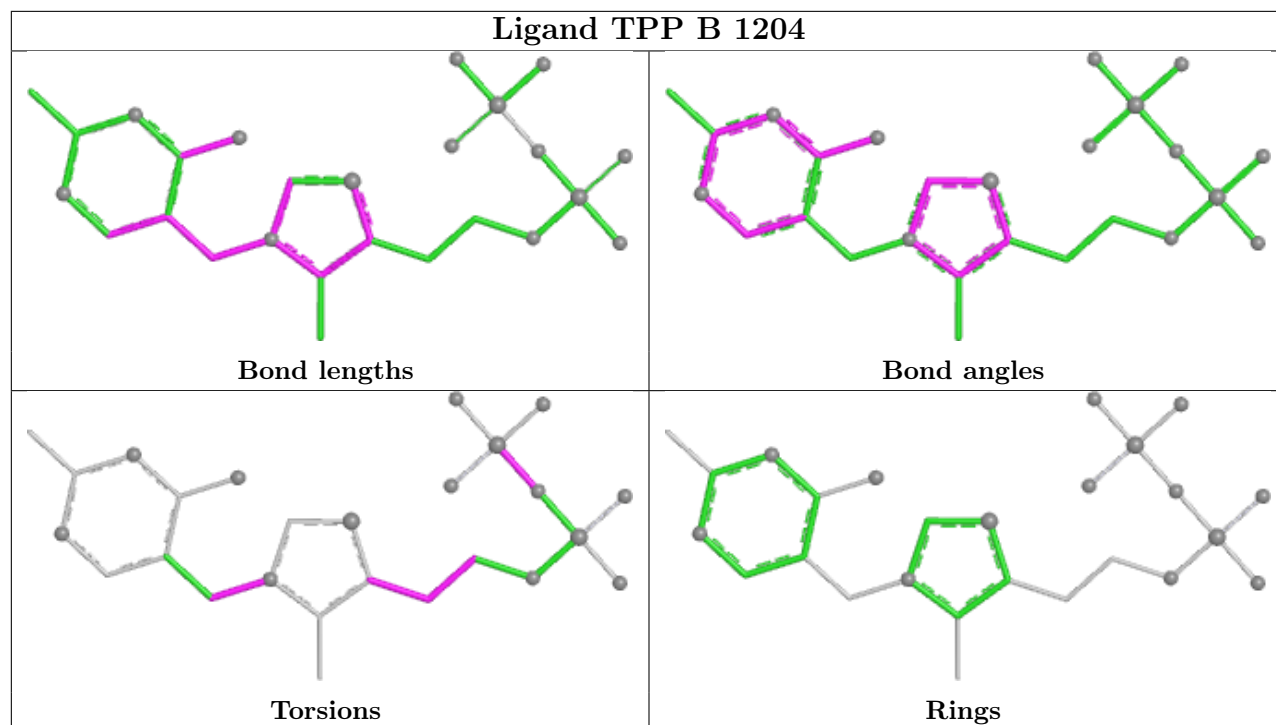
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1204	TPP	1	0

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.03	18 (1%) 72 68	36, 66, 125, 151	0
1	B	1169/1171 (99%)	0.02	23 (1%) 65 60	34, 66, 117, 171	0
1	C	1163/1171 (99%)	0.18	34 (2%) 53 48	36, 74, 130, 165	0
1	D	1157/1171 (98%)	0.20	27 (2%) 61 55	45, 77, 130, 170	0
1	E	1165/1171 (99%)	0.12	24 (2%) 63 58	29, 77, 128, 161	0
1	F	1158/1171 (98%)	0.19	27 (2%) 61 55	37, 78, 132, 188	0
All	All	6975/7026 (99%)	0.12	153 (2%) 62 57	29, 73, 128, 188	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	597	MET	4.8
1	C	1044	VAL	4.5
1	A	821	VAL	4.4
1	B	1143	PHE	4.3
1	D	586	THR	4.1
1	C	1145	GLU	3.9
1	D	1142	GLN	3.8
1	A	818	VAL	3.8
1	C	1071	ALA	3.6
1	E	656	PHE	3.6
1	D	1019	ALA	3.5
1	B	1071	ALA	3.4
1	A	1131	MET	3.4
1	C	901	ALA	3.4
1	E	655	THR	3.3
1	D	1143	PHE	3.3
1	F	1018	ALA	3.2
1	E	735	ILE	3.2
1	B	1150	LEU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	1144	PRO	3.2
1	A	735	ILE	3.2
1	B	1167	LYS	3.1
1	A	1170	GLU	3.1
1	E	467	PHE	3.1
1	F	1143	PHE	3.1
1	E	625	ALA	3.1
1	E	709	ALA	3.1
1	E	769	ALA	3.1
1	C	753	PRO	3.1
1	F	435	ILE	3.1
1	E	631	GLU	3.0
1	F	598	ASN	3.0
1	E	700	ALA	3.0
1	B	452	TYR	3.0
1	C	616	ALA	3.0
1	C	553	SER	2.9
1	D	1006	SER	2.9
1	B	747	ASN	2.9
1	A	1012	GLY	2.9
1	D	51	GLY	2.9
1	D	569	VAL	2.9
1	D	629	VAL	2.9
1	B	1023	PHE	2.9
1	F	159	LEU	2.8
1	B	1170	GLU	2.8
1	A	1140	LYS	2.8
1	D	435	ILE	2.8
1	C	572	VAL	2.8
1	B	1000	ASN	2.8
1	E	942	VAL	2.8
1	D	716	GLU	2.7
1	A	628	THR	2.7
1	F	586	THR	2.7
1	B	753	PRO	2.7
1	C	570	ILE	2.7
1	F	686	CYS	2.6
1	A	630	THR	2.6
1	F	626	ALA	2.6
1	A	820	LEU	2.5
1	C	452	TYR	2.5
1	C	1143	PHE	2.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	1170	GLU	2.5
1	B	1019	ALA	2.5
1	C	591	GLY	2.4
1	E	456	LYS	2.4
1	C	754	ALA	2.4
1	C	1000	ASN	2.4
1	C	623	ASP	2.4
1	F	104	PRO	2.4
1	E	997	VAL	2.4
1	E	1005	SER	2.4
1	D	622	VAL	2.4
1	F	627	ALA	2.4
1	F	1139	LEU	2.4
1	B	458	GLY	2.4
1	A	629	VAL	2.4
1	B	1014	VAL	2.4
1	B	700	ALA	2.4
1	C	1151	PHE	2.4
1	D	755	LYS	2.3
1	C	124	ASP	2.3
1	D	592	ASP	2.3
1	C	615	PRO	2.3
1	C	846	PRO	2.3
1	D	100	GLY	2.3
1	D	1023	PHE	2.3
1	E	1139	LEU	2.3
1	F	625	ALA	2.3
1	D	1153	LYS	2.3
1	C	747	ASN	2.3
1	C	630	THR	2.3
1	D	1000	ASN	2.3
1	B	1013	ALA	2.2
1	D	594	ILE	2.2
1	E	726	LYS	2.2
1	A	631	GLU	2.2
1	B	1145	GLU	2.2
1	E	739	PRO	2.2
1	C	767	VAL	2.2
1	E	711	LEU	2.2
1	F	251	LEU	2.2
1	C	619	ALA	2.2
1	D	1141	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	630	THR	2.2
1	F	1142	GLN	2.2
1	B	454	SER	2.2
1	D	940	GLY	2.2
1	C	852	VAL	2.2
1	D	1140	LYS	2.2
1	A	777	PHE	2.2
1	E	935	ILE	2.2
1	E	706	ALA	2.2
1	E	712	ALA	2.2
1	B	1121	THR	2.2
1	C	1001	THR	2.2
1	D	1097	TYR	2.2
1	A	1049	SER	2.2
1	C	993	LEU	2.2
1	D	1012	GLY	2.2
1	F	936	SER	2.2
1	F	569	VAL	2.2
1	E	570	ILE	2.2
1	A	452	TYR	2.2
1	C	746	GLY	2.2
1	D	1017	PHE	2.2
1	B	895	LEU	2.1
1	B	591	GLY	2.1
1	F	676	VAL	2.1
1	F	770	VAL	2.1
1	C	1033	ALA	2.1
1	C	521	ARG	2.1
1	B	1001	THR	2.1
1	F	628	THR	2.1
1	E	452	TYR	2.1
1	C	724	ILE	2.1
1	A	1147	ALA	2.1
1	F	630	THR	2.1
1	B	455	LYS	2.1
1	A	683	PRO	2.1
1	B	876	MET	2.1
1	F	454	SER	2.1
1	D	452	TYR	2.1
1	A	1014	VAL	2.1
1	E	821	VAL	2.1
1	C	515	ALA	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	754	ALA	2.0
1	F	700	ALA	2.0
1	F	1003	GLY	2.0
1	F	684	GLU	2.0
1	C	456	LYS	2.0
1	F	16	ALA	2.0
1	C	514	SER	2.0
1	D	584	VAL	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, 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	B	1207	5/5	0.85	0.16	87,87,88,89	0
5	SO4	F	1206	5/5	0.85	0.09	101,101,103,103	0
5	SO4	B	1206	5/5	0.86	0.10	93,95,95,96	0
5	SO4	D	1206	5/5	0.90	0.09	87,89,90,92	0
5	SO4	E	1206	5/5	0.91	0.08	79,80,82,83	0
5	SO4	A	1206	5/5	0.91	0.10	88,89,89,89	0
3	TPP	C	1204	26/26	0.92	0.09	57,70,80,87	0
2	SF4	C	1203	8/8	0.93	0.08	73,87,107,124	0
3	TPP	B	1204	26/26	0.94	0.08	59,70,83,87	0
3	TPP	A	1204	26/26	0.94	0.08	52,75,86,95	0
3	TPP	E	1204	26/26	0.94	0.08	44,70,77,82	0
2	SF4	A	1203	8/8	0.95	0.07	70,85,115,169	0
3	TPP	D	1204	26/26	0.95	0.07	58,64,73,82	0
5	SO4	C	1206	5/5	0.95	0.06	75,75,78,78	0
3	TPP	F	1204	26/26	0.96	0.07	48,68,71,77	0

*Continued on next page...*

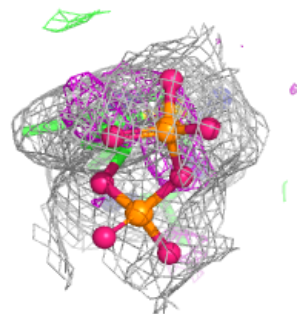
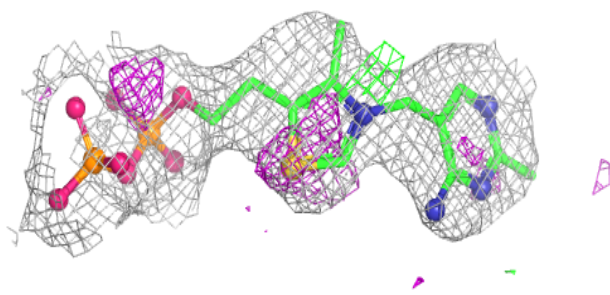
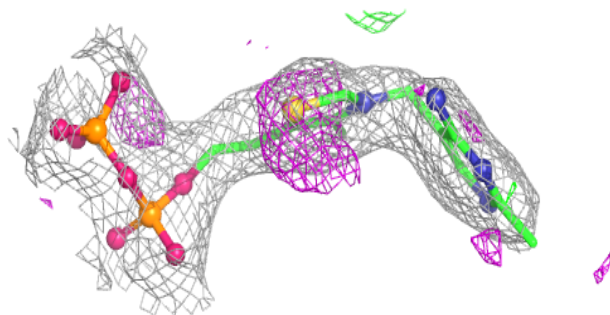
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	E	1203	8/8	0.96	0.06	63,95,138,162	0
2	SF4	B	1203	8/8	0.96	0.06	60,79,85,96	0
2	SF4	D	1202	8/8	0.96	0.09	73,82,95,121	0
2	SF4	D	1203	8/8	0.97	0.05	59,67,72,78	0
2	SF4	E	1202	8/8	0.97	0.05	80,88,105,113	0
2	SF4	A	1201	8/8	0.97	0.04	95,103,122,123	0
2	SF4	A	1202	8/8	0.97	0.05	75,81,86,88	0
2	SF4	B	1202	8/8	0.98	0.04	68,71,72,73	0
2	SF4	F	1201	8/8	0.98	0.04	88,92,105,106	0
2	SF4	F	1203	8/8	0.98	0.04	61,66,85,103	0
2	SF4	E	1201	8/8	0.98	0.03	95,97,110,115	0
4	MG	A	1205	1/1	0.98	0.05	44,44,44,44	0
2	SF4	B	1201	8/8	0.98	0.04	83,88,93,104	0
4	MG	E	1205	1/1	0.99	0.02	44,44,44,44	0
4	MG	F	1205	1/1	0.99	0.02	35,35,35,35	0
2	SF4	C	1202	8/8	0.99	0.03	72,76,81,82	0
2	SF4	C	1201	8/8	0.99	0.03	96,100,109,122	0
2	SF4	D	1201	8/8	0.99	0.04	73,76,81,84	0
2	SF4	F	1202	8/8	0.99	0.04	75,79,85,88	0
4	MG	B	1205	1/1	0.99	0.03	32,32,32,32	0
4	MG	C	1205	1/1	0.99	0.05	31,31,31,31	0
4	MG	D	1205	1/1	0.99	0.02	32,32,32,32	0

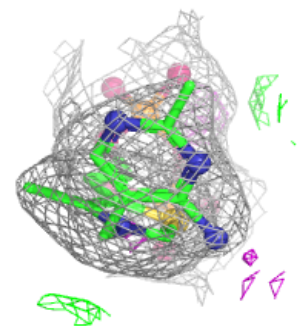
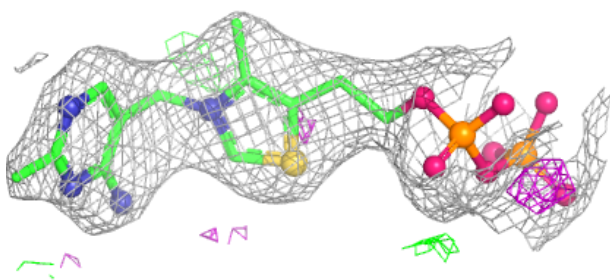
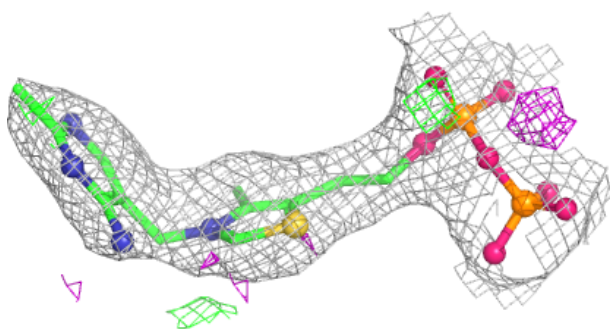
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

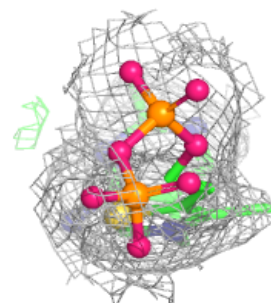
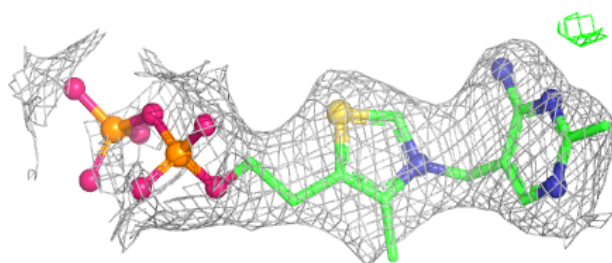
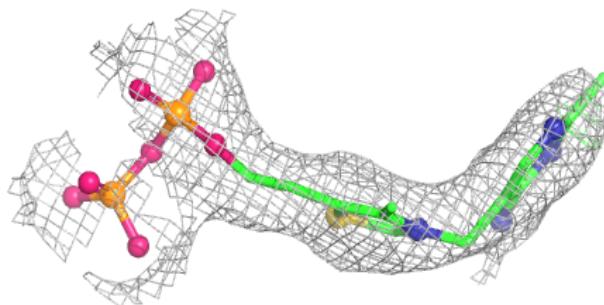
**Electron density around TPP B 1204:**

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

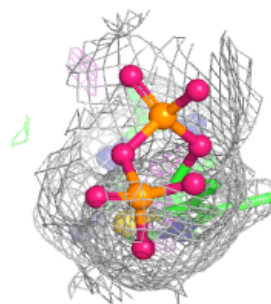
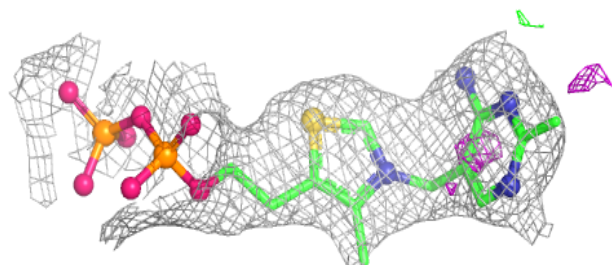
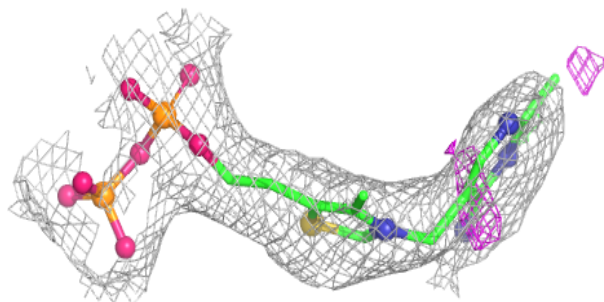


**Electron density around TPP A 1204:**

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

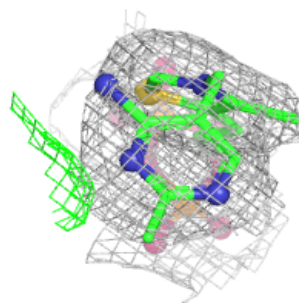
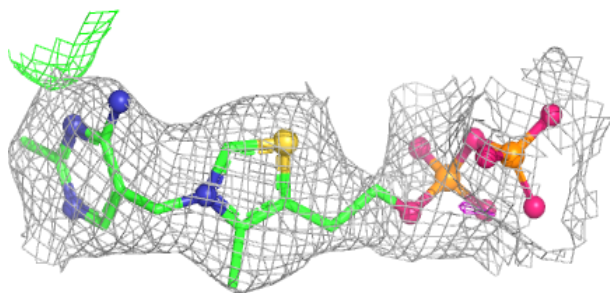
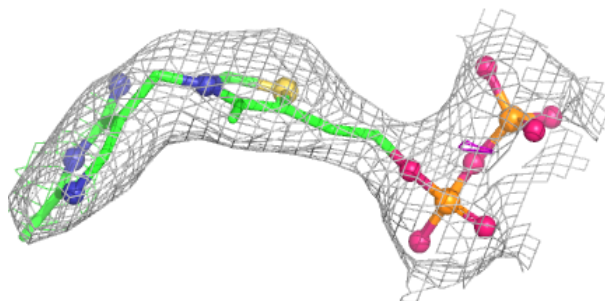
**Electron density around TPP E 1204:**

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

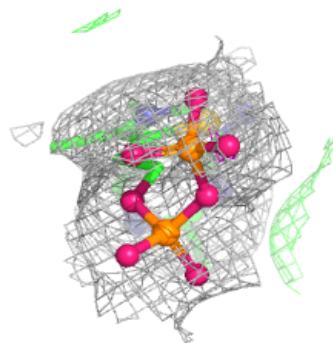
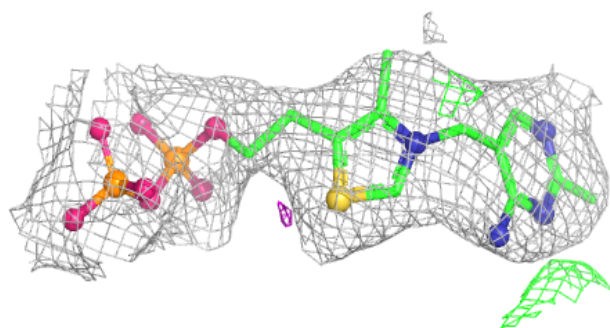
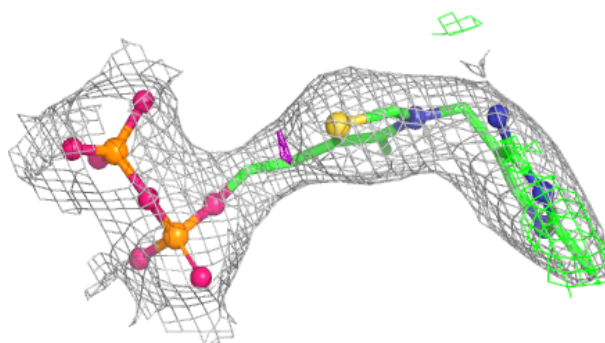


**Electron density around TPP D 1204:**

$2mF_o-DF_c$  (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.