



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:59 am BST

PDB ID : 6CIO  
Title : Pyruvate:ferredoxin oxidoreductase from Moorella thermoacetica with lactyl-TPP bound  
Authors : Chen, P.Y.-T.; Drennan, C.L.  
Deposited on : 2018-02-24  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

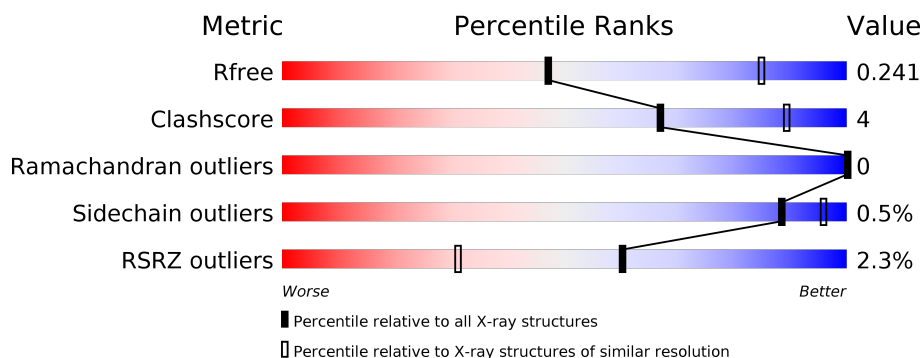
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>2%</div> <div>91%</div> <div>9%</div> </div>
1	B	1171	<div> <div>4%</div> <div>89%</div> <div>10%</div> </div>
1	C	1171	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	D	1171	<div> <div>%</div> <div>89%</div> <div>10%</div> </div>
1	E	1171	<div> <div>4%</div> <div>89%</div> <div>9%</div> </div>
1	F	1171	<div> <div>%</div> <div>87%</div> <div>12%</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](#)

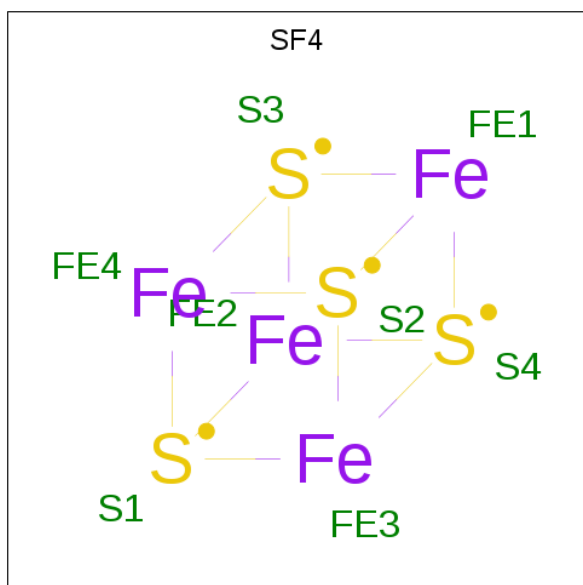
There are 7 unique types of molecules in this entry. The entry contains 53582 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

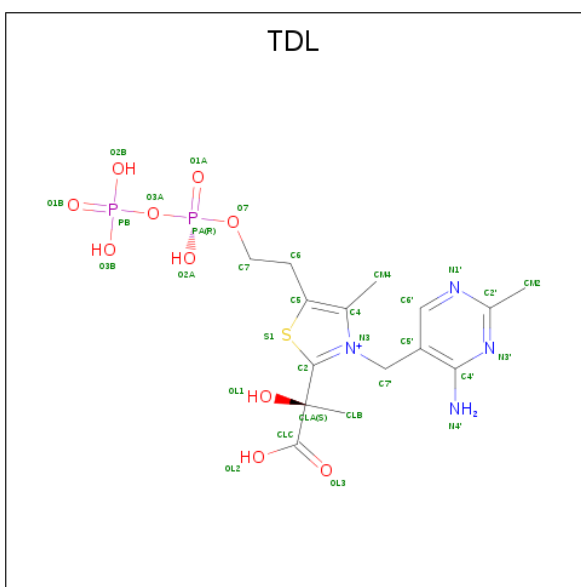
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1164	Total	C	N	O	S	0	0	0
			8878	5651	1510	1673	44			
1	B	1164	Total	C	N	O	S	0	0	0
			8879	5652	1510	1673	44			
1	C	1161	Total	C	N	O	S	0	0	0
			8879	5655	1509	1671	44			
1	D	1159	Total	C	N	O	S	0	0	0
			8853	5639	1503	1667	44			
1	E	1157	Total	C	N	O	S	0	0	0
			8840	5630	1504	1662	44			
1	F	1155	Total	C	N	O	S	0	0	0
			8834	5629	1500	1661	44			

- 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	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-HYDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDL) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0
3	C	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0
3	D	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0
3	F	1	Total 32	C 15	N 4	O 10	P 2	S 1	0	0

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

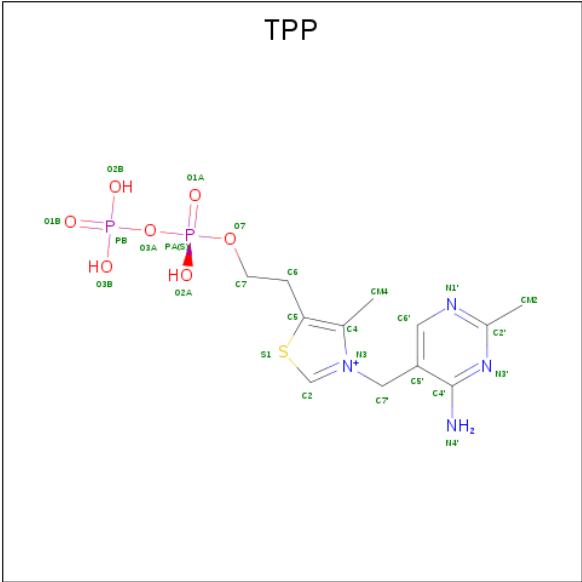
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- 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 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).



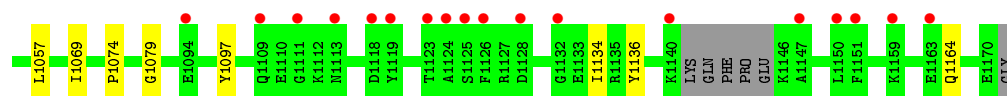
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
6	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 7 is water.

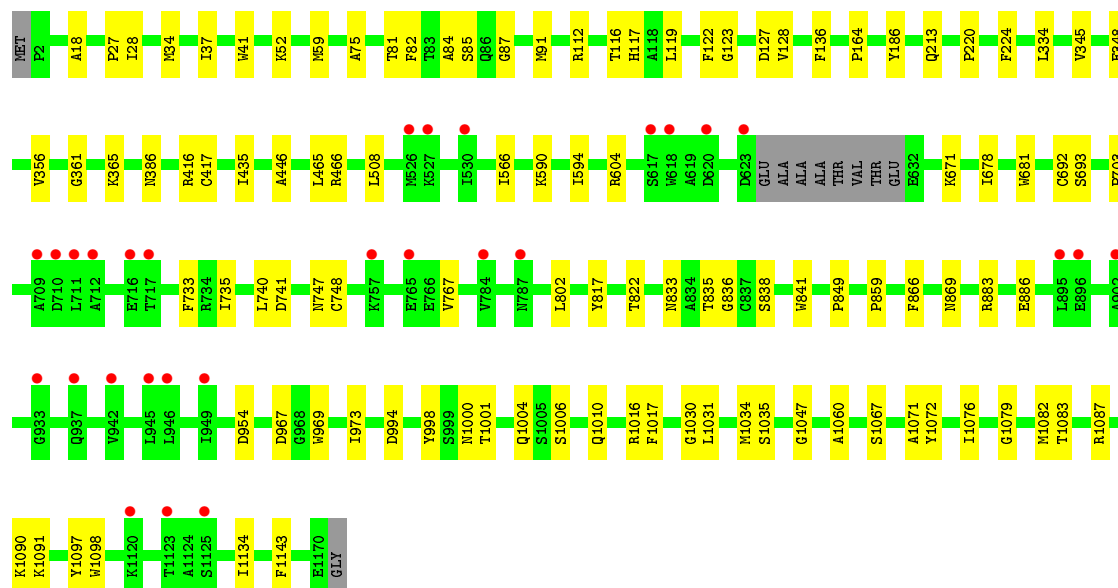
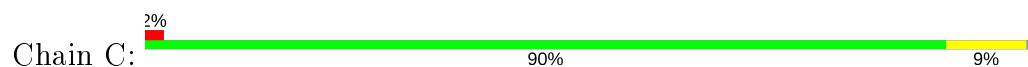
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	10	Total	O	0	0
			10	10		
7	C	11	Total	O	0	0
			11	11		
7	D	7	Total	O	0	0
			7	7		
7	E	13	Total	O	0	0
			13	13		
7	F	7	Total	O	0	0
			7	7		



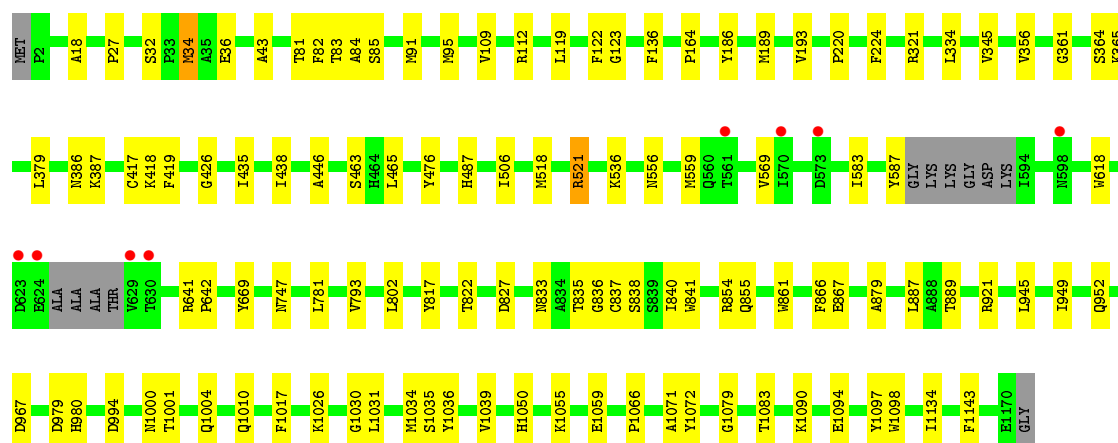
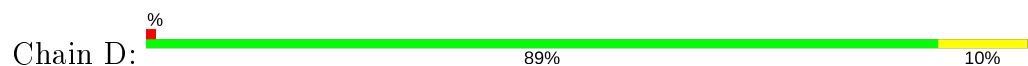




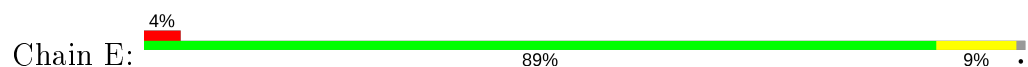
• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

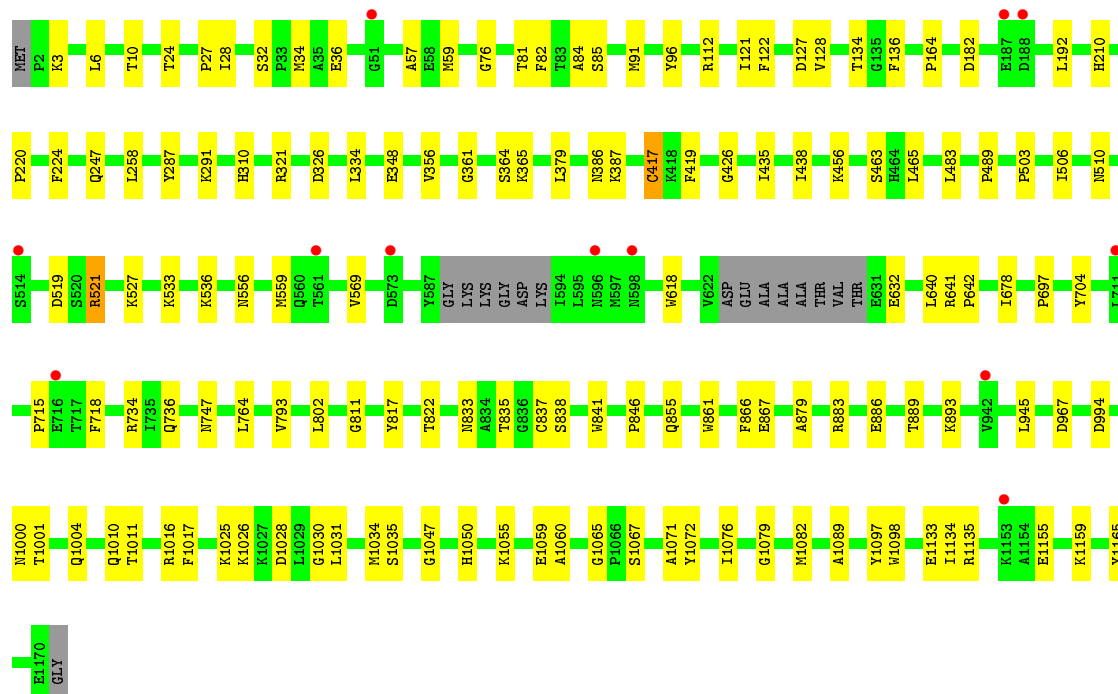


• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



• 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, $\alpha$ , $\beta$ , $\gamma$	340.39 Å 107.09 Å 239.56 Å 90.00° 109.67° 90.00°	Depositor
Resolution (Å)	48.45 – 3.00 48.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.45-3.00) 96.8 (48.45-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.207 , 0.241 0.207 , 0.241	Depositor DCC
$R_{free}$ test set	7867 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	53582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	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 65.58 % 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 6.9289e-06. 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: SO4, MG, TPP, SF4, TDL

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	0/9070	0.45	0/12296
1	B	0.26	0/9071	0.45	0/12297
1	C	0.26	0/9073	0.45	0/12298
1	D	0.26	0/9046	0.45	0/12266
1	E	0.26	0/9031	0.45	0/12239
1	F	0.26	0/9027	0.45	0/12238
All	All	0.26	0/54318	0.45	0/73634

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	8878	0	8806	63	0
1	B	8879	0	8807	78	0
1	C	8879	0	8819	70	0
1	D	8853	0	8768	74	0
1	E	8840	0	8786	68	0
1	F	8834	0	8769	87	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	2	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	32	0	19	6	0
3	C	32	0	19	8	0
3	D	32	0	19	6	0
3	F	32	0	19	6	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	B	26	0	16	0	0
6	E	26	0	16	0	0
7	A	6	0	0	0	0
7	B	10	0	0	0	0
7	C	11	0	0	1	0
7	D	7	0	0	0	0
7	E	13	0	0	2	0
7	F	7	0	0	1	0
All	All	53582	0	52863	412	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 (412) 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:O3	2.09	0.84
1:A:827:ASP:OD2	1:A:921:ARG:NH1	2.12	0.82
1:C:34:MET:HE3	1:C:82:PHE:HB3	1.63	0.80
3:A:1204:TDL:OL1	3:A:1204:TDL:N4'	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:TYR:O	1:B:1025:LYS:NZ	2.16	0.79
1:B:521:ARG:NH2	5:B:1207:SO4:S	2.55	0.79
1:C:802:LEU:HB2	1:C:822:THR:HB	1.64	0.78
3:D:1204:TDL:OL1	3:D:1204:TDL:N4'	2.18	0.74
3:F:1204:TDL:N4'	3:F:1204:TDL:OL1	2.20	0.74
1:A:34:MET:HE3	1:A:82:PHE:HB3	1.70	0.73
1:F:34:MET:HE3	1:F:82:PHE:HB3	1.70	0.73
1:F:1065:GLY:O	7:F:1301:HOH:O	2.05	0.73
1:F:435:ILE:HD11	1:F:465:LEU:HD22	1.71	0.72
1:E:34:MET:HE3	1:E:82:PHE:HB3	1.72	0.71
1:C:435:ILE:HD11	1:C:465:LEU:HD22	1.72	0.71
1:D:435:ILE:HD11	1:D:465:LEU:HD22	1.73	0.71
1:A:671:LYS:NZ	1:A:741:ASP:OD2	2.19	0.70
1:F:1026:LYS:HZ3	1:F:1098:TRP:HZ3	1.40	0.69
1:D:827:ASP:OD2	1:D:921:ARG:NH1	2.23	0.69
1:A:435:ILE:HD11	1:A:465:LEU:HD22	1.74	0.68
3:C:1204:TDL:N4'	3:C:1204:TDL:OL1	2.21	0.68
1:F:1055:LYS:HE2	1:F:1059:GLU:OE2	1.93	0.68
1:C:671:LYS:NZ	1:C:741:ASP:OD2	2.24	0.67
1:E:387:LYS:NZ	1:F:348:GLU:OE1	2.27	0.67
1:F:640:LEU:HD12	1:F:846:PRO:HG2	1.76	0.66
1:C:1076:ILE:HG22	1:C:1082:MET:HG3	1.78	0.66
1:A:967:ASP:HB3	1:A:994:ASP:HA	1.79	0.65
1:A:802:LEU:HB2	1:A:822:THR:HB	1.81	0.62
1:A:835:THR:HG22	3:A:1204:TDL:HLB2	1.81	0.62
1:A:21:GLU:OE2	1:A:202:ARG:NH1	2.29	0.62
1:F:802:LEU:HB2	1:F:822:THR:HB	1.80	0.62
1:E:706:ALA:HB2	1:E:781:LEU:HD21	1.82	0.61
1:F:27:PRO:HB3	1:F:1017:PHE:HE2	1.64	0.61
1:C:1035:SER:HB2	1:D:1031:LEU:HD23	1.83	0.60
1:D:27:PRO:HB3	1:D:1017:PHE:HE2	1.64	0.60
1:E:348:GLU:OE1	1:F:387:LYS:NZ	2.34	0.60
1:C:693:SER:OG	7:C:1301:HOH:O	2.16	0.60
1:E:954:ASP:OD2	1:F:210:HIS:NE2	2.33	0.60
1:B:435:ILE:HD11	1:B:465:LEU:HD22	1.82	0.60
1:B:592:ASP:O	1:B:596:ASN:ND2	2.29	0.60
1:F:793:VAL:HG21	1:F:1050:HIS:HB3	1.84	0.59
1:A:838:SER:HA	1:A:841:TRP:CE2	2.38	0.59
1:B:838:SER:HA	1:B:841:TRP:CE2	2.38	0.59
1:D:967:ASP:HB3	1:D:994:ASP:HA	1.85	0.59
1:F:967:ASP:HB3	1:F:994:ASP:HA	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1001:THR:O	1:E:1004:GLN:NE2	2.34	0.58
1:B:678:ILE:HD11	1:B:767:VAL:HG23	1.85	0.58
1:A:112:ARG:HH21	1:A:119:LEU:HD11	1.69	0.58
1:A:348:GLU:OE1	1:B:387:LYS:NZ	2.37	0.57
1:E:27:PRO:HB3	1:E:1017:PHE:HE2	1.69	0.57
1:C:866:PHE:CE2	3:C:1204:TDL:HM43	2.39	0.57
1:D:1055:LYS:HE3	1:D:1059:GLU:OE2	2.04	0.57
1:C:345:VAL:HB	1:D:334:LEU:HD21	1.86	0.57
1:C:1000:ASN:ND2	3:C:1204:TDL:HLB3	2.19	0.57
1:D:81:THR:HG21	1:D:91:MET:HE1	1.87	0.57
1:A:345:VAL:HB	1:B:334:LEU:HD21	1.87	0.56
1:B:887:LEU:HD13	1:B:952:GLN:HB2	1.87	0.56
1:E:694:LEU:HD22	1:E:793:VAL:HG13	1.87	0.56
1:F:419:PHE:HB2	1:F:463:SER:HB2	1.87	0.56
1:F:715:PRO:HG2	1:F:718:PHE:HB2	1.87	0.56
1:E:435:ILE:HD11	1:E:465:LEU:HD22	1.87	0.56
1:E:883:ARG:NH1	1:F:76:GLY:O	2.39	0.56
1:B:27:PRO:HB3	1:B:1017:PHE:HE2	1.71	0.56
1:D:43:ALA:HB1	1:D:1143:PHE:HZ	1.70	0.56
1:E:747:ASN:ND2	1:E:1083:THR:O	2.38	0.56
1:B:356:VAL:HG13	1:B:386:ASN:HA	1.87	0.55
1:D:835:THR:HG22	3:D:1204:TDL:HLB2	1.89	0.55
1:A:426:GLY:HA3	1:A:556:ASN:HB3	1.89	0.55
1:A:59:MET:HG3	1:A:65:ALA:HA	1.87	0.55
1:E:838:SER:HA	1:E:841:TRP:CE2	2.41	0.55
1:A:1000:ASN:HD22	3:A:1204:TDL:HLB3	1.71	0.55
1:D:583:ILE:HG23	1:D:587:TYR:HD2	1.71	0.55
1:E:802:LEU:HB2	1:E:822:THR:HB	1.89	0.55
1:E:345:VAL:HB	1:F:334:LEU:HD21	1.89	0.55
1:A:1000:ASN:ND2	3:A:1204:TDL:HLB3	2.22	0.54
1:E:967:ASP:HB3	1:E:994:ASP:HA	1.88	0.54
1:C:967:ASP:HB3	1:C:994:ASP:HA	1.87	0.54
1:A:177:GLU:OE2	1:A:447:GLN:NE2	2.37	0.54
1:C:883:ARG:NH2	1:C:886:GLU:OE1	2.32	0.54
1:B:1031:LEU:HD21	1:B:1164:GLN:HE22	1.71	0.54
1:C:81:THR:HG21	1:C:91:MET:HE1	1.88	0.54
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	1.90	0.54
1:C:671:LYS:HD2	1:C:740:LEU:HB2	1.89	0.54
1:D:1000:ASN:HD22	3:D:1204:TDL:HLB3	1.73	0.53
1:E:122:PHE:CE2	1:F:220:PRO:HD3	2.43	0.53
1:D:802:LEU:HB2	1:D:822:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:GLY:HA3	1:D:556:ASN:HB3	1.90	0.53
1:B:518:MET:HB3	1:B:618:TRP:HH2	1.72	0.53
1:A:590:LYS:HB3	1:A:594:ILE:HD12	1.89	0.53
1:D:487:HIS:CD2	1:D:559:MET:HG2	2.43	0.53
1:A:356:VAL:HG13	1:A:386:ASN:HA	1.89	0.53
1:F:426:GLY:HA3	1:F:556:ASN:HB3	1.90	0.53
1:B:793:VAL:HG21	1:B:1050:HIS:HB3	1.90	0.53
1:F:258:LEU:HD22	1:F:310:HIS:CG	2.44	0.52
1:A:419:PHE:HB2	1:A:463:SER:HB2	1.90	0.52
1:C:52:LYS:NZ	1:D:889:THR:OG1	2.41	0.52
1:C:802:LEU:HD13	1:C:859:PRO:HD3	1.92	0.52
1:E:419:PHE:HB2	1:E:463:SER:HB2	1.91	0.52
1:F:835:THR:HG22	3:F:1204:TDL:HLB2	1.91	0.52
1:C:112:ARG:HH21	1:C:119:LEU:HD11	1.75	0.52
1:F:81:THR:HG21	1:F:91:MET:HE1	1.91	0.52
1:A:1047:GLY:HA3	1:A:1089:ALA:HB3	1.92	0.52
1:F:356:VAL:HG13	1:F:386:ASN:HA	1.92	0.52
1:A:27:PRO:HB3	1:A:1017:PHE:HE2	1.75	0.52
1:A:1060:ALA:HB1	1:A:1067:SER:HB3	1.92	0.52
1:C:1010:GLN:HG3	1:C:1097:TYR:OH	2.10	0.52
1:C:348:GLU:OE1	1:D:387:LYS:NZ	2.43	0.51
1:C:678:ILE:HD11	1:C:767:VAL:HG23	1.91	0.51
1:F:838:SER:HA	1:F:841:TRP:CE2	2.45	0.51
1:B:81:THR:HG21	1:B:91:MET:HE1	1.91	0.51
1:E:204:ARG:NH2	7:E:1303:HOH:O	2.42	0.51
1:F:1155:GLU:HG2	1:F:1159:LYS:HE3	1.92	0.51
1:C:1079:GLY:HA3	1:C:1134:ILE:HB	1.91	0.51
1:A:85:SER:HA	1:A:127:ASP:HB3	1.92	0.51
1:A:220:PRO:HD3	1:B:122:PHE:CE2	2.45	0.51
1:B:802:LEU:HB2	1:B:822:THR:HB	1.92	0.51
1:C:1004:GLN:HG3	1:C:1016:ARG:HB2	1.93	0.51
1:F:1060:ALA:HB1	1:F:1067:SER:HB3	1.92	0.51
1:F:112:ARG:NH1	3:F:1204:TDL:OL3	2.43	0.51
1:E:1031:LEU:HD23	1:F:1035:SER:HB2	1.91	0.51
1:C:1004:GLN:HG2	1:C:1017:PHE:CE2	2.45	0.51
1:C:1031:LEU:HD23	1:D:1035:SER:HB2	1.93	0.51
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	1.93	0.50
1:C:112:ARG:NH2	1:C:119:LEU:HD11	2.26	0.50
1:A:1004:GLN:HG3	1:A:1016:ARG:HB2	1.92	0.50
1:A:112:ARG:NE	1:A:121:ILE:HA	2.27	0.50
1:F:866:PHE:CE2	3:F:1204:TDL:HM43	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ALA:HB2	1:B:186:TYR:CE1	2.46	0.50
1:B:752:CYS:HA	2:B:1201:SF4:S1	2.52	0.50
1:D:1090:LYS:HE2	1:D:1094:GLU:OE2	2.10	0.50
1:F:893:LYS:HB3	1:F:945:LEU:HD11	1.92	0.50
1:C:747:ASN:ND2	1:C:1083:THR:O	2.44	0.50
1:D:1072:TYR:HB2	1:D:1098:TRP:CE2	2.47	0.50
1:F:1028:ASP:OD2	1:F:1165:TYR:OH	2.25	0.50
1:F:1079:GLY:HA3	1:F:1134:ILE:HB	1.94	0.50
1:F:136:PHE:CE2	1:F:164:PRO:HB2	2.46	0.50
1:B:34:MET:HE3	1:B:82:PHE:HB3	1.93	0.49
1:E:1012:GLY:O	1:E:1139:LEU:HD22	2.12	0.49
1:E:52:LYS:NZ	1:F:889:THR:OG1	2.39	0.49
1:B:258:LEU:HD22	1:B:310:HIS:CG	2.47	0.49
1:B:122:PHE:HB3	1:B:364:SER:HB2	1.93	0.49
1:F:1001:THR:O	1:F:1004:GLN:NE2	2.44	0.49
1:F:883:ARG:NH1	1:F:886:GLU:OE2	2.35	0.49
1:C:835:THR:HG22	3:C:1204:TDL:HLB2	1.93	0.49
1:E:745:CYS:SG	1:E:746:GLY:N	2.85	0.49
1:F:1030:GLY:O	1:F:1034:MET:HG3	2.12	0.49
1:D:1079:GLY:HA3	1:D:1134:ILE:HB	1.94	0.49
1:C:220:PRO:HD3	1:D:122:PHE:CE2	2.48	0.49
1:D:838:SER:HA	1:D:841:TRP:CE2	2.47	0.49
1:E:678:ILE:HD12	1:E:764:LEU:HD13	1.92	0.49
1:F:489:PRO:HG3	1:F:510:ASN:O	2.12	0.49
1:B:85:SER:HA	1:B:127:ASP:HB3	1.94	0.49
1:E:85:SER:HA	1:E:127:ASP:HB3	1.94	0.49
1:A:1030:GLY:O	1:A:1034:MET:HG3	2.13	0.49
1:A:544:LYS:HE2	1:A:548:GLU:OE2	2.12	0.49
1:A:387:LYS:NZ	1:B:348:GLU:OE1	2.45	0.49
1:C:1072:TYR:HB2	1:C:1098:TRP:CE2	2.48	0.49
1:D:506:ILE:HG12	1:D:536:LYS:HE3	1.95	0.49
1:A:1035:SER:HB2	1:B:1031:LEU:HD23	1.95	0.49
1:C:435:ILE:HG23	1:C:446:ALA:HB1	1.94	0.48
1:E:678:ILE:HD13	1:E:739:PRO:HA	1.94	0.48
1:C:817:TYR:CZ	1:C:1071:ALA:HB1	2.48	0.48
1:C:998:TYR:CE1	1:C:1006:SER:HB2	2.48	0.48
1:D:793:VAL:HG21	1:D:1050:HIS:HB3	1.95	0.48
1:B:719:VAL:O	1:B:734:ARG:NH2	2.44	0.48
1:D:1000:ASN:ND2	3:D:1204:TDL:HLB3	2.27	0.48
1:E:27:PRO:HB3	1:E:1017:PHE:CE2	2.48	0.48
1:D:1004:GLN:HG2	1:D:1017:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:PHE:HB3	1:F:364:SER:HB2	1.96	0.48
1:A:435:ILE:HG23	1:A:446:ALA:HB1	1.96	0.48
1:E:1012:GLY:HA2	1:E:1150:LEU:HD13	1.95	0.48
1:B:692:CYS:HB2	1:B:748:CYS:HB2	1.94	0.48
1:D:641:ARG:NH1	1:D:669:TYR:O	2.45	0.48
1:A:836:GLY:HA2	3:A:1204:TDL:S1	2.53	0.48
1:D:356:VAL:HG13	1:D:386:ASN:HA	1.94	0.48
1:D:979:ASP:OD1	1:D:1036:TYR:OH	2.23	0.48
1:A:879:ALA:HB3	1:B:75:ALA:HB3	1.95	0.48
1:D:438:ILE:HD13	1:D:569:VAL:HG11	1.95	0.48
1:C:122:PHE:CE2	1:D:220:PRO:HD3	2.50	0.47
1:F:32:SER:O	1:F:36:GLU:HG3	2.14	0.47
1:F:632:GLU:OE2	1:F:641:ARG:NH2	2.30	0.47
1:B:518:MET:HB3	1:B:618:TRP:CH2	2.49	0.47
1:A:416:ARG:HG2	1:A:466:ARG:HG2	1.97	0.47
1:A:1004:GLN:HG2	1:A:1017:PHE:CE2	2.50	0.47
1:D:866:PHE:CE2	3:D:1204:TDL:HM43	2.49	0.47
1:E:356:VAL:HG13	1:E:386:ASN:HA	1.96	0.47
1:E:802:LEU:HD13	1:E:859:PRO:HD3	1.97	0.47
1:C:85:SER:HA	1:C:127:ASP:HB3	1.96	0.47
1:D:32:SER:O	1:D:36:GLU:HG3	2.15	0.47
1:A:112:ARG:NH2	1:A:119:LEU:HD11	2.30	0.47
1:A:18:ALA:HB2	1:A:186:TYR:CE1	2.50	0.47
1:A:814:GLU:HB3	1:A:993:LEU:HD13	1.96	0.47
1:E:37:ILE:HG13	1:E:41:TRP:CE2	2.50	0.47
1:B:827:ASP:OD1	1:B:853:ASN:ND2	2.48	0.47
1:C:1060:ALA:HB1	1:C:1067:SER:HB3	1.97	0.47
3:C:1204:TDL:C6'	3:C:1204:TDL:HM41	2.45	0.47
1:F:521:ARG:HD2	1:F:521:ARG:HA	1.61	0.47
1:A:361:GLY:HA2	1:A:365:LYS:HB3	1.96	0.46
1:D:887:LEU:HD13	1:D:952:GLN:HB2	1.96	0.46
1:F:438:ILE:HD13	1:F:569:VAL:HG11	1.96	0.46
1:A:1079:GLY:HA3	1:A:1134:ILE:HB	1.98	0.46
1:C:27:PRO:HB3	1:C:1017:PHE:HE2	1.80	0.46
1:E:81:THR:HG21	1:E:91:MET:HE1	1.96	0.46
1:F:510:ASN:HB2	1:F:559:MET:SD	2.55	0.46
1:E:1072:TYR:HB2	1:E:1098:TRP:CE2	2.50	0.46
1:C:1000:ASN:HD22	3:C:1204:TDL:HLB3	1.80	0.46
1:D:419:PHE:HB2	1:D:463:SER:HB2	1.97	0.46
1:D:945:LEU:O	1:D:949:ILE:HG12	2.15	0.46
1:E:1117:LEU:HD23	1:E:1120:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1000:ASN:HD22	3:F:1204:TDL:HLB3	1.80	0.46
1:F:855:GLN:N	1:F:855:GLN:OE1	2.48	0.46
1:D:817:TYR:CZ	1:D:1071:ALA:HB1	2.50	0.46
1:D:136:PHE:CE2	1:D:164:PRO:HB2	2.51	0.46
1:E:506:ILE:HG12	1:E:536:LYS:HE3	1.98	0.46
1:A:678:ILE:HD11	1:A:767:VAL:HG23	1.97	0.46
1:B:113:ALA:HB2	1:B:124:ASP:OD2	2.16	0.46
1:B:112:ARG:NH2	1:B:119:LEU:HD11	2.31	0.46
1:F:361:GLY:HA2	1:F:365:LYS:HB3	1.98	0.46
1:E:7:ASP:HA	1:E:177:GLU:O	2.16	0.46
1:B:855:GLN:N	1:B:855:GLN:OE1	2.49	0.46
1:A:113:ALA:HB2	1:A:124:ASP:OD2	2.16	0.46
1:C:136:PHE:CE2	1:C:164:PRO:HB2	2.50	0.46
1:F:96:TYR:CE1	1:F:134:THR:HA	2.51	0.45
1:E:213:GLN:HG3	1:F:861:TRP:HE3	1.80	0.45
1:E:122:PHE:HB3	1:E:364:SER:HB2	1.98	0.45
1:D:418:LYS:HE2	1:D:418:LYS:HB3	1.77	0.45
1:F:1133:GLU:OE2	1:F:1135:ARG:NE	2.44	0.45
1:A:27:PRO:HB3	1:A:1017:PHE:CE2	2.52	0.45
1:B:521:ARG:NH2	5:B:1207:SO4:O2	2.36	0.45
1:F:1000:ASN:ND2	3:F:1204:TDL:HLB3	2.31	0.45
1:D:855:GLN:N	1:D:855:GLN:OE1	2.49	0.45
1:B:112:ARG:HH21	1:B:119:LEU:HD11	1.81	0.45
1:F:519:ASP:OD1	1:F:618:TRP:NE1	2.46	0.45
1:B:435:ILE:HG23	1:B:446:ALA:HB1	1.98	0.45
1:C:693:SER:HB2	1:C:703:PRO:HD3	1.98	0.45
1:F:747:ASN:OD1	1:F:811:GLY:HA2	2.17	0.45
1:D:112:ARG:NH1	3:D:1204:TDL:OL3	2.49	0.45
1:D:18:ALA:HB2	1:D:186:TYR:CE1	2.51	0.45
1:E:220:PRO:HD3	1:F:122:PHE:CE2	2.52	0.45
1:A:855:GLN:OE1	1:A:855:GLN:N	2.50	0.45
1:A:81:THR:HG21	1:A:91:MET:HE1	1.99	0.45
1:E:1095:ALA:HB1	1:E:1126:PHE:HA	1.99	0.45
1:F:127:ASP:OD1	1:F:128:VAL:N	2.48	0.45
1:B:27:PRO:HB3	1:B:1017:PHE:CE2	2.52	0.45
1:E:66:ALA:HB2	1:E:91:MET:HE2	1.98	0.45
1:F:3:LYS:NZ	1:F:182:ASP:HB2	2.32	0.45
1:F:867:GLU:N	1:F:867:GLU:OE2	2.49	0.45
1:B:146:GLU:OE2	1:B:301:ARG:NH2	2.50	0.44
1:E:674:ILE:HG12	7:E:1313:HOH:O	2.16	0.44
1:F:678:ILE:HD11	1:F:764:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:LYS:HE2	1:E:194:ASP:HB2	2.00	0.44
1:F:456:LYS:HE2	1:F:837:CYS:SG	2.56	0.44
1:B:112:ARG:NE	1:B:121:ILE:HA	2.32	0.44
1:B:480:GLN:HA	1:B:500:GLY:O	2.16	0.44
1:C:112:ARG:HA	1:C:123:GLY:HA2	2.00	0.44
1:D:112:ARG:HA	1:D:123:GLY:HA2	1.99	0.44
1:D:43:ALA:HB1	1:D:1143:PHE:CZ	2.51	0.44
1:F:1004:GLN:HG2	1:F:1017:PHE:CE2	2.52	0.44
1:F:192:LEU:HD22	1:F:247:GLN:HB3	1.99	0.44
1:F:519:ASP:O	1:F:527:LYS:NZ	2.27	0.44
1:B:1004:GLN:HG2	1:B:1017:PHE:CE2	2.52	0.44
1:B:1097:TYR:HH	1:B:1136:TYR:HH	1.60	0.44
3:C:1204:TDL:H6'	3:C:1204:TDL:HM41	1.98	0.44
1:C:590:LYS:HB3	1:C:594:ILE:HD12	2.00	0.44
1:C:692:CYS:HB2	1:C:748:CYS:HB2	1.99	0.44
1:A:828:ARG:NH2	1:A:1061:GLU:OE2	2.50	0.44
1:B:18:ALA:HB2	1:B:186:TYR:CZ	2.52	0.44
1:B:431:ASN:HB3	1:B:465:LEU:HD11	2.00	0.44
1:E:417:CYS:HB2	1:E:419:PHE:CE1	2.53	0.44
1:E:501:ILE:HD13	1:E:535:LEU:HD13	1.99	0.44
1:A:866:PHE:CE2	3:A:1204:TDL:HM43	2.53	0.44
1:A:75:ALA:HB3	1:B:879:ALA:HB3	2.00	0.44
1:C:1087:ARG:HG2	1:C:1091:LYS:HE3	2.00	0.44
1:C:75:ALA:HB3	1:D:879:ALA:HB3	2.00	0.44
1:E:492:VAL:HG13	1:E:526:MET:SD	2.58	0.44
1:F:817:TYR:CZ	1:F:1071:ALA:HB1	2.53	0.44
1:F:85:SER:HA	1:F:127:ASP:HB3	1.99	0.44
1:A:1072:TYR:HB2	1:A:1098:TRP:CE2	2.53	0.43
1:B:512:THR:HG22	1:B:541:ASP:OD2	2.18	0.43
1:C:416:ARG:HG2	1:C:466:ARG:HG2	1.99	0.43
1:D:85:SER:HB2	1:D:112:ARG:HB3	2.00	0.43
1:F:1072:TYR:HB2	1:F:1098:TRP:CE2	2.53	0.43
1:E:18:ALA:HB2	1:E:186:TYR:CZ	2.53	0.43
1:F:1011:THR:OG1	1:F:1025:LYS:HA	2.17	0.43
1:A:1080:ILE:HG13	1:A:1082:MET:CE	2.49	0.43
1:D:1001:THR:O	1:D:1004:GLN:NE2	2.42	0.43
1:B:416:ARG:HG2	1:B:466:ARG:HG2	2.01	0.43
1:D:83:THR:O	1:D:109:VAL:HA	2.19	0.43
1:B:489:PRO:HG3	1:B:510:ASN:O	2.19	0.43
1:A:334:LEU:HD21	1:B:345:VAL:HB	1.99	0.43
1:A:935:ILE:HD13	1:A:947:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1057:LEU:HD23	1:B:1069:ILE:HD13	1.99	0.43
1:C:508:LEU:HD22	1:C:566:ILE:HD11	2.00	0.43
1:F:24:THR:HA	1:F:57:ALA:O	2.18	0.43
1:A:1139:LEU:HD21	1:A:1150:LEU:HD12	1.99	0.43
1:D:34:MET:HE3	1:D:82:PHE:HB3	1.99	0.43
1:E:140:SER:HB2	1:E:168:PHE:CZ	2.53	0.43
1:F:6:LEU:HD22	1:F:10:THR:HG21	2.01	0.43
1:B:521:ARG:HD2	1:B:521:ARG:HA	1.75	0.43
1:B:66:ALA:HB2	1:B:91:MET:HG2	2.01	0.43
1:D:18:ALA:HB2	1:D:186:TYR:CZ	2.54	0.43
1:B:189:MET:O	1:B:193:VAL:HG23	2.19	0.43
1:D:1039:VAL:HG22	1:D:1066:PRO:HG2	2.00	0.43
1:D:781:LEU:O	1:D:854:ARG:NH2	2.51	0.43
1:E:583:ILE:HG23	1:E:587:TYR:HD2	1.84	0.43
1:B:1010:GLN:HG3	1:B:1097:TYR:OH	2.19	0.42
1:C:59:MET:HA	1:D:980:HIS:NE2	2.34	0.42
1:F:28:ILE:HD13	1:F:84:ALA:O	2.19	0.42
1:A:480:GLN:HA	1:A:500:GLY:O	2.19	0.42
1:B:34:MET:HE3	1:B:34:MET:HB2	1.77	0.42
1:B:813:GLY:HA3	1:B:1074:PRO:HD2	2.00	0.42
1:D:1030:GLY:O	1:D:1034:MET:HG3	2.19	0.42
1:D:122:PHE:HB3	1:D:364:SER:HB2	2.00	0.42
1:A:373:LYS:HE2	1:A:405:GLU:OE2	2.20	0.42
1:B:122:PHE:HB3	1:B:364:SER:CB	2.50	0.42
1:C:34:MET:CE	1:C:82:PHE:HB3	2.44	0.42
1:D:867:GLU:OE2	1:D:867:GLU:N	2.47	0.42
1:A:438:ILE:HD13	1:A:569:VAL:HG11	2.01	0.42
1:B:558:ILE:HG23	1:B:605:ALA:HB2	2.01	0.42
1:B:803:LEU:HD12	1:B:849:PRO:HB2	2.02	0.42
1:B:814:GLU:HB3	1:B:993:LEU:HD13	2.02	0.42
1:C:604:ARG:HA	1:C:604:ARG:HD3	1.89	0.42
1:C:954:ASP:N	1:C:954:ASP:OD1	2.52	0.42
1:A:122:PHE:HB3	1:A:364:SER:HB2	2.00	0.42
1:C:1001:THR:O	1:C:1004:GLN:NE2	2.52	0.42
1:C:87:GLY:O	1:C:91:MET:HG3	2.19	0.42
1:B:455:LYS:HD3	1:B:672:ARG:CZ	2.49	0.42
1:C:866:PHE:CD2	1:C:973:ILE:HG21	2.54	0.42
1:C:334:LEU:HD21	1:D:345:VAL:HB	2.01	0.42
1:C:869:ASN:HB3	1:C:969:TRP:NE1	2.34	0.42
1:D:27:PRO:HB3	1:D:1017:PHE:CE2	2.49	0.42
1:E:747:ASN:OD1	1:E:811:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1076:ILE:HG22	1:F:1082:MET:HG3	2.02	0.42
1:B:671:LYS:NZ	1:B:741:ASP:OD2	2.38	0.42
1:C:836:GLY:HA2	3:C:1204:TDL:S1	2.60	0.42
1:E:583:ILE:HD13	1:E:598:ASN:HB3	2.01	0.42
1:E:855:GLN:N	1:E:855:GLN:OE1	2.53	0.42
1:F:1004:GLN:HG3	1:F:1016:ARG:HB2	2.02	0.42
1:B:63:ALA:HB2	1:B:90:LEU:HB3	2.01	0.42
1:C:1030:GLY:O	1:C:1034:MET:HG3	2.20	0.42
1:C:838:SER:HA	1:C:841:TRP:CE2	2.55	0.42
1:A:146:GLU:OE2	1:A:301:ARG:NH2	2.52	0.41
1:D:836:GLY:O	1:D:840:ILE:HG12	2.20	0.41
1:C:28:ILE:HD13	1:C:84:ALA:O	2.20	0.41
1:D:747:ASN:ND2	1:D:1083:THR:O	2.53	0.41
1:E:113:ALA:HB2	1:E:124:ASP:OD2	2.20	0.41
1:C:37:ILE:HG13	1:C:41:TRP:CE2	2.55	0.41
1:A:887:LEU:HD13	1:A:952:GLN:HB2	2.02	0.41
1:B:116:THR:OG1	1:B:117:HIS:N	2.53	0.41
1:B:422:LEU:HD22	1:B:423:GLY:H	1.85	0.41
1:F:112:ARG:NE	1:F:121:ILE:HA	2.35	0.41
1:F:503:PRO:HA	1:F:533:LYS:HB3	2.02	0.41
1:C:127:ASP:OD1	1:C:128:VAL:N	2.53	0.41
1:C:356:VAL:HG13	1:C:386:ASN:HA	2.02	0.41
1:D:435:ILE:HG23	1:D:446:ALA:HB1	2.00	0.41
1:D:521:ARG:HD2	1:D:521:ARG:HA	1.63	0.41
1:F:287:TYR:O	1:F:291:LYS:HD3	2.19	0.41
1:F:641:ARG:HB2	1:F:642:PRO:HD3	2.02	0.41
1:F:704:TYR:CE1	1:F:736:GLN:HB3	2.55	0.41
1:B:1030:GLY:O	1:B:1034:MET:HG3	2.21	0.41
1:C:361:GLY:HA2	1:C:365:LYS:HB3	2.03	0.41
1:D:641:ARG:HB2	1:D:642:PRO:HD3	2.03	0.41
1:E:671:LYS:HD2	1:E:740:LEU:HB2	2.03	0.41
1:E:803:LEU:HD12	1:E:849:PRO:HB2	2.02	0.41
1:E:28:ILE:HD13	1:E:84:ALA:O	2.21	0.41
1:C:213:GLN:HG3	1:D:861:TRP:HE3	1.85	0.41
1:D:84:ALA:HA	1:D:109:VAL:HG13	2.02	0.41
1:E:1030:GLY:O	1:E:1034:MET:HG3	2.21	0.41
1:F:1047:GLY:HA3	1:F:1089:ALA:HB3	2.02	0.41
1:B:681:TRP:CE3	1:B:683:PRO:HG3	2.56	0.41
1:C:1047:GLY:O	1:C:1090:LYS:HB2	2.21	0.41
1:C:681:TRP:CD1	1:C:735:ILE:HB	2.55	0.41
1:C:841:TRP:O	1:C:849:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:ILE:HG12	1:F:536:LYS:HE3	2.03	0.41
1:B:983:ALA:HB2	1:B:1036:TYR:CZ	2.56	0.41
1:C:116:THR:OG1	1:C:117:HIS:N	2.54	0.41
1:C:733:PHE:HE1	1:C:735:ILE:HG12	1.85	0.41
1:E:641:ARG:NH1	1:E:669:TYR:O	2.54	0.41
1:F:1010:GLN:HG3	1:F:1097:TYR:OH	2.20	0.41
1:E:1035:SER:HB2	1:F:1031:LEU:HD23	2.02	0.41
1:E:213:GLN:HG3	1:F:861:TRP:CE3	2.54	0.41
1:B:1001:THR:O	1:B:1004:GLN:NE2	2.48	0.41
1:D:1026:LYS:HZ3	1:D:1098:TRP:HZ3	1.69	0.41
1:D:112:ARG:NH2	1:D:119:LEU:HD11	2.36	0.41
1:E:361:GLY:HA2	1:E:365:LYS:HB3	2.03	0.41
1:E:678:ILE:HG23	1:E:679:PRO:HD2	2.02	0.41
1:F:697:PRO:HG2	1:F:811:GLY:HA2	2.03	0.41
1:A:1075:CYS:SG	1:A:1076:ILE:N	2.94	0.40
1:B:615:PRO:HD2	1:B:618:TRP:NE1	2.36	0.40
1:B:867:GLU:HB3	1:B:973:ILE:HG12	2.03	0.40
1:E:1008:ALA:O	1:E:1026:LYS:NZ	2.47	0.40
1:F:718:PHE:CZ	1:F:734:ARG:HD3	2.56	0.40
1:B:221:ASP:N	1:B:221:ASP:OD1	2.53	0.40
1:B:935:ILE:HD13	1:B:947:LEU:HD23	2.03	0.40
1:E:418:LYS:HE2	1:E:418:LYS:HB3	1.88	0.40
1:E:667:THR:HB	1:E:805:PHE:HB2	2.04	0.40
1:F:417:CYS:HA	1:F:483:LEU:O	2.22	0.40
1:D:189:MET:O	1:D:193:VAL:HG23	2.21	0.40
1:E:980:HIS:NE2	1:F:59:MET:HA	2.37	0.40
1:B:746:GLY:N	2:B:1202:SF4:S1	2.84	0.40
1:D:1010:GLN:HG3	1:D:1097:TYR:CZ	2.56	0.40
1:D:91:MET:O	1:D:95:MET:HG3	2.20	0.40
1:E:178:VAL:O	1:E:447:GLN:HA	2.22	0.40
1:B:1010:GLN:HG3	1:B:1097:TYR:CZ	2.56	0.40
1:B:967:ASP:HB3	1:B:994:ASP:HA	2.03	0.40
1:C:18:ALA:HB2	1:C:186:TYR:CZ	2.57	0.40
1:D:361:GLY:HA2	1:D:365:LYS:HB3	2.03	0.40
1:D:321:ARG:HB3	1:D:379:LEU:HD22	2.03	0.40
1:D:518:MET:HB3	1:D:618:TRP:CH2	2.56	0.40
1:E:189:MET:O	1:E:193:VAL:HG23	2.22	0.40
1:E:75:ALA:HB3	1:F:879:ALA:HB3	2.03	0.40
1:F:321:ARG:HB3	1:F:379:LEU:HD22	2.02	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	1160/1171 (99%)	1141 (98%)	19 (2%)	0	100	100
1	B	1160/1171 (99%)	1141 (98%)	19 (2%)	0	100	100
1	C	1157/1171 (99%)	1139 (98%)	18 (2%)	0	100	100
1	D	1153/1171 (98%)	1135 (98%)	18 (2%)	0	100	100
1	E	1151/1171 (98%)	1132 (98%)	19 (2%)	0	100	100
1	F	1149/1171 (98%)	1131 (98%)	18 (2%)	0	100	100
All	All	6930/7026 (99%)	6819 (98%)	111 (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	919/932 (99%)	916 (100%)	3 (0%)	92	97
1	B	919/932 (99%)	914 (100%)	5 (0%)	88	96
1	C	923/932 (99%)	919 (100%)	4 (0%)	91	97
1	D	918/932 (98%)	911 (99%)	7 (1%)	81	93
1	E	918/932 (98%)	913 (100%)	5 (0%)	88	96
1	F	918/932 (98%)	913 (100%)	5 (0%)	88	96
All	All	5515/5592 (99%)	5486 (100%)	29 (0%)	88	96

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	PHE
1	A	417	CYS
1	A	833	ASN
1	B	224	PHE
1	B	326	ASP
1	B	417	CYS
1	B	521	ARG
1	B	833	ASN
1	C	224	PHE
1	C	417	CYS
1	C	833	ASN
1	C	1143	PHE
1	D	34	MET
1	D	224	PHE
1	D	417	CYS
1	D	476	TYR
1	D	521	ARG
1	D	833	ASN
1	D	837	CYS
1	E	224	PHE
1	E	326	ASP
1	E	417	CYS
1	E	797	GLN
1	E	833	ASN
1	F	224	PHE
1	F	326	ASP
1	F	417	CYS
1	F	521	ARG
1	F	833	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	774	ASN
1	A	1000	ASN
1	B	1164	GLN
1	D	1000	ASN
1	F	1000	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	B	1207	-	4,4,4	0.13	0	6,6,6	0.13	0
3	TDL	D	1204	4	24,33,33	2.04	7 (29%)	28,51,51	1.55	8 (28%)
6	TPP	E	1204	4	22,27,27	2.05	6 (27%)	29,40,40	1.79	6 (20%)
2	SF4	F	1203	1	0,12,12	0.00	-	-		
2	SF4	A	1202	1	0,12,12	0.00	-	-		
2	SF4	B	1203	1	0,12,12	0.00	-	-		
2	SF4	C	1201	1	0,12,12	0.00	-	-		
5	SO4	F	1206	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SF4	D	1202	1	0,12,12	0.00	-	-		
5	SO4	D	1206	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SF4	E	1202	1	0,12,12	0.00	-	-		
5	SO4	C	1206	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SF4	D	1201	1	0,12,12	0.00	-	-		
2	SF4	C	1203	1	0,12,12	0.00	-	-		
3	TDL	A	1204	4	24,33,33	1.98	7 (29%)	28,51,51	1.47	5 (17%)
2	SF4	D	1203	1	0,12,12	0.00	-	-		
5	SO4	A	1206	-	4,4,4	0.15	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	TPP	B	1204	4	22,27,27	2.12	6 (27%)	29,40,40	1.95	8 (27%)
2	SF4	B	1202	1	0,12,12	0.00	-	-		
5	SO4	E	1206	-	4,4,4	0.14	0	6,6,6	0.08	0
3	TDL	C	1204	4	24,33,33	2.09	7 (29%)	28,51,51	1.50	6 (21%)
2	SF4	B	1201	1	0,12,12	0.00	-	-		
2	SF4	F	1202	1	0,12,12	0.00	-	-		
2	SF4	C	1202	1	0,12,12	0.00	-	-		
2	SF4	A	1203	1	0,12,12	0.00	-	-		
2	SF4	F	1201	1	0,12,12	0.00	-	-		
3	TDL	F	1204	4	24,33,33	2.08	7 (29%)	28,51,51	1.48	6 (21%)
2	SF4	E	1201	1	0,12,12	0.00	-	-		
2	SF4	A	1201	1	0,12,12	0.00	-	-		
5	SO4	B	1206	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SF4	E	1203	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
3	TDL	D	1204	4	-	4/16/29/29	0/2/2/2
6	TPP	E	1204	4	-	2/16/17/17	0/2/2/2
2	SF4	F	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	C	1201	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	D	1201	1	-	-	0/6/5/5
2	SF4	C	1203	1	-	-	0/6/5/5
3	TDL	A	1204	4	-	3/16/29/29	0/2/2/2
2	SF4	D	1203	1	-	-	0/6/5/5
6	TPP	B	1204	4	-	3/16/17/17	0/2/2/2
2	SF4	B	1202	1	-	-	0/6/5/5
3	TDL	C	1204	4	-	2/16/29/29	0/2/2/2
2	SF4	B	1201	1	-	-	0/6/5/5
2	SF4	F	1202	1	-	-	0/6/5/5
2	SF4	C	1202	1	-	-	0/6/5/5
2	SF4	A	1203	1	-	-	0/6/5/5
2	SF4	F	1201	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TDL	F	1204	4	-	4/16/29/29	0/2/2/2
2	SF4	E	1201	1	-	-	0/6/5/5
2	SF4	A	1201	1	-	-	0/6/5/5
2	SF4	E	1203	1	-	-	0/6/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1204	TPP	C4-N3	-4.93	1.35	1.39
6	B	1204	TPP	C4-N3	-4.90	1.35	1.39
3	C	1204	TDL	C6-C5	4.57	1.52	1.50
3	F	1204	TDL	C5-S1	4.53	1.82	1.74
3	D	1204	TDL	C5-S1	4.44	1.82	1.74
3	F	1204	TDL	C6-C5	4.39	1.52	1.50
3	C	1204	TDL	C5-S1	4.32	1.82	1.74
3	A	1204	TDL	C5-S1	4.26	1.82	1.74
3	D	1204	TDL	C6-C5	4.20	1.52	1.50
6	B	1204	TPP	C4'-N4'	3.90	1.43	1.34
3	C	1204	TDL	C7'-C5'	3.79	1.59	1.51
6	B	1204	TPP	C6-C5	3.78	1.52	1.50
6	E	1204	TPP	C4'-N4'	3.74	1.43	1.34
3	A	1204	TDL	C7'-C5'	3.68	1.58	1.51
3	F	1204	TDL	C7'-C5'	3.68	1.58	1.51
3	C	1204	TDL	CLB-CLA	3.65	1.57	1.53
3	D	1204	TDL	C4'-N4'	3.62	1.43	1.34
3	C	1204	TDL	C4'-N4'	3.62	1.43	1.34
3	D	1204	TDL	C7'-C5'	3.61	1.58	1.51
3	F	1204	TDL	CLB-CLA	3.60	1.57	1.53
6	B	1204	TPP	C7'-N3	-3.60	1.42	1.48
3	F	1204	TDL	C4'-N4'	3.59	1.43	1.34
3	A	1204	TDL	C6-C5	3.57	1.52	1.50
3	A	1204	TDL	C4'-N4'	3.51	1.43	1.34
3	D	1204	TDL	CLB-CLA	3.46	1.57	1.53
3	A	1204	TDL	CLB-CLA	3.34	1.57	1.53
6	E	1204	TPP	C7'-N3	-3.31	1.42	1.48
6	E	1204	TPP	C6-C5	3.26	1.52	1.50
6	E	1204	TPP	C7'-C5'	3.25	1.58	1.51
6	B	1204	TPP	C7'-C5'	3.23	1.57	1.51
3	A	1204	TDL	OL1-CLA	-2.48	1.38	1.43
3	A	1204	TDL	C6'-C5'	2.48	1.42	1.37
3	D	1204	TDL	C6'-C5'	2.45	1.42	1.37
3	F	1204	TDL	OL1-CLA	-2.44	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1204	TDL	OL1-CLA	-2.42	1.38	1.43
3	C	1204	TDL	C6'-C5'	2.37	1.42	1.37
3	F	1204	TDL	C6'-C5'	2.36	1.42	1.37
6	E	1204	TPP	C6'-C5'	2.29	1.42	1.37
6	B	1204	TPP	C6'-C5'	2.28	1.42	1.37
3	C	1204	TDL	OL1-CLA	-2.27	1.39	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1204	TPP	C6-C5-C4	-6.31	122.37	127.43
6	E	1204	TPP	C6-C5-C4	-5.90	122.69	127.43
6	E	1204	TPP	C6'-N1'-C2'	3.14	121.31	115.96
3	C	1204	TDL	C5-C4-N3	3.14	114.22	107.66
3	A	1204	TDL	C5-C4-N3	3.08	114.09	107.66
3	F	1204	TDL	C5-C4-N3	3.06	114.05	107.66
3	D	1204	TDL	C5-C4-N3	3.00	113.92	107.66
6	B	1204	TPP	C6'-N1'-C2'	2.99	121.05	115.96
3	C	1204	TDL	PA-O3A-PB	-2.99	122.57	132.83
3	C	1204	TDL	C6'-N1'-C2'	2.98	121.03	115.96
3	A	1204	TDL	C6'-N1'-C2'	2.94	120.97	115.96
3	F	1204	TDL	C6'-N1'-C2'	2.87	120.84	115.96
6	E	1204	TPP	C5'-C6'-N1'	-2.86	119.06	123.82
3	D	1204	TDL	C6'-N1'-C2'	2.82	120.76	115.96
6	B	1204	TPP	N4'-C4'-N3'	2.78	120.96	117.03
6	B	1204	TPP	C5'-C6'-N1'	-2.71	119.31	123.82
3	D	1204	TDL	C5'-C7'-N3	2.70	117.72	113.26
3	D	1204	TDL	PA-O3A-PB	-2.66	123.71	132.83
3	A	1204	TDL	PA-O3A-PB	-2.55	124.07	132.83
3	F	1204	TDL	PA-O3A-PB	-2.52	124.19	132.83
6	B	1204	TPP	CM4-C4-N3	2.51	125.73	122.53
6	E	1204	TPP	PA-O3A-PB	-2.39	124.62	132.83
3	D	1204	TDL	CM2-C2'-N1'	2.33	119.70	117.14
6	B	1204	TPP	PA-O3A-PB	-2.32	124.85	132.83
3	D	1204	TDL	C2'-N3'-C4'	2.26	121.61	118.08
3	A	1204	TDL	C5'-C6'-N1'	-2.26	120.06	123.82
3	D	1204	TDL	N1'-C2'-N3'	-2.25	121.67	125.54
3	D	1204	TDL	C5'-C6'-N1'	-2.22	120.13	123.82
3	F	1204	TDL	C5'-C6'-N1'	-2.21	120.13	123.82
3	F	1204	TDL	N1'-C2'-N3'	-2.18	121.78	125.54
3	C	1204	TDL	N1'-C2'-N3'	-2.18	121.79	125.54
3	A	1204	TDL	N1'-C2'-N3'	-2.16	121.82	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1204	TDL	C2'-N3'-C4'	2.13	121.40	118.08
3	C	1204	TDL	C5'-C6'-N1'	-2.12	120.29	123.82
6	B	1204	TPP	N1'-C2'-N3'	-2.12	121.90	125.54
6	E	1204	TPP	N4'-C4'-N3'	2.11	120.02	117.03
3	C	1204	TDL	C2'-N3'-C4'	2.07	121.31	118.08
6	B	1204	TPP	C2'-N3'-C4'	2.01	121.22	118.08
6	E	1204	TPP	N1'-C2'-N3'	-2.01	122.08	125.54

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1204	TDL	C4-C5-C6-C7
6	E	1204	TPP	C4-C5-C6-C7
3	A	1204	TDL	C7-O7-PA-O1A
3	C	1204	TDL	C4-C5-C6-C7
3	D	1204	TDL	PA-O3A-PB-O1B
3	A	1204	TDL	PA-O3A-PB-O1B
3	F	1204	TDL	PB-O3A-PA-O7
3	D	1204	TDL	PA-O3A-PB-O3B
3	A	1204	TDL	C4-C5-C6-C7
3	F	1204	TDL	C4-C5-C6-C7
3	F	1204	TDL	PA-O3A-PB-O1B
3	C	1204	TDL	PB-O3A-PA-O7
6	B	1204	TPP	PA-O3A-PB-O3B
6	B	1204	TPP	C7-O7-PA-O3A
3	D	1204	TDL	C7-O7-PA-O1A
6	E	1204	TPP	C7-O7-PA-O1A
3	F	1204	TDL	C7-O7-PA-O1A
6	B	1204	TPP	C4-C5-C6-C7

There are no ring outliers.

7 monomers are involved in 31 short contacts:

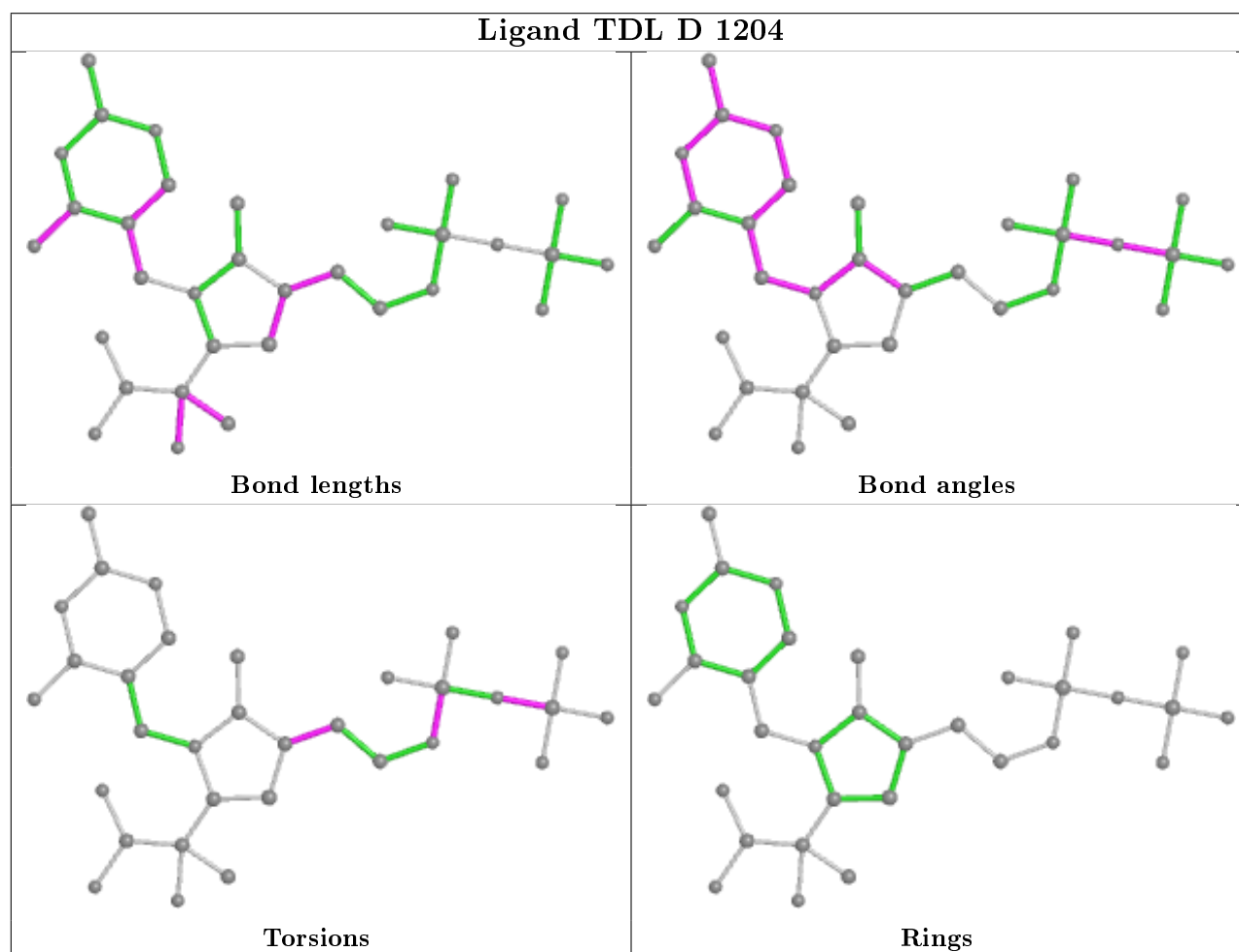
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1207	SO4	3	0
3	D	1204	TDL	6	0
3	A	1204	TDL	6	0
2	B	1202	SF4	1	0
3	C	1204	TDL	8	0
2	B	1201	SF4	1	0

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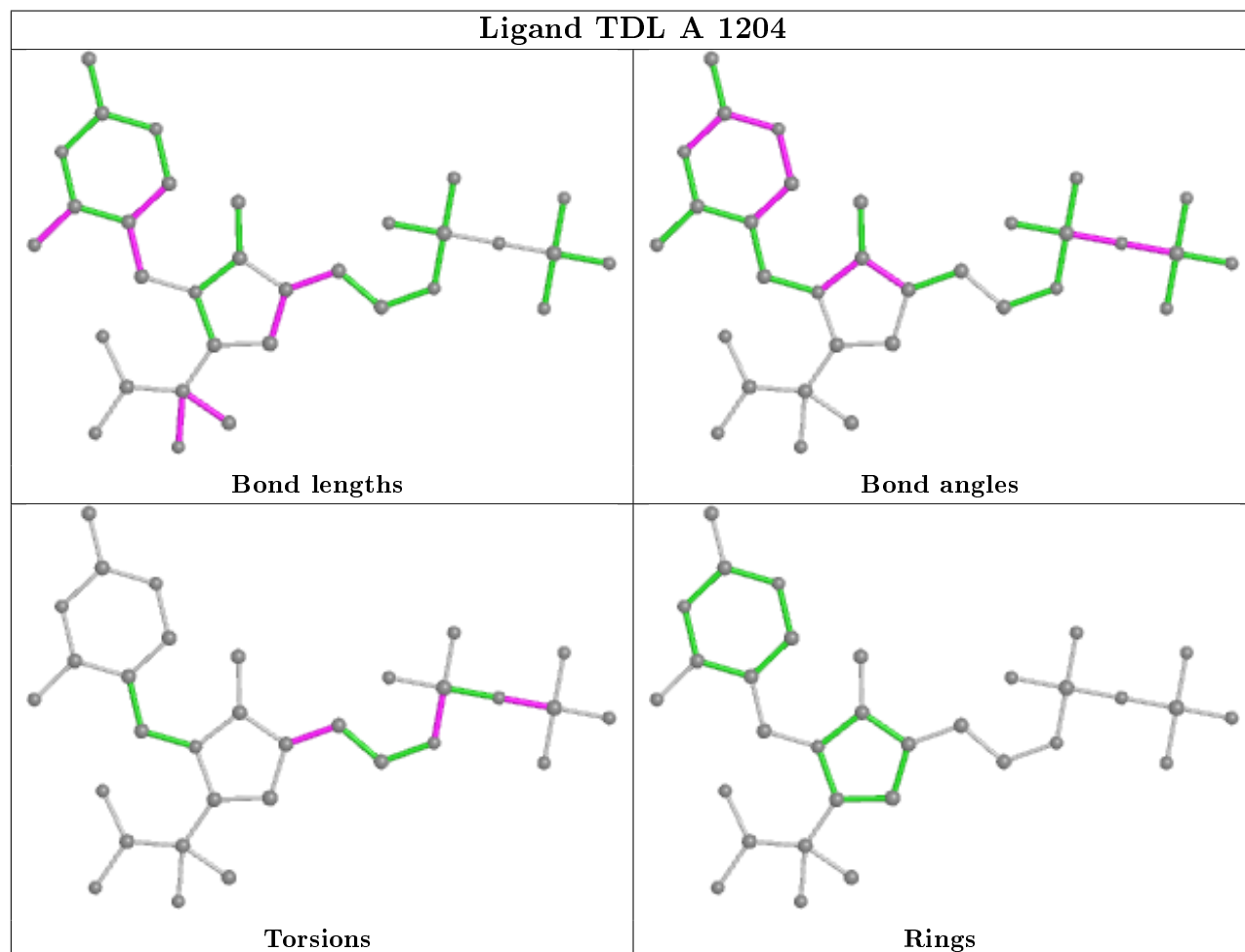
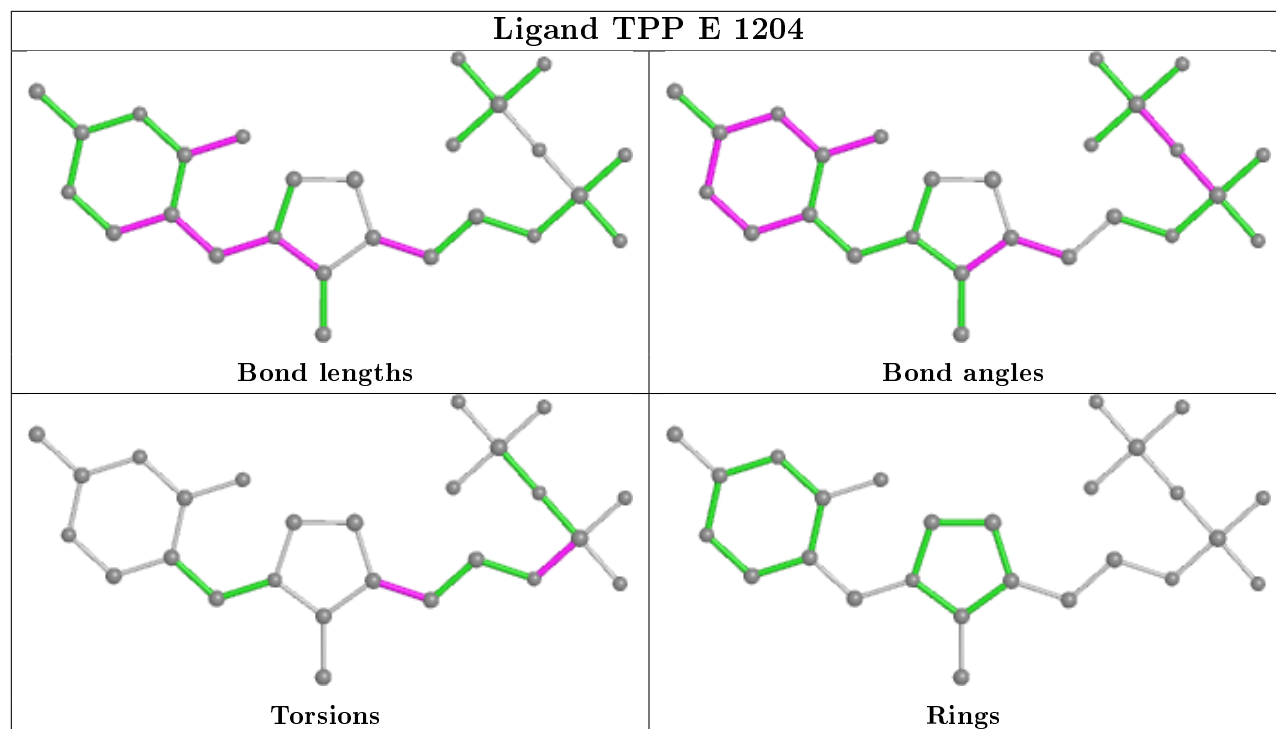
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1204	TDL	6	0

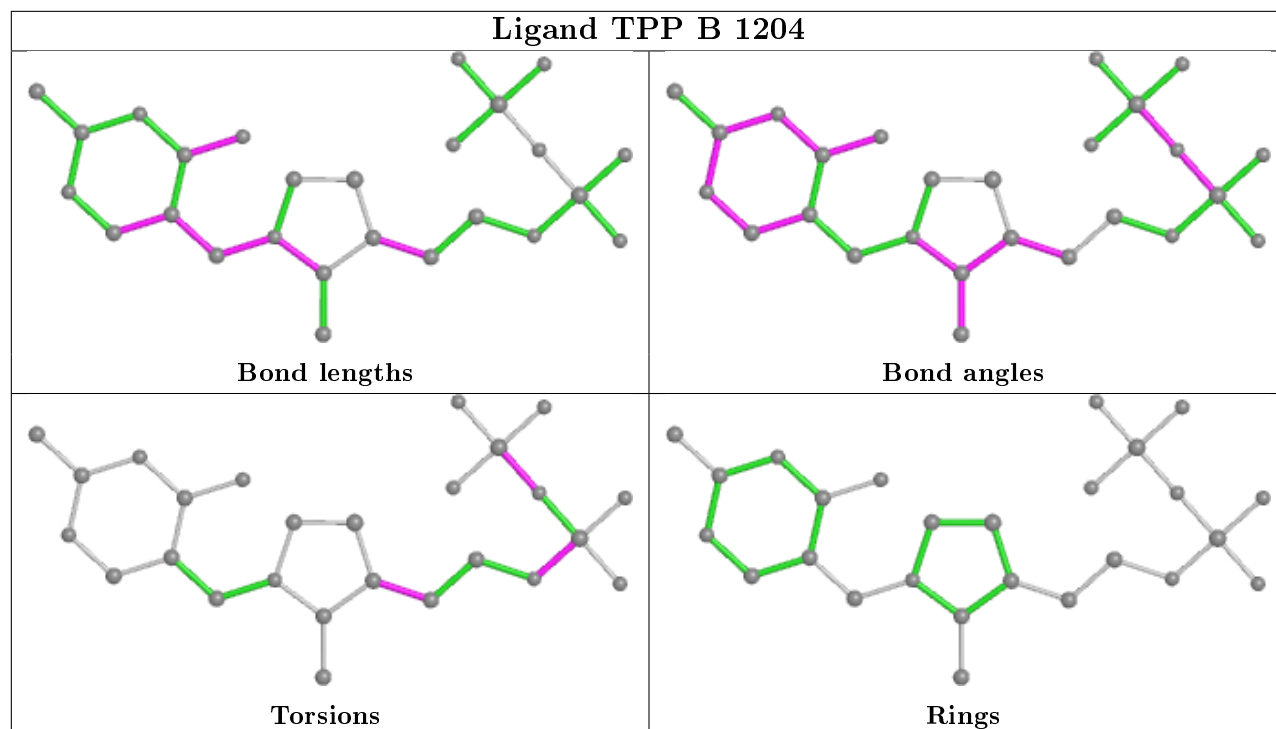
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



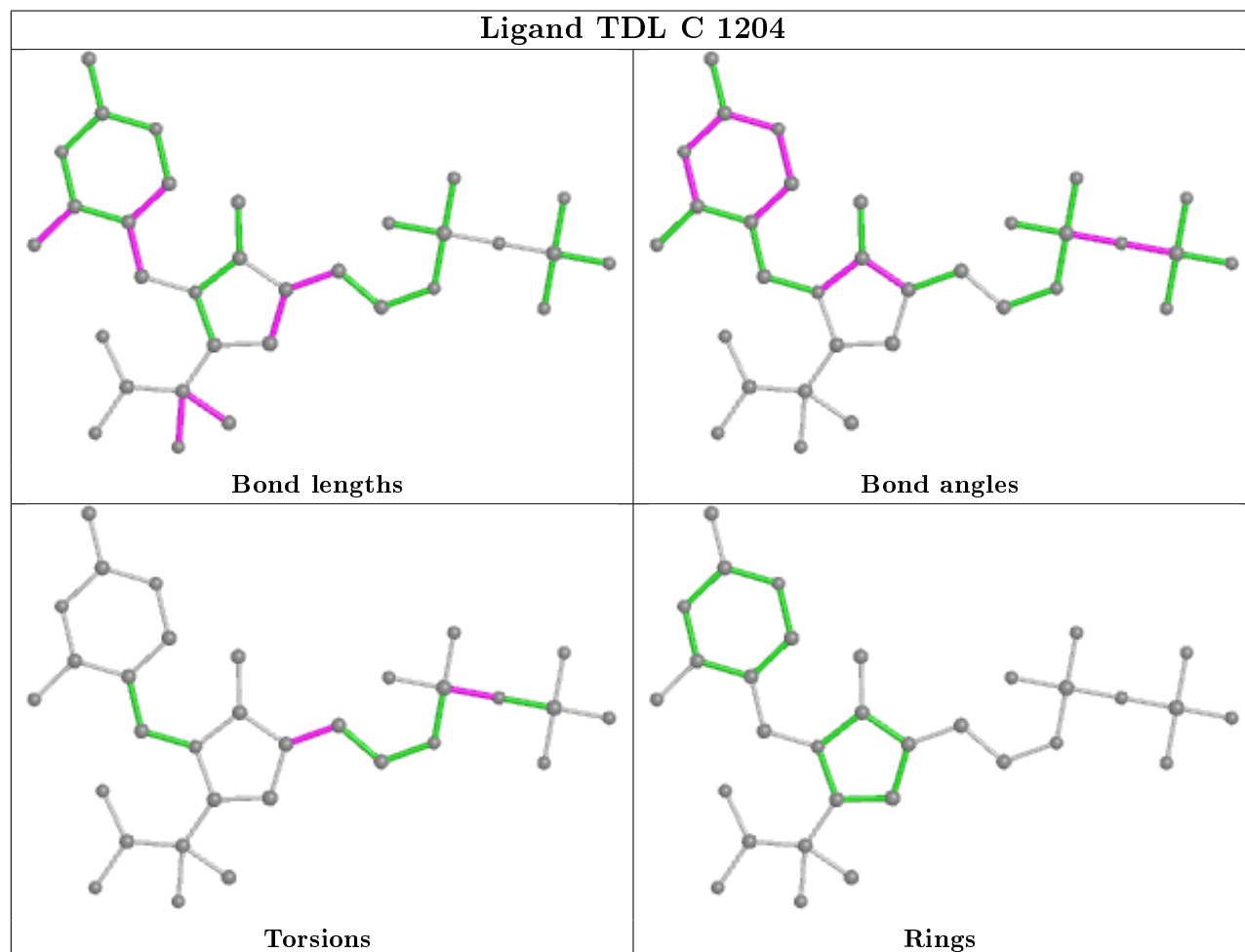


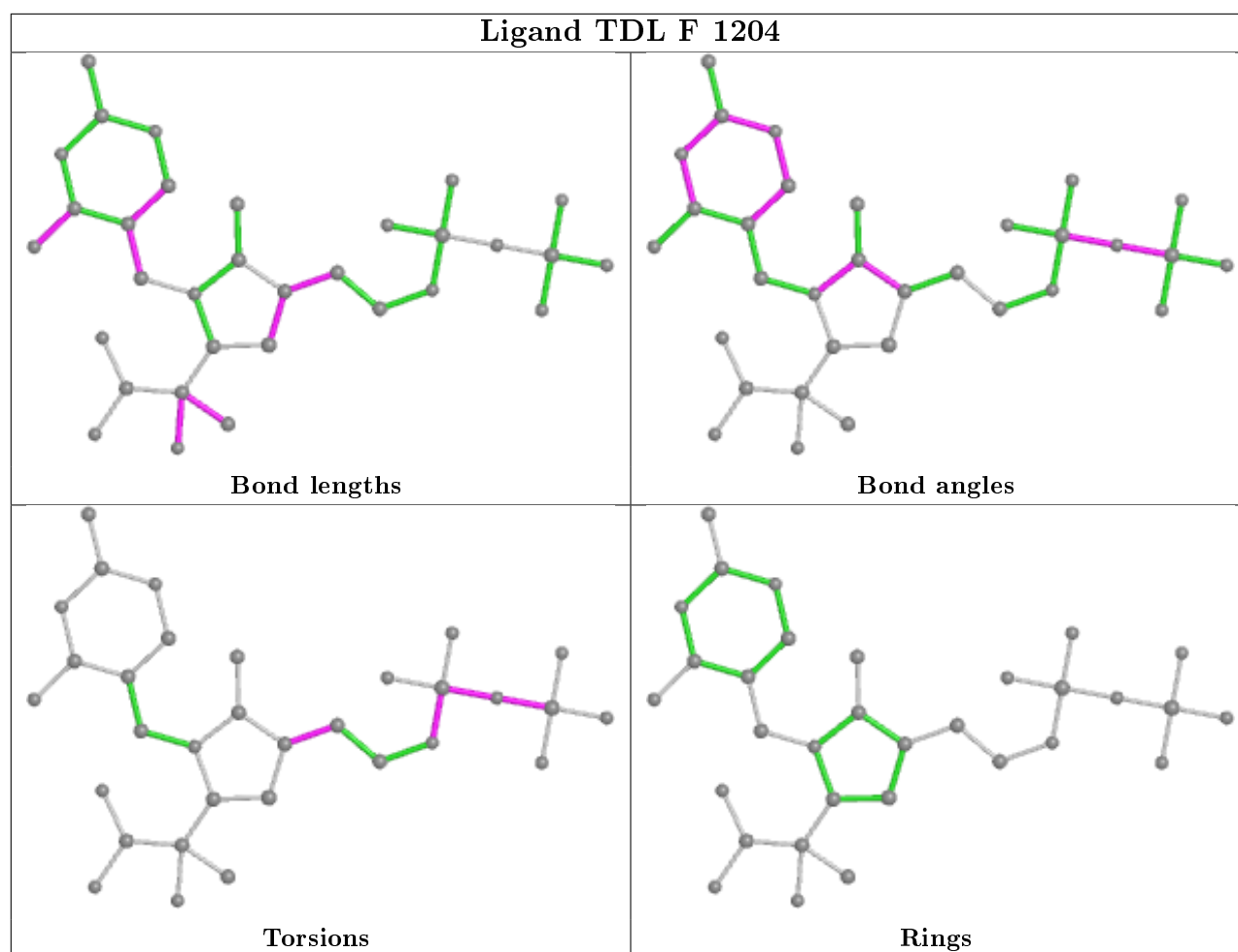


## Ligand TPP B 1204



## Ligand TDL C 1204





## 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	1164/1171 (99%)	-0.19	25 (2%)	63	34	27, 65, 117, 152	0
1	B	1164/1171 (99%)	-0.12	41 (3%)	44	18	24, 72, 127, 166	0
1	C	1161/1171 (99%)	-0.16	29 (2%)	57	29	26, 69, 116, 154	0
1	D	1159/1171 (98%)	-0.16	8 (0%)	87	69	33, 75, 124, 171	0
1	E	1157/1171 (98%)	0.01	46 (3%)	38	15	31, 75, 127, 158	0
1	F	1155/1171 (98%)	-0.07	12 (1%)	82	59	40, 79, 131, 187	0
All	All	6960/7026 (99%)	-0.12	161 (2%)	60	31	24, 73, 125, 187	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1128	ASP	4.9
1	B	686	CYS	4.7
1	E	716	GLU	4.2
1	B	910	TRP	4.0
1	E	684	GLU	3.9
1	F	561	THR	3.9
1	B	1125	SER	3.9
1	B	726	LYS	3.9
1	A	1127	ARG	3.8
1	E	782	PRO	3.7
1	F	188	ASP	3.7
1	A	1049	SER	3.6
1	E	780	GLN	3.6
1	E	594	ILE	3.5
1	E	891	ILE	3.5
1	A	1109	GLN	3.5
1	B	1119	TYR	3.4
1	E	617	SER	3.4
1	E	795	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	708	PRO	3.4
1	E	894	ALA	3.4
1	B	589	LYS	3.3
1	E	855	GLN	3.3
1	A	942	VAL	3.3
1	B	898	PRO	3.3
1	E	717	THR	3.2
1	B	679	PRO	3.2
1	F	598	ASN	3.2
1	A	1136	TYR	3.2
1	B	902	ALA	3.2
1	F	573	ASP	3.1
1	A	1122	PRO	3.1
1	A	1128	ASP	3.1
1	B	710	ASP	3.1
1	E	784	VAL	3.1
1	C	895	LEU	3.1
1	E	713	GLY	3.0
1	E	932	PRO	3.0
1	C	623	ASP	3.0
1	C	949	ILE	3.0
1	B	733	PHE	3.0
1	E	907	CYS	3.0
1	B	1151	PHE	2.9
1	A	1121	THR	2.9
1	B	1126	PHE	2.9
1	C	945	LEU	2.9
1	B	1147	ALA	2.9
1	B	1050	HIS	2.9
1	B	1132	GLY	2.9
1	E	715	PRO	2.8
1	B	728	ALA	2.8
1	B	1051	SER	2.8
1	F	51	GLY	2.8
1	C	1123	THR	2.8
1	C	526	MET	2.8
1	C	1125	SER	2.8
1	A	716	GLU	2.8
1	E	730	GLY	2.8
1	E	1106	GLN	2.8
1	E	735	ILE	2.8
1	A	1131	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	590	LYS	2.8
1	B	1109	GLN	2.7
1	B	1113	ASN	2.7
1	E	787	ASN	2.7
1	A	919	ARG	2.7
1	C	784	VAL	2.7
1	C	620	ASP	2.6
1	D	624	GLU	2.6
1	C	896	GLU	2.6
1	C	787	ASN	2.6
1	A	589	LYS	2.6
1	D	630	THR	2.6
1	E	1109	GLN	2.6
1	E	935	ILE	2.6
1	B	894	ALA	2.6
1	E	620	ASP	2.6
1	C	527	LYS	2.5
1	B	783	GLU	2.5
1	E	899	VAL	2.5
1	B	794	LYS	2.5
1	B	906	ALA	2.5
1	A	790	PRO	2.5
1	E	519	ASP	2.5
1	B	1159	LYS	2.5
1	F	716	GLU	2.5
1	E	682	GLN	2.5
1	B	1123	THR	2.5
1	A	1095	ALA	2.5
1	C	617	SER	2.5
1	E	518	MET	2.4
1	B	1150	LEU	2.4
1	C	711	LEU	2.4
1	E	936	SER	2.4
1	E	1164	GLN	2.4
1	E	1012	GLY	2.4
1	E	720	THR	2.4
1	E	728	ALA	2.4
1	E	678	ILE	2.4
1	A	1111	GLY	2.4
1	A	1113	ASN	2.4
1	B	1163	GLU	2.4
1	B	684	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	187	GLU	2.4
1	D	573	ASP	2.4
1	B	976	GLY	2.4
1	C	946	LEU	2.4
1	B	716	GLU	2.3
1	B	1094	GLU	2.3
1	B	812	CYS	2.3
1	E	931	LEU	2.3
1	E	598	ASN	2.3
1	D	598	ASN	2.3
1	C	709	ALA	2.3
1	D	623	ASP	2.3
1	C	757	LYS	2.3
1	C	942	VAL	2.3
1	C	710	ASP	2.3
1	E	710	ASP	2.2
1	B	1140	LYS	2.2
1	F	942	VAL	2.2
1	A	949	ILE	2.2
1	B	1124	ALA	2.2
1	E	680	GLN	2.2
1	F	711	LEU	2.2
1	C	1120	LYS	2.2
1	C	933	GLY	2.2
1	E	714	ALA	2.2
1	A	946	LEU	2.2
1	B	1054	MET	2.2
1	A	1130	LEU	2.2
1	E	1150	LEU	2.2
1	A	1163	GLU	2.2
1	C	530	ILE	2.2
1	B	1111	GLY	2.2
1	C	618	TRP	2.2
1	B	1118	ASP	2.2
1	E	1054	MET	2.2
1	A	974	GLY	2.2
1	C	765	GLU	2.1
1	A	1125	SER	2.1
1	C	717	THR	2.1
1	A	941	GLU	2.1
1	E	589	LYS	2.1
1	B	968	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	596	ASN	2.1
1	C	937	GLN	2.1
1	D	561	THR	2.1
1	C	902	ALA	2.1
1	F	1153	LYS	2.1
1	C	712	ALA	2.1
1	D	629	VAL	2.1
1	A	686	CYS	2.1
1	E	520	SER	2.1
1	F	514	SER	2.1
1	E	621	ALA	2.0
1	D	570	ILE	2.0
1	A	1100	LEU	2.0
1	C	716	GLU	2.0
1	E	511	SER	2.0
1	E	781	LEU	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 carbohydrates 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	F	1206	5/5	0.90	0.17	106,106,108,108	0
4	MG	E	1205	1/1	0.90	0.13	26,26,26,26	0
5	SO4	C	1206	5/5	0.91	0.24	89,89,92,94	0
5	SO4	B	1206	5/5	0.92	0.18	84,91,92,94	0
5	SO4	A	1206	5/5	0.94	0.13	83,83,84,86	0
5	SO4	D	1206	5/5	0.94	0.16	107,107,108,108	0
5	SO4	B	1207	5/5	0.94	0.23	71,77,78,80	0

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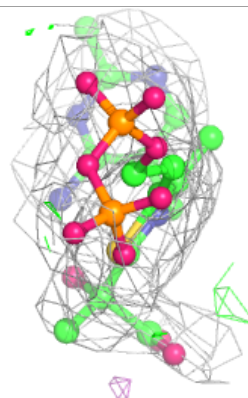
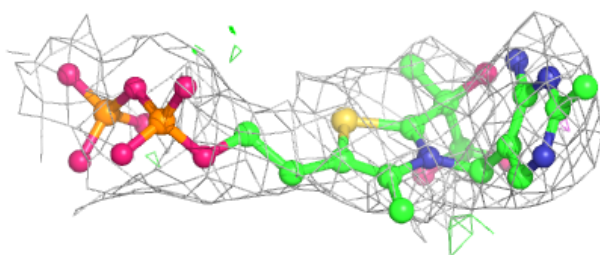
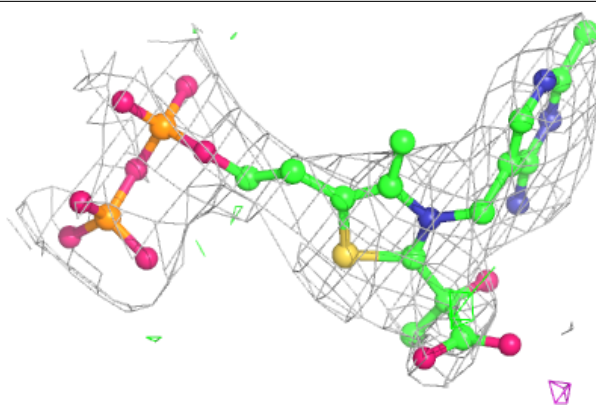
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	E	1206	5/5	0.95	0.19	78,85,87,87	0
4	MG	C	1205	1/1	0.96	0.09	26,26,26,26	0
3	TDL	C	1204	32/32	0.96	0.22	41,54,70,76	3
6	TPP	E	1204	26/26	0.96	0.21	51,66,75,78	0
3	TDL	F	1204	32/32	0.96	0.26	52,61,74,79	0
4	MG	D	1205	1/1	0.96	0.12	22,22,22,22	0
3	TDL	A	1204	32/32	0.96	0.29	56,61,80,85	0
6	TPP	B	1204	26/26	0.97	0.26	58,68,78,88	0
2	SF4	B	1202	8/8	0.97	0.12	77,109,137,188	0
2	SF4	B	1201	8/8	0.97	0.08	93,121,175,180	0
2	SF4	C	1203	8/8	0.98	0.16	44,64,73,89	0
4	MG	A	1205	1/1	0.98	0.20	32,32,32,32	0
4	MG	B	1205	1/1	0.98	0.18	39,39,39,39	0
3	TDL	D	1204	32/32	0.98	0.25	44,62,80,84	0
2	SF4	A	1202	8/8	0.98	0.12	60,66,68,72	0
2	SF4	F	1201	8/8	0.98	0.12	80,84,86,97	0
2	SF4	E	1202	8/8	0.98	0.12	85,108,144,175	0
2	SF4	B	1203	8/8	0.98	0.13	57,71,79,85	0
4	MG	F	1205	1/1	0.98	0.16	21,21,21,21	0
2	SF4	A	1201	8/8	0.98	0.09	83,105,118,147	0
2	SF4	D	1201	8/8	0.98	0.14	71,75,97,129	0
2	SF4	A	1203	8/8	0.99	0.13	47,71,78,79	0
2	SF4	D	1202	8/8	0.99	0.14	63,64,70,83	0
2	SF4	C	1201	8/8	0.99	0.08	70,83,92,104	0
2	SF4	D	1203	8/8	0.99	0.19	49,50,52,74	0
2	SF4	F	1203	8/8	0.99	0.19	53,55,65,67	0
2	SF4	E	1201	8/8	0.99	0.09	92,125,144,172	0
2	SF4	F	1202	8/8	0.99	0.15	64,67,72,102	0
2	SF4	C	1202	8/8	0.99	0.14	64,76,92,97	0
2	SF4	E	1203	8/8	0.99	0.14	59,81,104,107	0

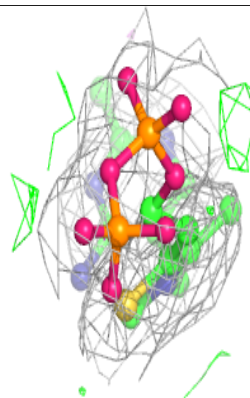
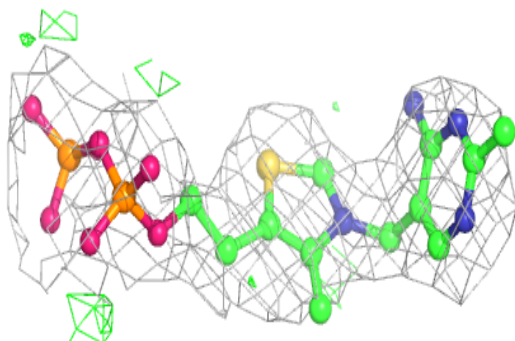
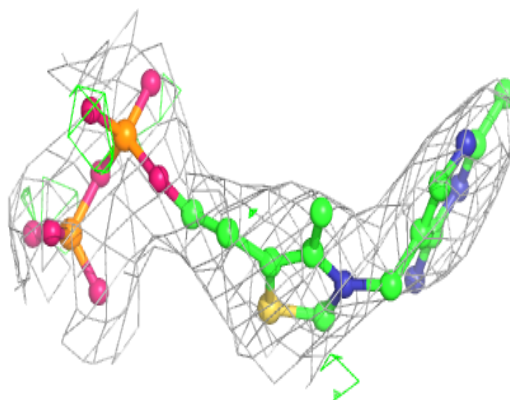
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TDL 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)

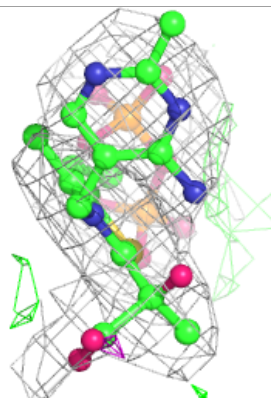
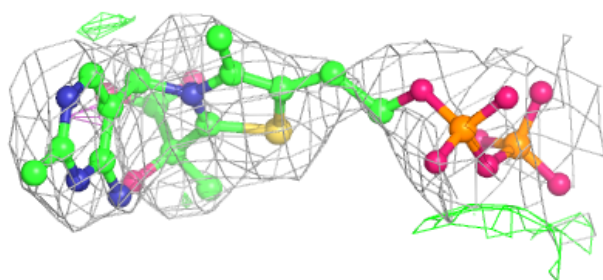
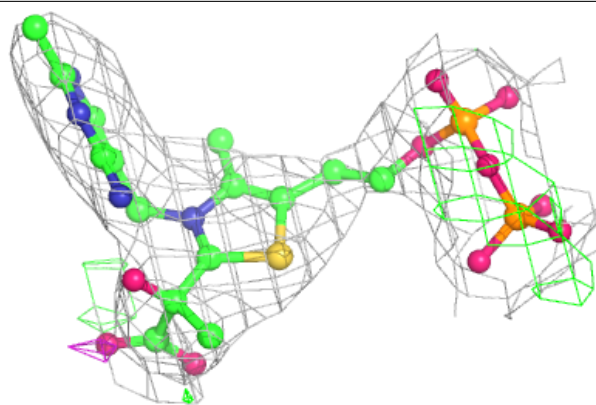
**Electron density around TPP E 1204:**

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

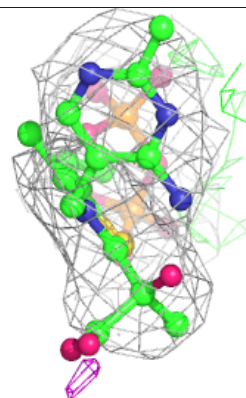
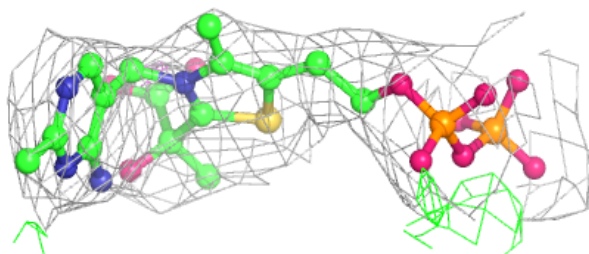
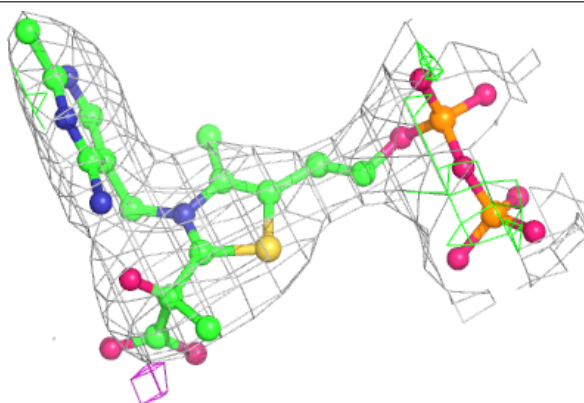


**Electron density around TDL F 1204:**

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

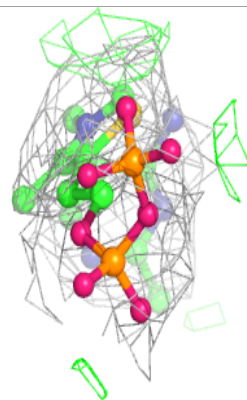
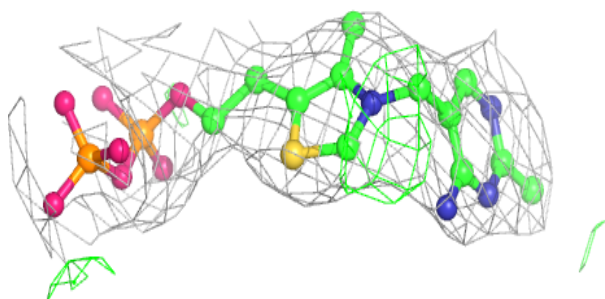
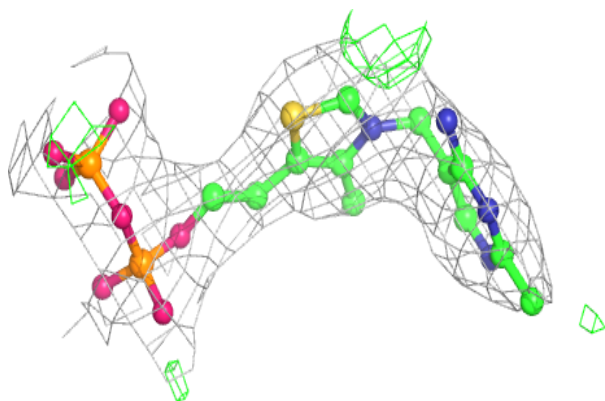
**Electron density around TDL A 1204:**

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

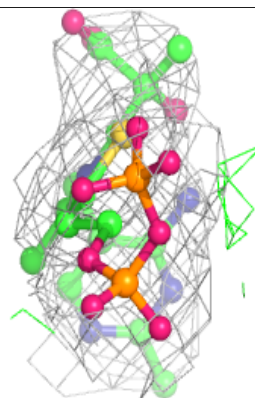
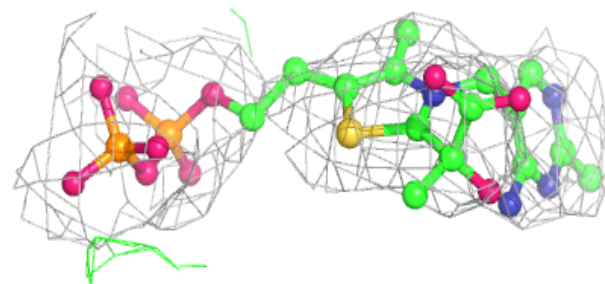
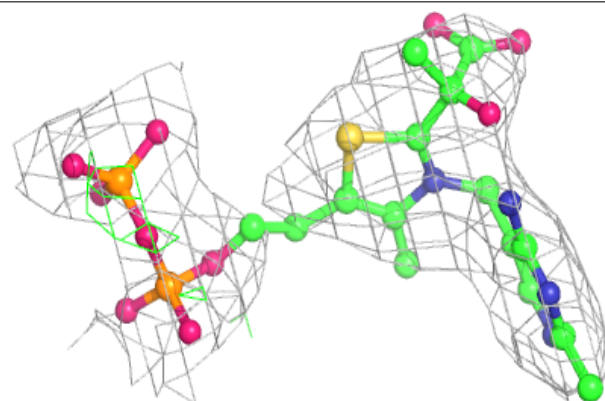


**Electron density around TPP B 1204:**

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

**Electron density around TDL 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.