



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 10:06 PM EDT

PDB ID : 6CIP
Title : Pyruvate:ferredoxin oxidoreductase from Moorella thermoacetica with acetyl-TPP bound
Authors : Chen, P.Y.-T.; Drennan, C.L.
Deposited on : 2018-02-24
Resolution : 3.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

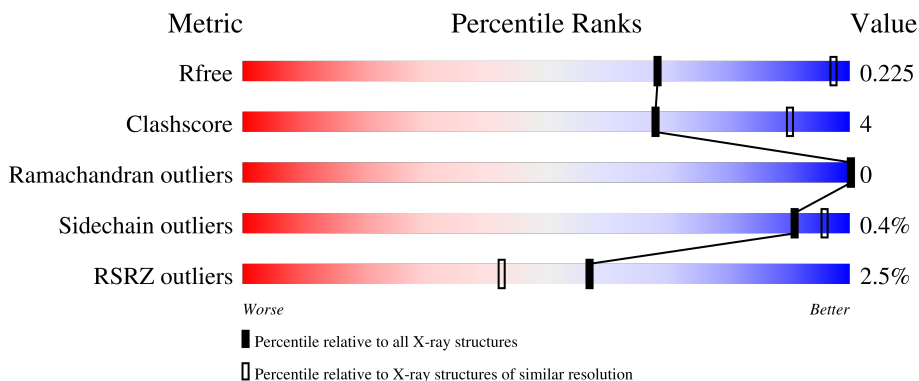
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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.



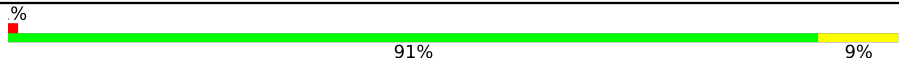
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1171	
1	B	1171	
1	C	1171	
1	D	1171	
1	E	1171	

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Mol	Chain	Length	Quality of chain
1	F	1171	 A horizontal bar chart representing the quality of the chain. The bar is primarily green, indicating a high quality score of 91%. A small yellow segment at the end indicates a lower quality score of 9%. The percentage values '91%' and '9%' are printed below the bar. A small red square is visible at the start of the bar.

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](#)

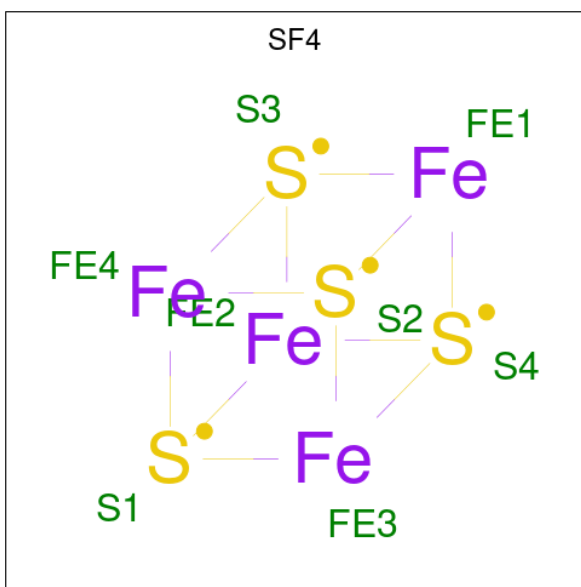
There are 6 unique types of molecules in this entry. The entry contains 52992 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

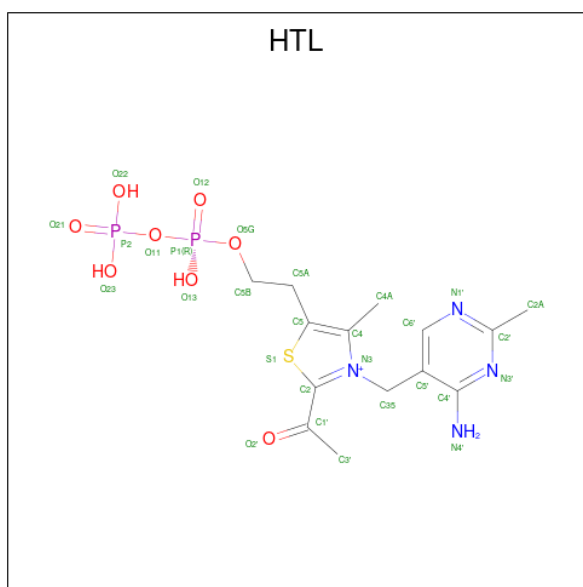
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1165	Total 8779	C 5586	N 1485	O 1665	S 43	0	0	0
1	B	1165	Total 8728	C 5555	N 1476	O 1654	S 43	0	0	0
1	C	1163	Total 8763	C 5576	N 1481	O 1662	S 44	0	0	0
1	D	1164	Total 8767	C 5585	N 1483	O 1655	S 44	0	0	0
1	E	1164	Total 8788	C 5592	N 1486	O 1666	S 44	0	0	0
1	F	1169	Total 8781	C 5589	N 1486	O 1662	S 44	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$) (labeled as "Ligand of Interest" by depositor).

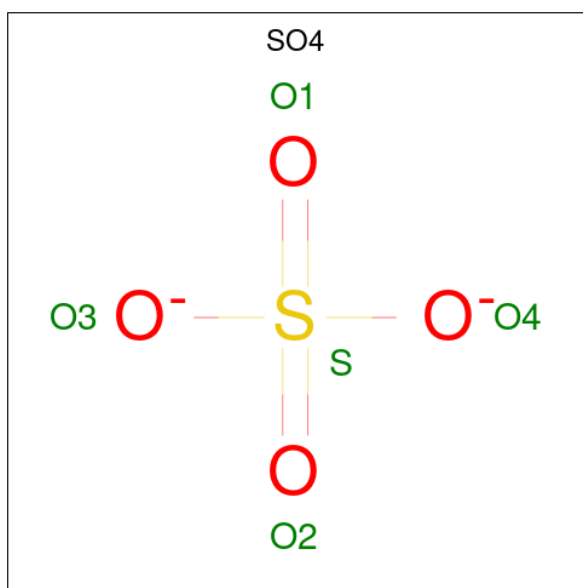


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
3	E	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
3	F	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	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	D	1	Total	Mg	0	0
			1	1		
4	E	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: O₄S).



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	4	Total	O	0	0
			4	4		
6	B	3	Total	O	0	0
			3	3		
6	C	4	Total	O	0	0
			4	4		
6	D	3	Total	O	0	0
			3	3		

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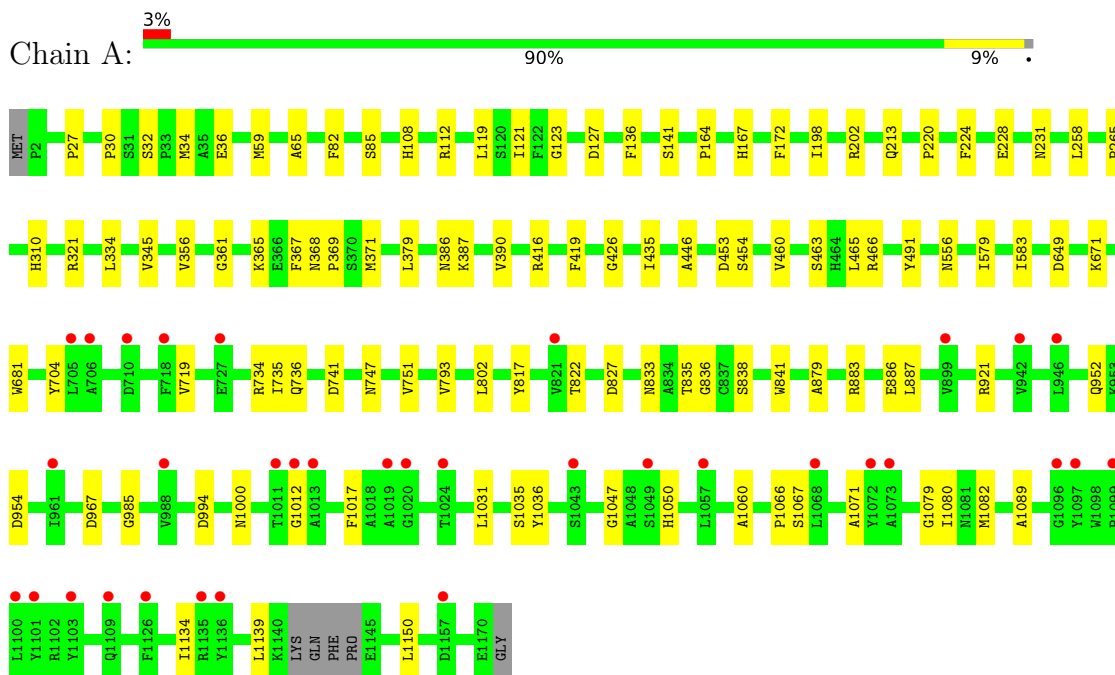
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	8	Total O 8 8	0	0
6	F	5	Total O 5 5	0	0

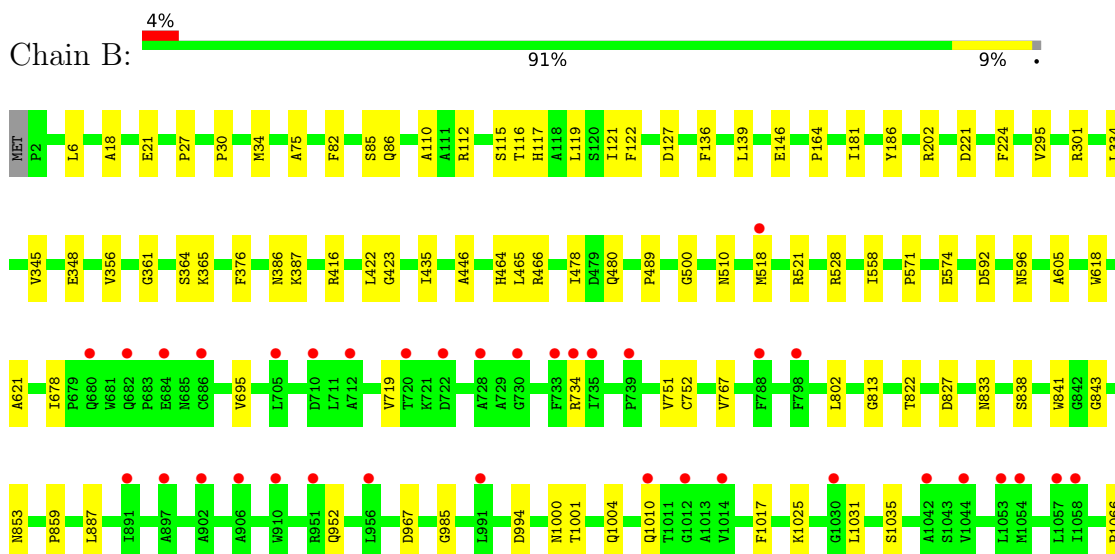
3 Residue-property plots

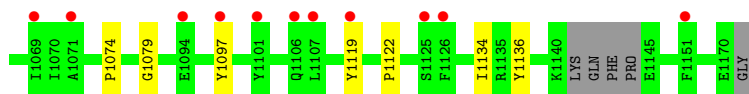
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

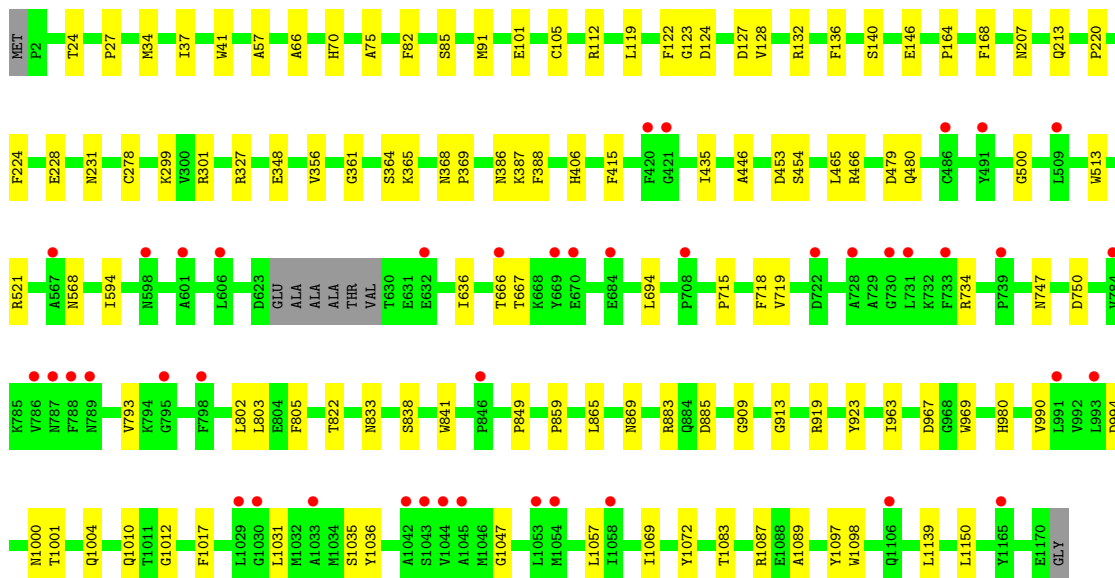
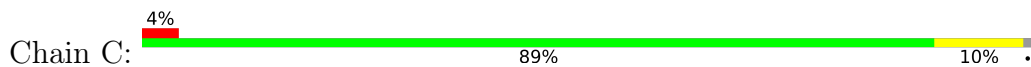


• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

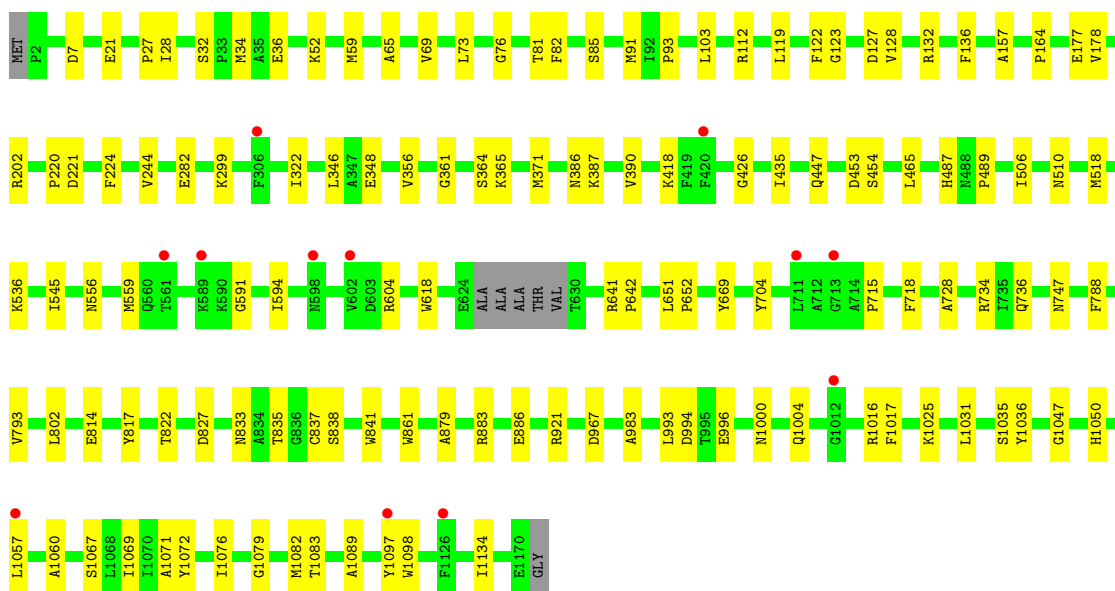
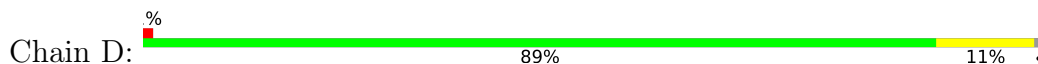




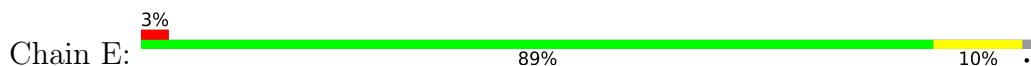
● Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

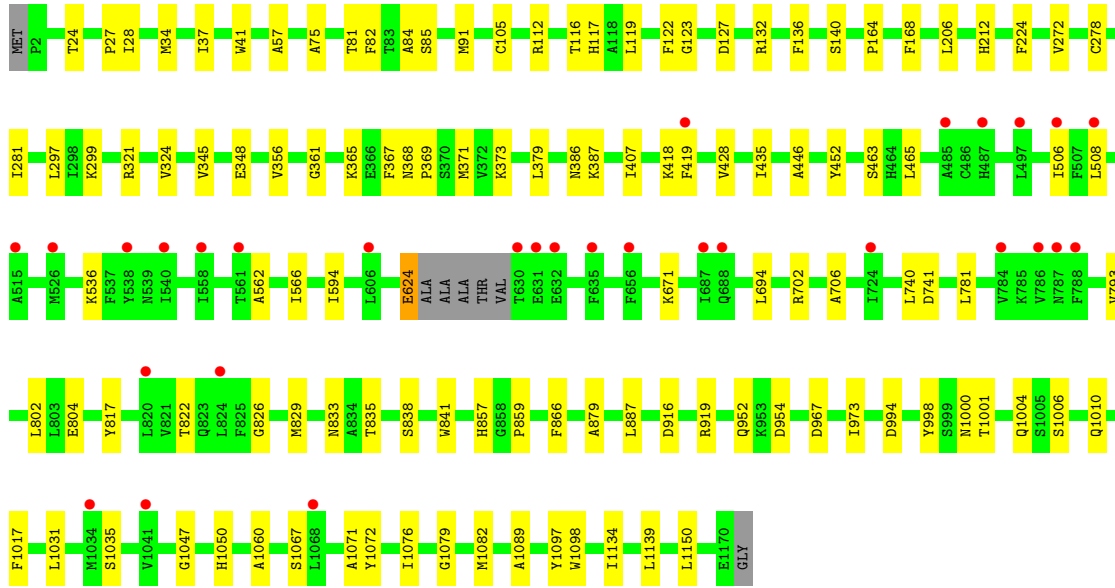


● Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

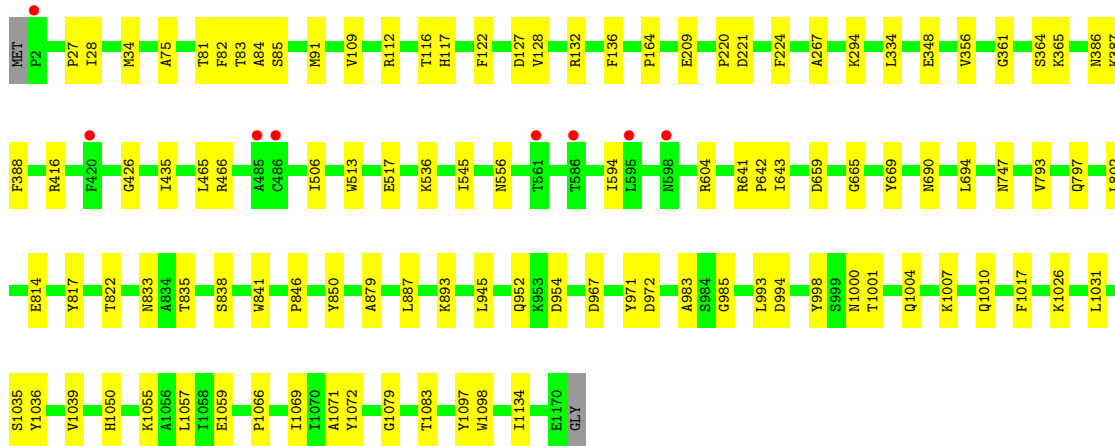
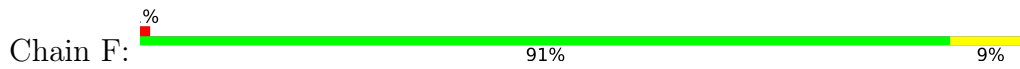


● Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





● 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, α , β , γ	342.00Å 108.26Å 240.44Å 90.00° 109.32° 90.00°	Depositor
Resolution (Å)	97.45 – 3.19 97.45 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.7 (97.45-3.19) 95.7 (97.45-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.187 , 0.225 0.188 , 0.225	Depositor DCC
R_{free} test set	6633 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtrriage
Anisotropy	0.574	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52992	wwPDB-VP
Average B, all atoms (Å ²)	103.0	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 60.84 % 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 1.4327e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, SO4, HTL

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	0.26	0/8971	0.45	0/12194
1	B	0.26	0/8920	0.45	0/12134
1	C	0.27	0/8956	0.45	0/12176
1	D	0.26	0/8961	0.46	0/12180
1	E	0.27	0/8981	0.45	0/12205
1	F	0.26	0/8975	0.45	0/12205
All	All	0.26	0/53764	0.45	0/73094

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

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	8779	0	8547	68	0
1	B	8728	0	8454	70	0
1	C	8763	0	8523	74	0
1	D	8767	0	8542	79	0
1	E	8788	0	8568	71	0
1	F	8781	0	8535	67	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	1	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	29	0	18	5	0
3	B	29	0	18	3	0
3	C	29	0	18	3	0
3	D	29	0	18	5	0
3	E	29	0	18	3	0
3	F	29	0	18	5	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	4	0	0	0	0
6	B	3	0	0	0	0
6	C	4	0	0	1	0
6	D	3	0	0	0	0
6	E	8	0	0	0	0
6	F	5	0	0	0	0
All	All	52992	0	51277	399	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 (399) 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:E:34:MET:HE3	1:E:82:PHE:HB3	1.54	0.88
1:C:34:MET:HE3	1:C:82:PHE:HB3	1.54	0.88
1:B:521:ARG:NH1	5:B:1207:SO4:S	2.52	0.82
1:B:521:ARG:NH1	5:B:1207:SO4:O2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:MET:HE3	1:B:82:PHE:HB3	1.61	0.80
1:D:435:ILE:HD11	1:D:465:LEU:HD22	1.65	0.77
1:E:802:LEU:HB2	1:E:822:THR:HB	1.66	0.76
1:A:34:MET:HE3	1:A:82:PHE:HB3	1.66	0.76
1:F:435:ILE:HD11	1:F:465:LEU:HD22	1.67	0.76
1:F:34:MET:HE3	1:F:82:PHE:HB3	1.68	0.76
1:F:27:PRO:HB3	1:F:1017:PHE:HE2	1.52	0.73
1:D:1057:LEU:HD23	1:D:1069:ILE:HD13	1.69	0.73
1:B:521:ARG:NH1	5:B:1207:SO4:O3	2.24	0.71
1:D:793:VAL:HG21	1:D:1050:HIS:HB3	1.73	0.69
1:C:435:ILE:HD11	1:C:465:LEU:HD22	1.73	0.69
1:B:592:ASP:O	1:B:596:ASN:ND2	2.26	0.69
1:E:112:ARG:HH21	1:E:119:LEU:HD11	1.57	0.69
1:F:802:LEU:HB2	1:F:822:THR:HB	1.76	0.68
1:A:435:ILE:HD11	1:A:465:LEU:HD22	1.76	0.67
1:B:435:ILE:HD11	1:B:465:LEU:HD22	1.77	0.67
1:E:435:ILE:HD11	1:E:465:LEU:HD22	1.77	0.66
1:D:802:LEU:HB2	1:D:822:THR:HB	1.76	0.66
1:D:27:PRO:HB3	1:D:1017:PHE:HE2	1.61	0.65
1:C:913:GLY:HA3	1:C:919:ARG:HE	1.63	0.63
1:C:750:ASP:OD1	1:C:1087:ARG:NH2	2.31	0.63
1:D:81:THR:HG21	1:D:91:MET:HE1	1.80	0.62
1:C:387:LYS:NZ	1:D:348:GLU:OE1	2.28	0.62
1:E:671:LYS:NZ	1:E:741:ASP:OD2	2.24	0.62
1:B:827:ASP:OD1	1:B:853:ASN:ND2	2.32	0.62
1:E:967:ASP:HB3	1:E:994:ASP:HA	1.81	0.61
1:F:1057:LEU:HD23	1:F:1069:ILE:HD13	1.82	0.61
1:A:827:ASP:OD2	1:A:921:ARG:NH1	2.28	0.61
1:A:802:LEU:HB2	1:A:822:THR:HB	1.83	0.61
1:C:348:GLU:OE1	1:D:387:LYS:NZ	2.33	0.60
1:E:702:ARG:NH2	1:E:804:GLU:OE1	2.30	0.60
1:F:967:ASP:HB3	1:F:994:ASP:HA	1.83	0.59
1:A:1012:GLY:HA2	1:A:1150:LEU:HD13	1.84	0.59
1:D:967:ASP:HB3	1:D:994:ASP:HA	1.83	0.59
1:D:883:ARG:NH2	1:D:886:GLU:OE2	2.30	0.58
1:E:1079:GLY:HA3	1:E:1134:ILE:HB	1.85	0.58
1:A:1036:TYR:O	1:B:1025:LYS:NZ	2.34	0.57
1:B:356:VAL:HG13	1:B:386:ASN:HA	1.86	0.57
1:B:27:PRO:HB3	1:B:1017:PHE:HE2	1.69	0.57
3:B:1204:HTL:H4'2	3:B:1204:HTL:C1'	2.17	0.57
1:D:835:THR:HG22	3:D:1204:HTL:H3'2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:706:ALA:HB2	1:E:781:LEU:HD21	1.87	0.57
1:F:893:LYS:HB3	1:F:945:LEU:HD11	1.86	0.57
1:A:967:ASP:HB3	1:A:994:ASP:HA	1.87	0.57
1:C:1031:LEU:HD23	1:D:1035:SER:HB2	1.87	0.57
3:C:1204:HTL:H4'2	3:C:1204:HTL:C1'	2.18	0.57
1:F:27:PRO:HB3	1:F:1017:PHE:CE2	2.38	0.57
1:C:356:VAL:HG13	1:C:386:ASN:HA	1.87	0.56
1:E:112:ARG:NH2	1:E:119:LEU:HD11	2.19	0.56
1:A:426:GLY:HA3	1:A:556:ASN:HB3	1.88	0.56
1:F:506:ILE:HG12	1:F:536:LYS:HE3	1.87	0.56
3:A:1204:HTL:C1'	3:A:1204:HTL:H4'2	2.18	0.56
1:F:81:THR:HG21	1:F:91:MET:HE1	1.88	0.56
3:D:1204:HTL:H4'2	3:D:1204:HTL:C1'	2.19	0.56
1:B:1000:ASN:HD22	3:B:1204:HTL:H3'3	1.71	0.55
1:C:66:ALA:HB2	1:C:91:MET:HE2	1.88	0.55
1:C:122:PHE:CE2	1:D:220:PRO:HD3	2.41	0.55
1:B:838:SER:HA	1:B:841:TRP:CE2	2.41	0.55
1:A:838:SER:HA	1:A:841:TRP:CE2	2.41	0.55
1:A:1060:ALA:HB1	1:A:1067:SER:HB3	1.89	0.54
1:A:671:LYS:NZ	1:A:741:ASP:OD2	2.29	0.54
1:B:21:GLU:OE1	1:B:202:ARG:NH2	2.40	0.54
1:D:747:ASN:ND2	1:D:1083:THR:O	2.39	0.54
1:A:361:GLY:HA2	1:A:365:LYS:HB3	1.90	0.54
1:E:1076:ILE:HG22	1:E:1082:MET:HG3	1.89	0.54
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	1.89	0.54
1:C:513:TRP:CD2	1:C:521:ARG:HG2	2.42	0.54
1:D:817:TYR:CZ	1:D:1071:ALA:HB1	2.43	0.54
1:A:1000:ASN:ND2	3:A:1204:HTL:H3'3	2.23	0.53
1:B:146:GLU:OE2	1:B:301:ARG:NH2	2.41	0.53
1:D:1060:ALA:HB1	1:D:1067:SER:HB3	1.91	0.53
1:E:508:LEU:HD22	1:E:566:ILE:HD11	1.90	0.53
1:C:207:ASN:N	6:C:1301:HOH:O	2.41	0.53
1:E:1060:ALA:HB1	1:E:1067:SER:HB3	1.91	0.53
1:E:1072:TYR:HB2	1:E:1098:TRP:CE2	2.44	0.53
1:F:793:VAL:HG21	1:F:1050:HIS:HB3	1.91	0.53
1:D:426:GLY:HA3	1:D:556:ASN:HB3	1.91	0.53
1:B:528:ARG:NH1	1:B:621:ALA:O	2.40	0.53
1:E:802:LEU:HD13	1:E:859:PRO:HD3	1.91	0.53
1:A:85:SER:HA	1:A:127:ASP:HB3	1.91	0.52
1:B:1000:ASN:ND2	3:B:1204:HTL:H3'3	2.24	0.52
1:E:140:SER:HB2	1:E:168:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:SER:HA	1:B:127:ASP:HB3	1.90	0.52
3:F:1204:HTL:C1'	3:F:1204:HTL:H4'2	2.22	0.52
1:A:220:PRO:HD3	1:B:122:PHE:CE2	2.45	0.52
1:A:887:LEU:HD13	1:A:952:GLN:HB2	1.91	0.52
1:D:356:VAL:HG13	1:D:386:ASN:HA	1.91	0.52
1:F:1079:GLY:HA3	1:F:1134:ILE:HB	1.90	0.52
1:C:747:ASN:ND2	1:C:1083:THR:O	2.43	0.52
1:A:356:VAL:HG13	1:A:386:ASN:HA	1.91	0.52
1:E:419:PHE:HB2	1:E:463:SER:HB2	1.91	0.52
1:A:112:ARG:HH21	1:A:119:LEU:HD11	1.75	0.51
1:B:422:LEU:HD22	1:B:423:GLY:H	1.76	0.51
1:E:356:VAL:HG13	1:E:386:ASN:HA	1.92	0.51
1:A:387:LYS:NZ	1:B:348:GLU:OE1	2.44	0.51
1:B:416:ARG:HG2	1:B:466:ARG:HG2	1.93	0.51
1:C:122:PHE:HB3	1:C:364:SER:HB2	1.91	0.51
1:D:506:ILE:HG12	1:D:536:LYS:HE3	1.93	0.51
1:F:356:VAL:HG13	1:F:386:ASN:HA	1.92	0.51
1:F:641:ARG:NH1	1:F:669:TYR:O	2.40	0.51
1:F:1004:GLN:HG2	1:F:1017:PHE:CE2	2.46	0.51
1:C:27:PRO:HB3	1:C:1017:PHE:HE2	1.75	0.51
1:E:1010:GLN:HG3	1:E:1097:TYR:OH	2.10	0.51
1:B:112:ARG:HH21	1:B:119:LEU:HD11	1.76	0.51
1:C:1057:LEU:HD23	1:C:1069:ILE:HD13	1.92	0.51
1:A:460:VAL:HG22	1:A:491:TYR:CZ	2.46	0.51
1:F:1072:TYR:HB2	1:F:1098:TRP:CE2	2.46	0.51
1:E:1000:ASN:ND2	3:E:1204:HTL:H3'3	2.25	0.51
1:A:1035:SER:HB2	1:B:1031:LEU:HD23	1.93	0.51
1:E:1047:GLY:HA3	1:E:1089:ALA:HB3	1.91	0.51
1:A:265:PRO:HB2	1:C:568:ASN:ND2	2.25	0.50
1:E:1035:SER:HB2	1:F:1031:LEU:HD23	1.93	0.50
1:A:321:ARG:HB3	1:A:379:LEU:HD22	1.93	0.50
1:D:136:PHE:CE2	1:D:164:PRO:HB2	2.45	0.50
1:D:715:PRO:HG2	1:D:718:PHE:HB2	1.93	0.50
1:C:228:GLU:OE2	1:C:231:ASN:ND2	2.40	0.50
1:C:967:ASP:HB3	1:C:994:ASP:HA	1.94	0.50
1:D:704:TYR:CE1	1:D:736:GLN:HB3	2.46	0.50
1:E:361:GLY:HA2	1:E:365:LYS:HB3	1.94	0.50
1:B:678:ILE:HD11	1:B:767:VAL:HG23	1.93	0.50
1:C:1047:GLY:HA3	1:C:1089:ALA:HB3	1.93	0.50
1:F:838:SER:HA	1:F:841:TRP:CE2	2.45	0.50
1:C:1001:THR:O	1:C:1004:GLN:NE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:887:LEU:HD13	1:E:952:GLN:HB2	1.93	0.50
1:A:883:ARG:NH2	1:A:886:GLU:OE1	2.38	0.50
1:D:1004:GLN:HG3	1:D:1016:ARG:HB2	1.94	0.50
1:A:416:ARG:HG2	1:A:466:ARG:HG2	1.94	0.49
1:B:6:LEU:HD12	1:B:181:ILE:HD11	1.94	0.49
1:D:518:MET:HB3	1:D:618:TRP:CH2	2.47	0.49
1:C:85:SER:HA	1:C:127:ASP:HB3	1.94	0.49
1:D:591:GLY:H	1:D:594:ILE:HD11	1.76	0.49
1:F:1039:VAL:HG22	1:F:1066:PRO:HG2	1.95	0.49
1:E:1004:GLN:HG2	1:E:1017:PHE:CE2	2.48	0.49
1:A:435:ILE:HG23	1:A:446:ALA:HB1	1.95	0.49
1:B:18:ALA:HB2	1:B:186:TYR:CE1	2.47	0.49
1:D:996:GLU:OE1	1:D:1097:TYR:OH	2.27	0.49
1:E:136:PHE:CE2	1:E:164:PRO:HB2	2.45	0.49
1:A:817:TYR:CZ	1:A:1071:ALA:HB1	2.47	0.49
1:D:838:SER:HA	1:D:841:TRP:CE2	2.48	0.49
1:F:545:ILE:HG23	1:F:604:ARG:HD2	1.94	0.49
1:C:838:SER:HA	1:C:841:TRP:CE2	2.47	0.49
1:D:827:ASP:OD2	1:D:921:ARG:NH1	2.35	0.49
1:E:122:PHE:CE2	1:F:220:PRO:HD3	2.48	0.49
1:A:141:SER:HG	1:A:167:HIS:HE2	1.61	0.48
1:A:835:THR:HG22	3:A:1204:HTL:H3'2	1.95	0.48
1:C:715:PRO:HG2	1:C:718:PHE:HB2	1.95	0.48
1:F:817:TYR:CZ	1:F:1071:ALA:HB1	2.48	0.48
1:D:1079:GLY:HA3	1:D:1134:ILE:HB	1.95	0.48
1:E:435:ILE:HG23	1:E:446:ALA:HB1	1.96	0.48
3:E:1204:HTL:H4'2	3:E:1204:HTL:C1'	2.25	0.48
1:A:345:VAL:HB	1:B:334:LEU:HD21	1.95	0.48
1:D:545:ILE:HG23	1:D:604:ARG:HD2	1.94	0.48
1:F:361:GLY:HA2	1:F:365:LYS:HB3	1.95	0.48
1:A:1031:LEU:HD12	1:B:1035:SER:HB3	1.95	0.48
1:C:694:LEU:HD22	1:C:793:VAL:HG13	1.95	0.48
1:E:1031:LEU:HD23	1:F:1035:SER:HB2	1.95	0.48
1:B:1004:GLN:HG2	1:B:1017:PHE:CE2	2.49	0.48
1:C:37:ILE:HG13	1:C:41:TRP:CE2	2.49	0.48
1:C:885:ASP:CG	1:D:52:LYS:HZ2	2.17	0.48
1:C:1000:ASN:ND2	3:C:1204:HTL:H3'3	2.29	0.48
1:E:506:ILE:HG12	1:E:536:LYS:HE3	1.96	0.47
1:F:136:PHE:CE2	1:F:164:PRO:HB2	2.49	0.47
1:F:1010:GLN:HG3	1:F:1097:TYR:OH	2.14	0.47
1:C:1072:TYR:HB2	1:C:1098:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:PRO:HB3	1:E:1017:PHE:HE2	1.79	0.47
1:B:361:GLY:HA2	1:B:365:LYS:HB3	1.96	0.47
1:D:1000:ASN:HD22	3:D:1204:HTL:H3'3	1.80	0.47
1:F:835:THR:HG22	3:F:1204:HTL:H3'2	1.96	0.47
1:B:719:VAL:O	1:B:734:ARG:NH2	2.47	0.47
1:A:368:ASN:HB2	1:A:369:PRO:HD2	1.97	0.47
1:A:681:TRP:CE2	1:A:735:ILE:HB	2.50	0.47
1:B:887:LEU:HD13	1:B:952:GLN:HB2	1.95	0.47
1:C:27:PRO:HB3	1:C:1017:PHE:CE2	2.50	0.47
1:D:1004:GLN:HG2	1:D:1017:PHE:CE2	2.50	0.47
1:F:972:ASP:OD2	1:F:998:TYR:OH	2.25	0.47
1:C:112:ARG:NH2	1:C:119:LEU:HD11	2.28	0.47
1:F:887:LEU:HD13	1:F:952:GLN:HB2	1.96	0.47
1:C:869:ASN:HB3	1:C:969:TRP:CE2	2.50	0.47
1:C:667:THR:HB	1:C:805:PHE:HB2	1.96	0.47
1:E:85:SER:HA	1:E:127:ASP:HB3	1.96	0.47
1:F:1001:THR:O	1:F:1004:GLN:NE2	2.45	0.47
1:D:34:MET:HE3	1:D:82:PHE:HB3	1.96	0.46
1:C:415:PHE:O	1:C:466:ARG:HA	2.14	0.46
1:C:719:VAL:O	1:C:734:ARG:NH2	2.47	0.46
1:A:836:GLY:HA2	3:A:1204:HTL:S1	2.56	0.46
1:B:122:PHE:HB3	1:B:364:SER:HB2	1.97	0.46
1:C:435:ILE:HG23	1:C:446:ALA:HB1	1.96	0.46
1:D:361:GLY:HA2	1:D:365:LYS:HB3	1.96	0.46
1:A:1139:LEU:HD21	1:A:1150:LEU:HD12	1.98	0.46
1:D:157:ALA:HA	1:D:244:VAL:HG21	1.97	0.46
1:D:1072:TYR:HB2	1:D:1098:TRP:CE2	2.50	0.46
1:C:146:GLU:OE2	1:C:301:ARG:NH2	2.49	0.46
1:E:321:ARG:HB3	1:E:379:LEU:HD22	1.98	0.46
1:B:695:VAL:HG21	1:B:751:VAL:HG21	1.97	0.46
1:C:70:HIS:HE2	1:C:101:GLU:CD	2.19	0.46
1:D:453:ASP:OD1	1:D:454:SER:N	2.49	0.46
1:D:127:ASP:OD1	1:D:128:VAL:N	2.47	0.46
1:A:704:TYR:CE1	1:A:736:GLN:HB3	2.51	0.46
1:A:1000:ASN:HD22	3:A:1204:HTL:H3'3	1.80	0.45
1:C:802:LEU:HD13	1:C:859:PRO:HD3	1.99	0.45
1:D:122:PHE:HB3	1:D:364:SER:HB2	1.98	0.45
1:F:83:THR:O	1:F:109:VAL:HA	2.16	0.45
1:B:464:HIS:HB3	1:B:478:ILE:HG13	1.99	0.45
1:B:752:CYS:HA	2:B:1201:SF4:S1	2.56	0.45
1:D:1076:ILE:HG22	1:D:1082:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:HB3	1:A:1017:PHE:HE2	1.81	0.45
1:B:1097:TYR:HH	1:B:1136:TYR:HH	1.62	0.45
1:E:373:LYS:HD2	1:E:407:ILE:HD13	1.98	0.45
1:B:386:ASN:OD1	1:B:387:LYS:N	2.49	0.45
1:D:322:ILE:HD12	1:D:346:LEU:HD11	1.99	0.45
1:E:24:THR:HA	1:E:57:ALA:O	2.17	0.45
1:E:879:ALA:HB3	1:F:75:ALA:HB3	1.97	0.45
1:A:85:SER:HB2	1:A:112:ARG:HB3	1.99	0.45
1:D:418:LYS:HE2	1:D:418:LYS:HB3	1.81	0.45
1:E:817:TYR:CZ	1:E:1071:ALA:HB1	2.52	0.45
1:A:879:ALA:HB3	1:B:75:ALA:HB3	1.97	0.45
1:A:985:GLY:HA2	1:A:1066:PRO:HD3	1.98	0.45
1:B:558:ILE:HG23	1:B:605:ALA:HB2	1.99	0.45
1:B:985:GLY:HA2	1:B:1066:PRO:HD3	1.99	0.45
1:C:356:VAL:HG12	1:C:388:PHE:HE2	1.81	0.45
1:F:426:GLY:HA3	1:F:556:ASN:HB3	1.99	0.45
1:B:480:GLN:HA	1:B:500:GLY:O	2.17	0.45
1:E:116:THR:OG1	1:E:117:HIS:N	2.50	0.45
1:E:272:VAL:HB	1:E:324:VAL:HG22	1.99	0.45
1:A:112:ARG:NE	1:A:121:ILE:HA	2.32	0.45
1:B:27:PRO:HB3	1:B:1017:PHE:CE2	2.52	0.45
1:E:367:PHE:HA	1:E:371:MET:SD	2.57	0.45
1:C:75:ALA:HB3	1:D:879:ALA:HB3	1.98	0.45
1:C:140:SER:HB2	1:C:168:PHE:CZ	2.52	0.45
1:A:136:PHE:CE2	1:A:164:PRO:HB2	2.52	0.44
1:B:295:VAL:HB	1:B:376:PHE:CE1	2.52	0.44
1:D:21:GLU:OE2	1:D:202:ARG:NH2	2.50	0.44
1:E:81:THR:HG21	1:E:91:MET:HE1	1.98	0.44
1:E:671:LYS:HD2	1:E:740:LEU:HB2	1.98	0.44
1:F:28:ILE:HA	3:F:1204:HTL:H351	2.00	0.44
1:F:747:ASN:ND2	1:F:1083:THR:O	2.50	0.44
1:B:1001:THR:O	1:B:1004:GLN:NE2	2.50	0.44
1:C:802:LEU:HB2	1:C:822:THR:HB	1.99	0.44
1:F:694:LEU:HD22	1:F:793:VAL:HG13	1.98	0.44
1:A:719:VAL:O	1:A:734:ARG:NH2	2.46	0.44
1:C:1012:GLY:HA2	1:C:1150:LEU:HD13	1.99	0.44
1:E:562:ALA:O	1:E:566:ILE:HG12	2.18	0.44
1:B:30:PRO:HG2	1:B:110:ALA:HB1	2.00	0.44
1:C:220:PRO:HD3	1:D:122:PHE:CE2	2.53	0.44
1:E:112:ARG:HA	1:E:123:GLY:HA2	2.00	0.44
1:B:967:ASP:HB3	1:B:994:ASP:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:GLN:HG3	1:B:1097:TYR:OH	2.18	0.44
1:E:368:ASN:HB2	1:E:369:PRO:HD2	1.98	0.44
1:E:998:TYR:CE1	1:E:1006:SER:HB2	2.52	0.44
1:C:480:GLN:HA	1:C:500:GLY:O	2.16	0.44
1:C:963:ILE:HB	1:C:990:VAL:HG22	2.00	0.44
1:A:579:ILE:O	1:A:583:ILE:HG13	2.18	0.44
1:C:980:HIS:NE2	1:D:59:MET:HA	2.33	0.44
1:C:1000:ASN:HD22	3:C:1204:HTL:H3'3	1.83	0.44
1:E:866:PHE:CD2	1:E:973:ILE:HG21	2.53	0.44
1:F:814:GLU:HB3	1:F:993:LEU:HD13	2.00	0.44
1:A:82:PHE:HD1	1:A:108:HIS:HB2	1.82	0.43
1:A:1047:GLY:HA3	1:A:1089:ALA:HB3	2.00	0.43
1:F:85:SER:HB2	1:F:112:ARG:HB3	2.00	0.43
1:F:1055:LYS:HE2	1:F:1059:GLU:OE2	2.18	0.43
1:C:803:LEU:HD12	1:C:849:PRO:HB2	2.01	0.43
1:D:73:LEU:HD13	1:D:103:LEU:HB3	1.99	0.43
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	2.00	0.43
1:D:1000:ASN:ND2	3:D:1204:HTL:H3'3	2.33	0.43
1:C:368:ASN:HB2	1:C:369:PRO:HD2	2.00	0.43
1:C:1035:SER:HB2	1:D:1031:LEU:HD23	2.00	0.43
1:D:32:SER:O	1:D:36:GLU:HG3	2.17	0.43
1:E:387:LYS:NZ	1:F:348:GLU:OE1	2.51	0.43
1:F:1000:ASN:HD22	3:F:1204:HTL:H3'3	1.83	0.43
1:A:30:PRO:HB3	1:A:172:PHE:CE2	2.53	0.43
1:A:112:ARG:HA	1:A:123:GLY:HA2	2.00	0.43
1:A:258:LEU:HD12	1:A:310:HIS:CG	2.53	0.43
1:B:802:LEU:HB2	1:B:822:THR:HB	2.01	0.43
1:D:221:ASP:N	1:D:221:ASP:OD1	2.51	0.43
1:D:983:ALA:HB2	1:D:1036:TYR:CZ	2.54	0.43
1:B:521:ARG:HA	1:B:521:ARG:HD2	1.89	0.43
1:D:518:MET:HB3	1:D:618:TRP:HH2	1.83	0.43
1:E:694:LEU:HD22	1:E:793:VAL:HG13	2.01	0.43
1:E:838:SER:HA	1:E:841:TRP:CE2	2.53	0.43
1:C:453:ASP:OD1	1:C:454:SER:N	2.50	0.43
1:E:105:CYS:HB3	1:E:164:PRO:HB3	2.00	0.43
1:F:122:PHE:HB3	1:F:364:SER:HB2	2.01	0.43
1:F:985:GLY:HA2	1:F:1066:PRO:HD3	2.01	0.43
1:A:213:GLN:NE2	1:B:843:GLY:HA2	2.34	0.43
1:A:747:ASN:O	1:A:751:VAL:HG23	2.19	0.43
1:C:112:ARG:HA	1:C:123:GLY:HA2	2.00	0.43
1:C:361:GLY:HA2	1:C:365:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:883:ARG:NH1	1:D:76:GLY:O	2.52	0.43
1:C:1010:GLN:HG3	1:C:1097:TYR:OH	2.19	0.43
1:E:428:VAL:HG11	1:E:452:TYR:OH	2.19	0.43
1:E:916:ASP:HB3	1:E:919:ARG:HB2	2.00	0.43
1:F:84:ALA:HA	1:F:109:VAL:HG13	2.01	0.43
1:B:112:ARG:NH2	1:B:119:LEU:HD11	2.32	0.43
1:B:1010:GLN:HG3	1:B:1097:TYR:HH	1.84	0.43
1:B:1119:TYR:HE2	1:B:1122:PRO:HA	1.82	0.43
1:D:112:ARG:NH2	1:D:119:LEU:HD11	2.34	0.43
1:E:75:ALA:HB3	1:F:879:ALA:HB3	2.01	0.43
1:A:34:MET:CE	1:A:82:PHE:HB3	2.45	0.43
1:D:282:GLU:OE1	1:D:299:LYS:NZ	2.42	0.43
1:D:1047:GLY:HA3	1:D:1089:ALA:HB3	2.01	0.42
1:E:281:ILE:HG21	1:E:297:LEU:HD13	2.00	0.42
1:E:954:ASP:OD1	1:E:954:ASP:N	2.50	0.42
1:F:127:ASP:OD1	1:F:128:VAL:N	2.49	0.42
1:F:267:ALA:HA	1:F:294:LYS:HB3	2.01	0.42
1:C:213:GLN:HG3	1:D:861:TRP:HE3	1.84	0.42
1:C:1036:TYR:O	1:D:1025:LYS:NZ	2.50	0.42
1:B:489:PRO:HG3	1:B:510:ASN:O	2.19	0.42
1:B:136:PHE:CE2	1:B:164:PRO:HB2	2.55	0.42
1:E:278:CYS:HB3	1:E:299:LYS:HG2	2.01	0.42
1:E:1001:THR:O	1:E:1004:GLN:NE2	2.52	0.42
1:F:643:ILE:HG21	1:F:846:PRO:HD3	2.00	0.42
1:A:419:PHE:HB2	1:A:463:SER:HB2	2.00	0.42
1:B:85:SER:HB2	1:B:112:ARG:HB3	2.02	0.42
1:B:221:ASP:OD1	1:B:221:ASP:N	2.51	0.42
1:E:28:ILE:HD13	1:E:84:ALA:O	2.20	0.42
1:B:518:MET:HB3	1:B:618:TRP:HH2	1.84	0.42
1:B:813:GLY:HA3	1:B:1074:PRO:HD2	2.01	0.42
1:C:865:LEU:HD13	1:D:93:PRO:HB2	2.01	0.42
1:D:728:ALA:HB2	1:D:788:PHE:HE2	1.84	0.42
1:E:624:GLU:H	1:E:624:GLU:HG3	1.72	0.42
1:B:112:ARG:NE	1:B:121:ILE:HA	2.35	0.42
1:B:571:PRO:HB2	1:B:574:GLU:HG3	2.02	0.42
1:F:983:ALA:HB2	1:F:1036:TYR:CZ	2.55	0.42
1:C:112:ARG:HH21	1:C:119:LEU:HD11	1.85	0.41
1:E:857:HIS:ND1	1:F:209:GLU:HG2	2.35	0.41
1:B:86:GLN:OE1	1:B:115:SER:N	2.41	0.41
1:D:7:ASP:HA	1:D:177:GLU:O	2.20	0.41
1:D:641:ARG:HB2	1:D:642:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:793:VAL:HG21	1:E:1050:HIS:HB3	2.02	0.41
1:C:105:CYS:HB3	1:C:164:PRO:HB3	2.02	0.41
1:D:487:HIS:CD2	1:D:559:MET:HG2	2.54	0.41
1:E:206:LEU:HD23	1:E:212:HIS:CE1	2.55	0.41
1:E:835:THR:HG22	3:E:1204:HTL:H3'2	2.02	0.41
1:F:954:ASP:OD1	1:F:954:ASP:N	2.52	0.41
1:A:334:LEU:HD21	1:B:345:VAL:HB	2.02	0.41
1:A:386:ASN:OD1	1:A:387:LYS:N	2.53	0.41
1:B:139:LEU:HD12	1:B:301:ARG:O	2.21	0.41
1:C:909:GLY:HA3	1:C:923:TYR:CE1	2.54	0.41
1:D:27:PRO:HB3	1:D:1017:PHE:CE2	2.49	0.41
1:C:1004:GLN:HG2	1:C:1017:PHE:CE2	2.56	0.41
1:F:85:SER:HA	1:F:127:ASP:HB3	2.02	0.41
1:F:221:ASP:OD1	1:F:221:ASP:N	2.51	0.41
1:F:1000:ASN:ND2	3:F:1204:HTL:H3'3	2.35	0.41
1:A:954:ASP:OD1	1:A:954:ASP:N	2.53	0.41
1:B:116:THR:OG1	1:B:117:HIS:N	2.53	0.41
1:D:651:LEU:HA	1:D:652:PRO:HD3	1.90	0.41
1:F:116:THR:OG1	1:F:117:HIS:N	2.53	0.41
1:F:659:ASP:N	1:F:659:ASP:OD1	2.53	0.41
1:F:665:GLY:N	1:F:850:TYR:O	2.52	0.41
1:F:356:VAL:HG12	1:F:388:PHE:HE1	1.85	0.41
1:A:32:SER:O	1:A:36:GLU:HG3	2.20	0.41
1:A:1079:GLY:HA3	1:A:1134:ILE:HB	2.01	0.41
1:E:37:ILE:HG13	1:E:41:TRP:CE2	2.55	0.41
1:F:641:ARG:HB2	1:F:642:PRO:HD3	2.03	0.41
1:A:59:MET:HG3	1:A:65:ALA:HA	2.03	0.41
1:B:802:LEU:HD13	1:B:859:PRO:HD3	2.02	0.41
1:C:127:ASP:OD1	1:C:128:VAL:N	2.53	0.41
1:C:278:CYS:HB3	1:C:299:LYS:HG2	2.03	0.41
1:C:406:HIS:NE2	1:C:479:ASP:HB2	2.35	0.41
1:C:1012:GLY:O	1:C:1139:LEU:HD22	2.20	0.41
1:D:371:MET:HB3	1:D:390:VAL:CG1	2.50	0.41
1:D:489:PRO:HG3	1:D:510:ASN:O	2.21	0.41
1:D:641:ARG:NH1	1:D:669:TYR:O	2.53	0.41
1:E:1139:LEU:HD21	1:E:1150:LEU:HD12	2.02	0.41
1:F:416:ARG:HG2	1:F:466:ARG:HG2	2.03	0.41
1:C:132:ARG:HH11	1:D:132:ARG:HH11	1.69	0.41
1:D:814:GLU:HB3	1:D:993:LEU:HD13	2.02	0.41
1:E:348:GLU:OE1	1:F:387:LYS:NZ	2.54	0.41
1:F:971:TYR:O	1:F:1007:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:OE2	1:A:231:ASN:ND2	2.45	0.40
1:B:435:ILE:HG23	1:B:446:ALA:HB1	2.03	0.40
1:C:24:THR:HA	1:C:57:ALA:O	2.21	0.40
1:C:213:GLN:HG3	1:D:861:TRP:CE3	2.56	0.40
1:D:178:VAL:O	1:D:447:GLN:HA	2.22	0.40
1:D:718:PHE:CZ	1:D:734:ARG:HD3	2.56	0.40
1:F:513:TRP:HE3	1:F:517:GLU:OE1	2.04	0.40
1:F:1026:LYS:NZ	1:F:1098:TRP:HZ3	2.19	0.40
1:A:213:GLN:HE22	1:B:843:GLY:HA2	1.87	0.40
1:A:367:PHE:HA	1:A:371:MET:SD	2.61	0.40
1:C:136:PHE:CE2	1:C:164:PRO:HB2	2.56	0.40
1:D:28:ILE:HA	3:D:1204:HTL:H351	2.03	0.40
1:E:826:GLY:HA2	1:E:829:MET:HG2	2.03	0.40
1:A:793:VAL:HG21	1:A:1050:HIS:HB3	2.03	0.40
1:C:124:ASP:HB2	1:C:327:ARG:O	2.21	0.40
1:E:132:ARG:HH11	1:F:132:ARG:HH11	1.69	0.40
1:E:418:LYS:HE2	1:E:418:LYS:HB3	1.76	0.40
1:F:690:ASN:HB3	1:F:797:GLN:HB2	2.04	0.40
1:A:112:ARG:NH2	1:A:119:LEU:HD11	2.35	0.40
1:A:453:ASP:OD1	1:A:454:SER:N	2.54	0.40
1:D:65:ALA:O	1:D:69:VAL:HG23	2.22	0.40
1:D:85:SER:HA	1:D:127:ASP:HB3	2.03	0.40
1:A:198:ILE:O	1:A:202:ARG:HG2	2.21	0.40
1:C:636:ILE:HD11	1:C:666:THR:HG22	2.03	0.40
1:D:112:ARG:HA	1:D:123:GLY:HA2	2.02	0.40
1:E:345:VAL:HB	1:F:334:LEU:HD21	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	1161/1171 (99%)	1144 (98%)	17 (2%)	0	100	100
1	B	1161/1171 (99%)	1142 (98%)	19 (2%)	0	100	100
1	C	1159/1171 (99%)	1139 (98%)	20 (2%)	0	100	100
1	D	1160/1171 (99%)	1140 (98%)	20 (2%)	0	100	100
1	E	1160/1171 (99%)	1140 (98%)	20 (2%)	0	100	100
1	F	1167/1171 (100%)	1146 (98%)	21 (2%)	0	100	100
All	All	6968/7026 (99%)	6851 (98%)	117 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	889/932 (95%)	885 (100%)	4 (0%)	91	96
1	B	877/932 (94%)	875 (100%)	2 (0%)	93	98
1	C	889/932 (95%)	886 (100%)	3 (0%)	92	97
1	D	888/932 (95%)	885 (100%)	3 (0%)	92	97
1	E	894/932 (96%)	890 (100%)	4 (0%)	91	96
1	F	886/932 (95%)	883 (100%)	3 (0%)	92	97
All	All	5323/5592 (95%)	5304 (100%)	19 (0%)	91	96

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	PHE
1	A	390	VAL
1	A	649	ASP
1	A	833	ASN
1	B	224	PHE
1	B	833	ASN
1	C	224	PHE

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Mol	Chain	Res	Type
1	C	594	ILE
1	C	833	ASN
1	D	224	PHE
1	D	833	ASN
1	D	837	CYS
1	E	224	PHE
1	E	594	ILE
1	E	624	GLU
1	E	833	ASN
1	F	224	PHE
1	F	594	ILE
1	F	833	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1000	ASN
1	B	213	GLN
1	B	1000	ASN
1	C	1000	ASN
1	D	539	ASN
1	D	1000	ASN
1	E	433	ASN
1	E	560	GLN
1	E	1000	ASN
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 monosaccharides 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
2	SF4	B	1201	1	0,12,12	-	-	-	-	-
3	HTL	E	1204	4	23,30,30	1.84	5 (21%)	31,45,45	2.69	7 (22%)
5	SO4	D	1206	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	C	1206	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SF4	D	1202	1	0,12,12	-	-	-	-	-
2	SF4	A	1203	1	0,12,12	-	-	-	-	-
3	HTL	C	1204	4	23,30,30	1.72	5 (21%)	31,45,45	2.77	8 (25%)
2	SF4	B	1203	1	0,12,12	-	-	-	-	-
2	SF4	C	1201	1	0,12,12	-	-	-	-	-
2	SF4	F	1201	1	0,12,12	-	-	-	-	-
2	SF4	E	1202	1	0,12,12	-	-	-	-	-
2	SF4	A	1201	1	0,12,12	-	-	-	-	-
5	SO4	E	1206	-	4,4,4	0.14	0	6,6,6	0.14	0
3	HTL	B	1204	4	23,30,30	1.67	5 (21%)	31,45,45	2.63	8 (25%)
2	SF4	C	1203	1	0,12,12	-	-	-	-	-
2	SF4	B	1202	1	0,12,12	-	-	-	-	-
3	HTL	D	1204	4	23,30,30	1.89	5 (21%)	31,45,45	2.51	7 (22%)
5	SO4	B	1206	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SF4	F	1203	1	0,12,12	-	-	-	-	-
3	HTL	A	1204	4	23,30,30	1.73	5 (21%)	31,45,45	2.57	5 (16%)
2	SF4	D	1201	1	0,12,12	-	-	-	-	-
2	SF4	E	1203	1	0,12,12	-	-	-	-	-
2	SF4	C	1202	1	0,12,12	-	-	-	-	-
2	SF4	D	1203	1	0,12,12	-	-	-	-	-
3	HTL	F	1204	4	23,30,30	1.91	5 (21%)	31,45,45	2.54	8 (25%)
2	SF4	F	1202	1	0,12,12	-	-	-	-	-
5	SO4	B	1207	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SF4	A	1202	1	0,12,12	-	-	-	-	-
5	SO4	A	1206	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SF4	E	1201	1	0,12,12	-	-	-	-	-
5	SO4	F	1206	-	4,4,4	0.15	0	6,6,6	0.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HTL	E	1204	4	-	1/16/21/21	0/2/2/2
2	SF4	B	1201	1	-	-	0/6/5/5
2	SF4	D	1202	1	-	-	0/6/5/5
2	SF4	A	1203	1	-	-	0/6/5/5
3	HTL	C	1204	4	-	2/16/21/21	0/2/2/2
2	SF4	B	1203	1	-	-	0/6/5/5
2	SF4	C	1201	1	-	-	0/6/5/5
2	SF4	F	1201	1	-	-	0/6/5/5
2	SF4	E	1202	1	-	-	0/6/5/5
2	SF4	A	1201	1	-	-	0/6/5/5
3	HTL	B	1204	4	-	2/16/21/21	0/2/2/2
2	SF4	C	1203	1	-	-	0/6/5/5
2	SF4	B	1202	1	-	-	0/6/5/5
3	HTL	D	1204	4	-	2/16/21/21	0/2/2/2
2	SF4	F	1203	1	-	-	0/6/5/5
3	HTL	A	1204	4	-	1/16/21/21	0/2/2/2
2	SF4	D	1201	1	-	-	0/6/5/5
2	SF4	E	1203	1	-	-	0/6/5/5
2	SF4	C	1202	1	-	-	0/6/5/5
2	SF4	D	1203	1	-	-	0/6/5/5
3	HTL	F	1204	4	-	2/16/21/21	0/2/2/2
2	SF4	F	1202	1	-	-	0/6/5/5
2	SF4	A	1202	1	-	-	0/6/5/5
2	SF4	E	1201	1	-	-	0/6/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1204	HTL	C5A-C5	4.81	1.53	1.50
3	D	1204	HTL	C5A-C5	4.59	1.52	1.50
3	E	1204	HTL	C5A-C5	4.14	1.52	1.50
3	F	1204	HTL	C35-C5'	3.88	1.59	1.51
3	E	1204	HTL	C4'-N4'	3.82	1.43	1.34
3	F	1204	HTL	C4'-N4'	3.76	1.43	1.34
3	E	1204	HTL	C5-S1	3.72	1.81	1.74
3	D	1204	HTL	C5-S1	3.72	1.81	1.74
3	D	1204	HTL	C4'-N4'	3.72	1.43	1.34
3	E	1204	HTL	C35-C5'	3.71	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	HTL	C4'-N4'	3.70	1.43	1.34
3	F	1204	HTL	C5-S1	3.70	1.81	1.74
3	C	1204	HTL	C35-C5'	3.70	1.58	1.51
3	A	1204	HTL	C35-C5'	3.69	1.58	1.51
3	C	1204	HTL	C5-S1	3.69	1.81	1.74
3	A	1204	HTL	C4'-N4'	3.68	1.43	1.34
3	B	1204	HTL	C35-C5'	3.67	1.58	1.51
3	D	1204	HTL	C35-C5'	3.66	1.58	1.51
3	C	1204	HTL	C4'-N4'	3.64	1.43	1.34
3	B	1204	HTL	C5-S1	3.63	1.80	1.74
3	A	1204	HTL	C5-S1	3.54	1.80	1.74
3	A	1204	HTL	C5A-C5	3.21	1.52	1.50
3	C	1204	HTL	C5A-C5	2.93	1.52	1.50
3	A	1204	HTL	C6'-C5'	2.62	1.43	1.37
3	F	1204	HTL	C6'-C5'	2.47	1.42	1.37
3	B	1204	HTL	C5A-C5	2.46	1.52	1.50
3	D	1204	HTL	C6'-C5'	2.45	1.42	1.37
3	B	1204	HTL	C6'-C5'	2.38	1.42	1.37
3	C	1204	HTL	C6'-C5'	2.37	1.42	1.37
3	E	1204	HTL	C6'-C5'	2.36	1.42	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1204	HTL	C4-N3-C2	13.38	116.08	108.64
3	E	1204	HTL	C4-N3-C2	12.70	115.70	108.64
3	B	1204	HTL	C4-N3-C2	12.33	115.50	108.64
3	A	1204	HTL	C4-N3-C2	12.14	115.39	108.64
3	F	1204	HTL	C4-N3-C2	11.73	115.17	108.64
3	D	1204	HTL	C4-N3-C2	11.55	115.07	108.64
3	E	1204	HTL	P1-O11-P2	-3.52	120.76	132.83
3	D	1204	HTL	C5-C4-N3	3.23	114.42	107.66
3	F	1204	HTL	C5-C4-N3	3.21	114.36	107.66
3	E	1204	HTL	C5-C4-N3	3.08	114.10	107.66
3	A	1204	HTL	C5-C4-N3	3.06	114.05	107.66
3	B	1204	HTL	C6'-N1'-C2'	3.05	121.16	115.96
3	F	1204	HTL	C6'-N1'-C2'	3.05	121.15	115.96
3	D	1204	HTL	C6'-N1'-C2'	3.01	121.09	115.96
3	C	1204	HTL	C6'-N1'-C2'	2.97	121.01	115.96
3	E	1204	HTL	C6'-N1'-C2'	2.90	120.89	115.96
3	A	1204	HTL	P1-O11-P2	-2.85	123.04	132.83
3	B	1204	HTL	P1-O11-P2	-2.85	123.05	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	HTL	C5-C4-N3	2.83	113.57	107.66
3	C	1204	HTL	C5-C4-N3	2.78	113.47	107.66
3	A	1204	HTL	C6'-N1'-C2'	2.74	120.63	115.96
3	F	1204	HTL	P1-O11-P2	-2.69	123.59	132.83
3	D	1204	HTL	P1-O11-P2	-2.60	123.92	132.83
3	C	1204	HTL	C5'-C6'-N1'	-2.49	119.68	123.82
3	C	1204	HTL	P1-O11-P2	-2.46	124.39	132.83
3	B	1204	HTL	N1'-C2'-N3'	-2.37	121.46	125.54
3	B	1204	HTL	C5'-C6'-N1'	-2.36	119.88	123.82
3	D	1204	HTL	C5'-C6'-N1'	-2.35	119.91	123.82
3	F	1204	HTL	N1'-C2'-N3'	-2.34	121.51	125.54
3	C	1204	HTL	C2A-C2'-N1'	2.29	119.65	117.14
3	A	1204	HTL	C5'-C6'-N1'	-2.27	120.04	123.82
3	B	1204	HTL	C2'-N3'-C4'	2.22	121.55	118.08
3	B	1204	HTL	C2A-C2'-N1'	2.20	119.56	117.14
3	F	1204	HTL	C2'-N3'-C4'	2.20	121.51	118.08
3	E	1204	HTL	C5'-C6'-N1'	-2.20	120.16	123.82
3	D	1204	HTL	N1'-C2'-N3'	-2.18	121.78	125.54
3	F	1204	HTL	C5'-C6'-N1'	-2.17	120.21	123.82
3	E	1204	HTL	C2'-N3'-C4'	2.16	121.45	118.08
3	C	1204	HTL	N1'-C2'-N3'	-2.13	121.88	125.54
3	E	1204	HTL	N1'-C2'-N3'	-2.12	121.90	125.54
3	F	1204	HTL	C4A-C4-C5	-2.08	123.05	127.60
3	C	1204	HTL	C2'-N3'-C4'	2.05	121.27	118.08
3	D	1204	HTL	C4A-C4-C5	-2.04	123.13	127.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

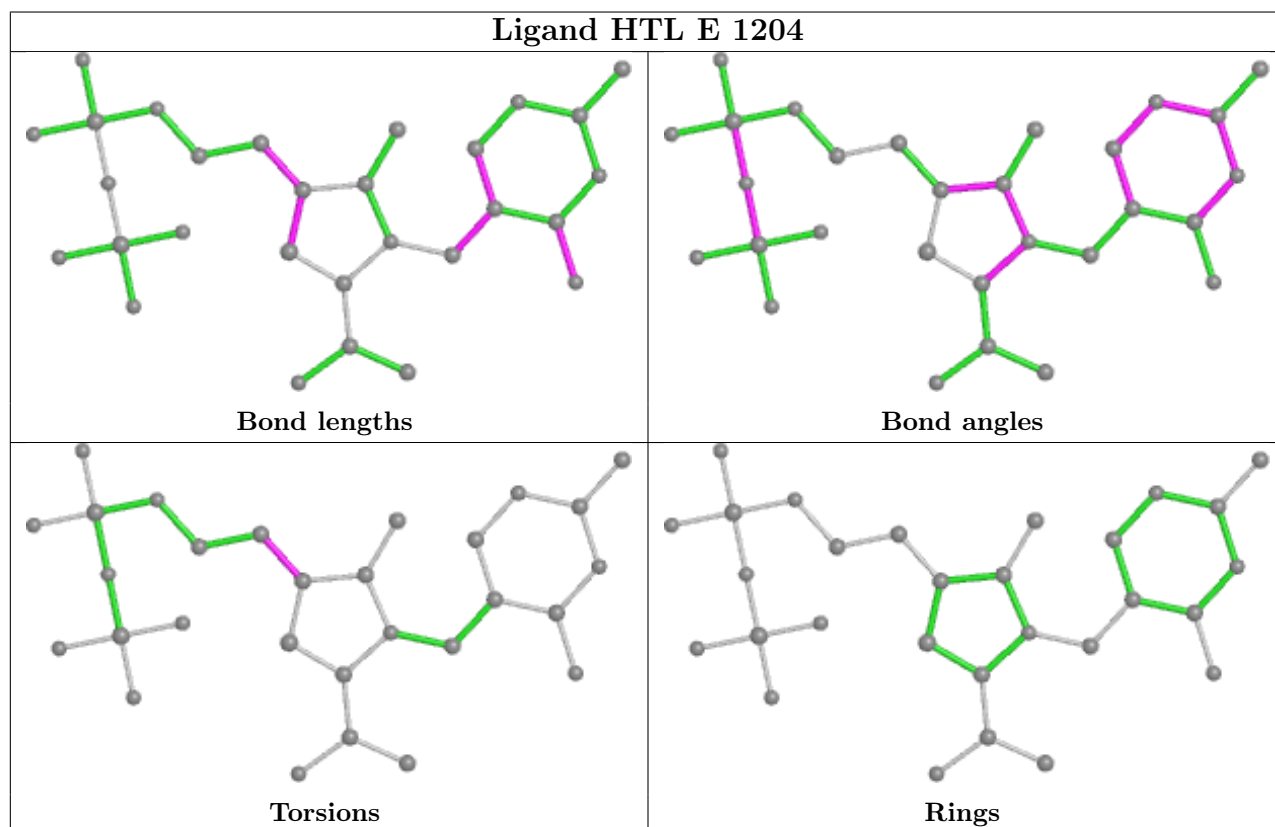
Mol	Chain	Res	Type	Atoms
3	C	1204	HTL	P2-O11-P1-O5G
3	B	1204	HTL	P2-O11-P1-O5G
3	D	1204	HTL	P2-O11-P1-O5G
3	F	1204	HTL	P2-O11-P1-O5G
3	A	1204	HTL	C4-C5-C5A-C5B
3	B	1204	HTL	C4-C5-C5A-C5B
3	C	1204	HTL	C4-C5-C5A-C5B
3	D	1204	HTL	C4-C5-C5A-C5B
3	E	1204	HTL	C4-C5-C5A-C5B
3	F	1204	HTL	C4-C5-C5A-C5B

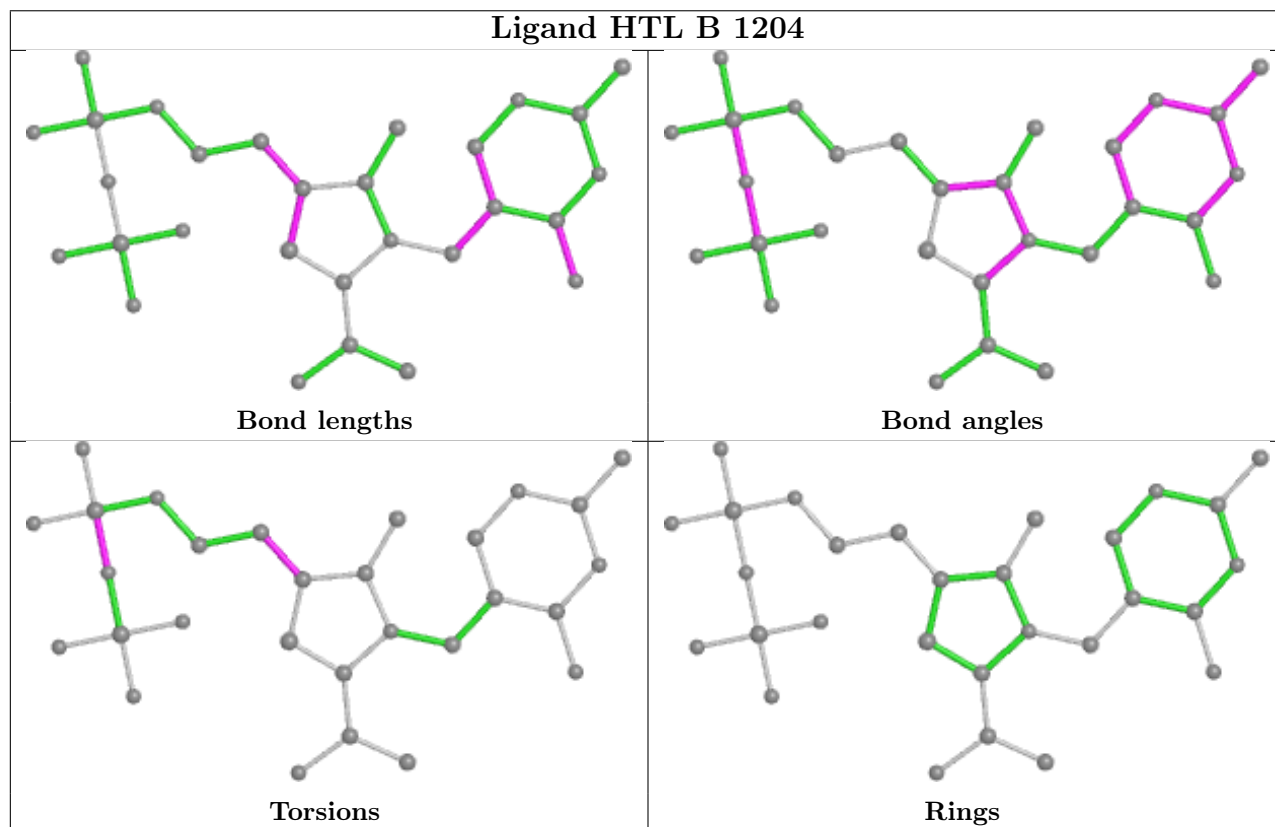
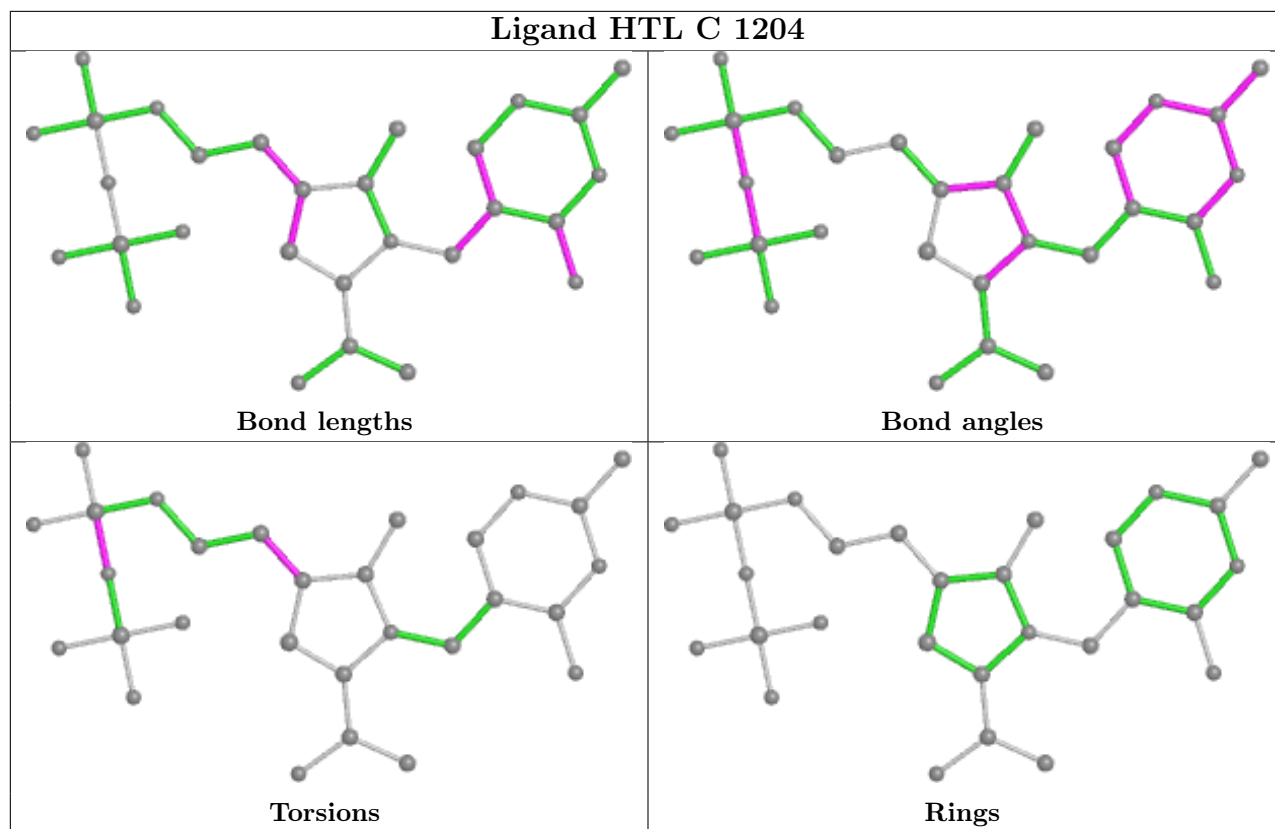
There are no ring outliers.

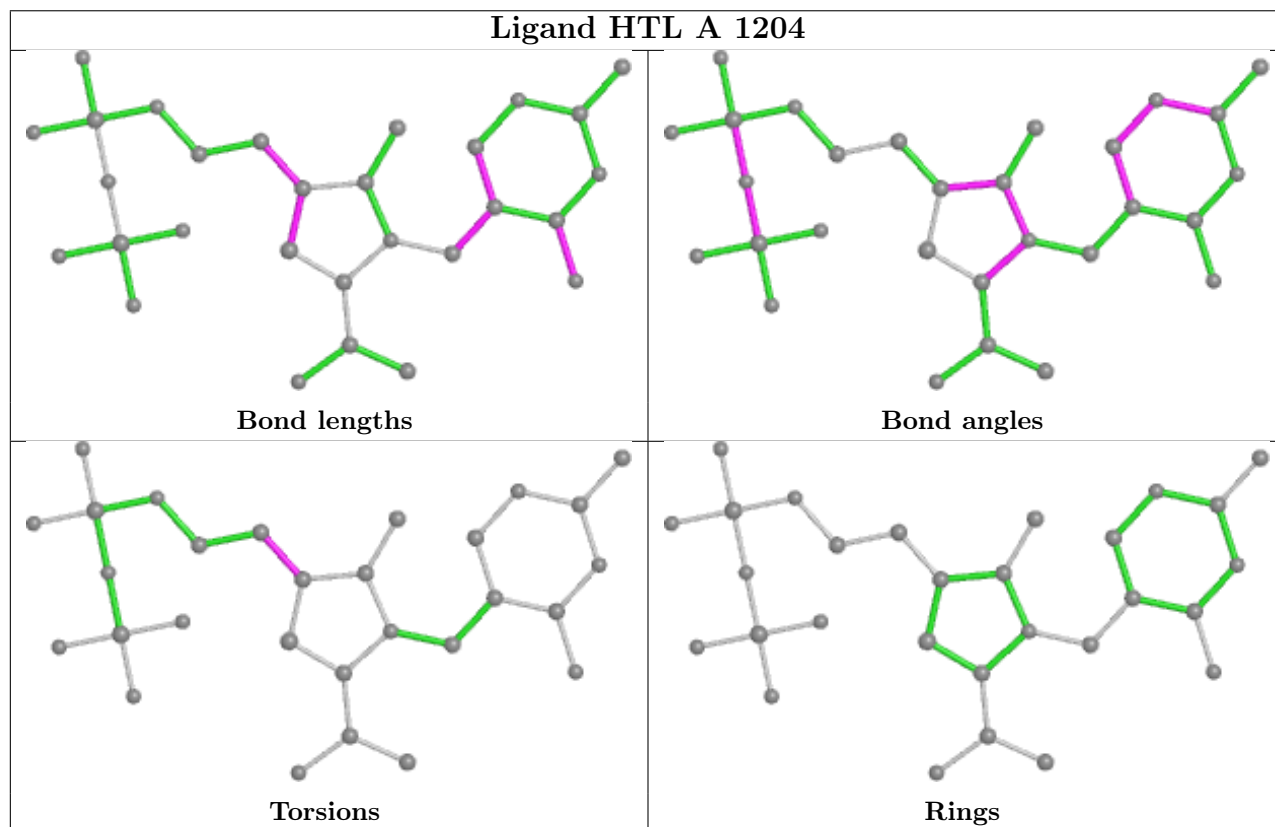
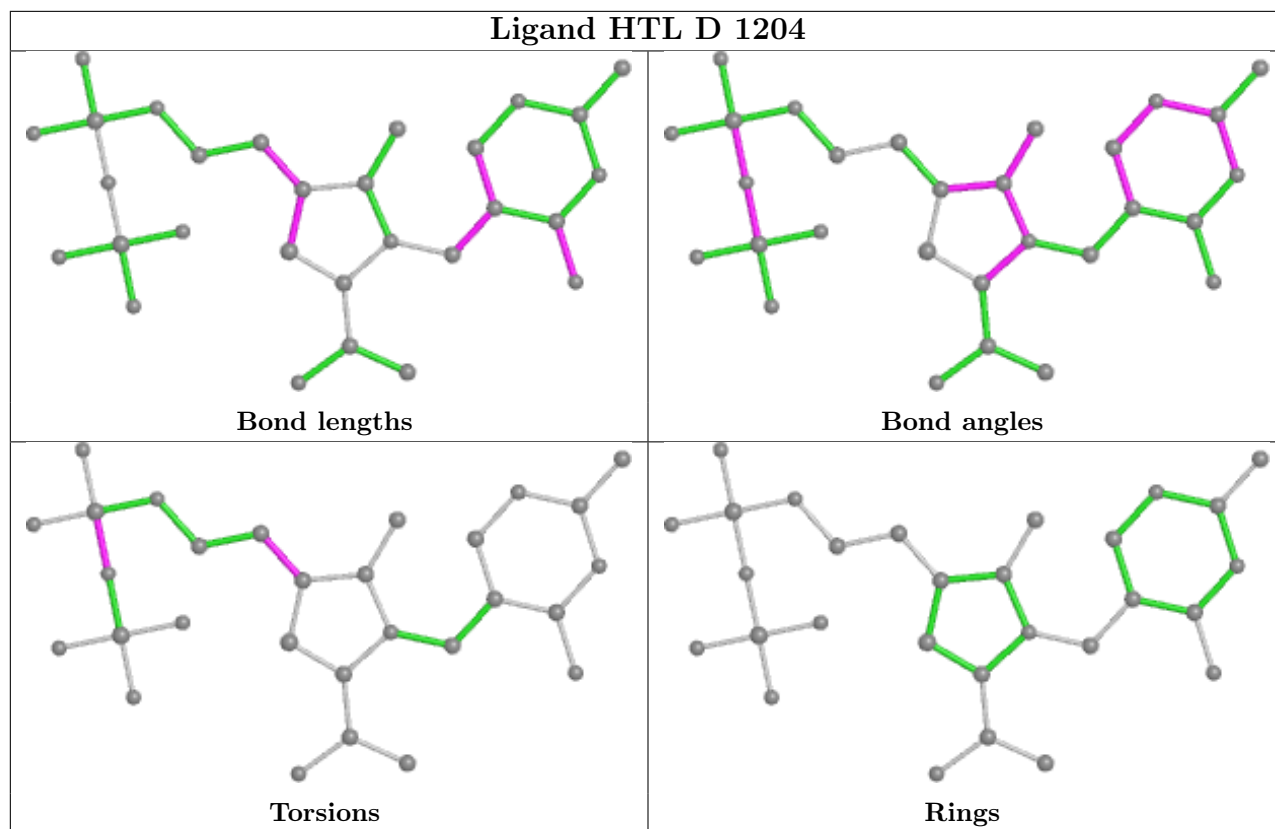
8 monomers are involved in 28 short contacts:

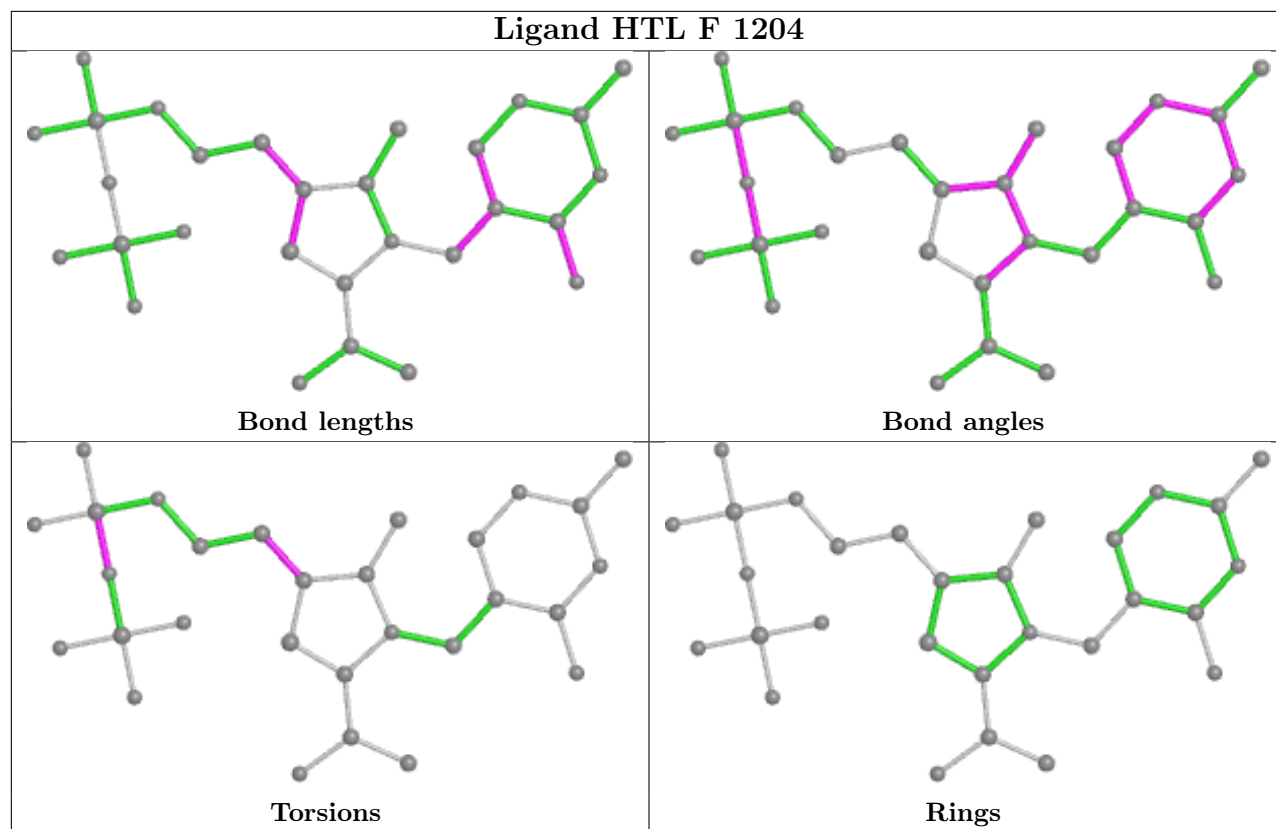
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	SF4	1	0
3	E	1204	HTL	3	0
3	C	1204	HTL	3	0
3	B	1204	HTL	3	0
3	D	1204	HTL	5	0
3	A	1204	HTL	5	0
3	F	1204	HTL	5	0
5	B	1207	SO4	3	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1165/1171 (99%)	-0.03	34 (2%)	51 35	60, 98, 165, 217	0
1	B	1165/1171 (99%)	0.04	47 (4%)	38 24	58, 101, 168, 225	0
1	C	1163/1171 (99%)	0.07	43 (3%)	41 26	52, 101, 169, 213	0
1	D	1164/1171 (99%)	-0.09	12 (1%)	82 72	61, 103, 161, 233	0
1	E	1164/1171 (99%)	-0.05	30 (2%)	56 40	46, 91, 153, 224	0
1	F	1169/1171 (99%)	-0.15	8 (0%)	87 81	45, 96, 154, 270	0
All	All	6990/7026 (99%)	-0.03	174 (2%)	57 43	45, 99, 163, 270	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	598	ASN	6.2
1	B	1126	PHE	5.2
1	F	561	THR	5.0
1	C	1044	VAL	5.0
1	B	734	ARG	4.8
1	E	784	VAL	4.8
1	B	684	GLU	4.6
1	B	733	PHE	4.6
1	C	788	PHE	4.5
1	C	730	GLY	4.3
1	B	710	ASP	4.3
1	D	713	GLY	4.1
1	B	910	TRP	4.0
1	E	508	LEU	4.0
1	C	787	ASN	4.0
1	C	789	ASN	3.9
1	F	598	ASN	3.9
1	C	1029	LEU	3.9
1	E	788	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	786	VAL	3.8
1	E	631	GLU	3.7
1	C	846	PRO	3.7
1	B	1125	SER	3.6
1	A	1012	GLY	3.5
1	A	705	LEU	3.5
1	A	899	VAL	3.4
1	B	1094	GLU	3.4
1	D	561	THR	3.4
1	A	1073	ALA	3.3
1	B	1058	ILE	3.3
1	A	1136	TYR	3.3
1	C	1042	ALA	3.3
1	C	991	LEU	3.3
1	B	1057	LEU	3.2
1	E	630	THR	3.2
1	E	558	ILE	3.2
1	E	540	ILE	3.2
1	B	728	ALA	3.2
1	C	598	ASN	3.2
1	A	946	LEU	3.1
1	B	1010	GLN	3.1
1	E	787	ASN	3.1
1	A	1100	LEU	3.1
1	E	606	LEU	3.1
1	A	1126	PHE	3.1
1	E	1034	MET	3.1
1	B	1044	VAL	3.1
1	C	784	VAL	3.1
1	C	1043	SER	3.1
1	B	735	ILE	3.0
1	C	786	VAL	3.0
1	A	1103	TYR	3.0
1	C	993	LEU	3.0
1	C	632	GLU	3.0
1	B	788	PHE	3.0
1	D	711	LEU	2.9
1	A	706	ALA	2.9
1	A	1068	LEU	2.9
1	B	897	ALA	2.9
1	B	720	THR	2.9
1	F	420	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1119	TYR	2.9
1	B	798	PHE	2.8
1	B	1069	ILE	2.8
1	B	891	ILE	2.8
1	C	708	PRO	2.8
1	B	686	CYS	2.8
1	B	1014	VAL	2.8
1	C	728	ALA	2.8
1	B	680	GLN	2.7
1	D	1012	GLY	2.7
1	A	1057	LEU	2.7
1	A	1020	GLY	2.7
1	C	733	PHE	2.7
1	A	1101	TYR	2.7
1	B	956	LEU	2.7
1	C	1054	MET	2.7
1	A	1096	GLY	2.6
1	B	1054	MET	2.6
1	B	1030	GLY	2.6
1	C	722	ASP	2.6
1	C	666	THR	2.6
1	A	1072	TYR	2.6
1	B	902	ALA	2.6
1	A	1024	THR	2.6
1	B	1106	GLN	2.6
1	A	1019	ALA	2.6
1	E	1041	VAL	2.6
1	C	486	CYS	2.6
1	D	420	PHE	2.6
1	B	1042	ALA	2.6
1	B	1012	GLY	2.5
1	E	561	THR	2.5
1	E	656	PHE	2.5
1	D	306	PHE	2.5
1	A	961	ILE	2.5
1	B	991	LEU	2.5
1	C	1106	GLN	2.5
1	C	420	PHE	2.5
1	C	1053	LEU	2.5
1	E	1068	LEU	2.5
1	E	419	PHE	2.5
1	B	730	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1049	SER	2.4
1	C	509	LEU	2.4
1	C	795	GLY	2.4
1	C	1030	GLY	2.4
1	E	487	HIS	2.4
1	C	421	GLY	2.4
1	F	586	THR	2.4
1	A	1011	THR	2.4
1	C	669	TYR	2.3
1	F	595	LEU	2.3
1	C	1058	ILE	2.3
1	B	682	GLN	2.3
1	D	589	LYS	2.3
1	D	602	VAL	2.3
1	E	688	GLN	2.3
1	C	1033	ALA	2.3
1	F	485	ALA	2.3
1	C	1165	TYR	2.3
1	A	1013	ALA	2.3
1	D	1126	PHE	2.3
1	B	722	ASP	2.3
1	B	906	ALA	2.3
1	B	705	LEU	2.3
1	B	1107	LEU	2.2
1	E	820	LEU	2.2
1	C	601	ALA	2.2
1	F	486	CYS	2.2
1	E	635	PHE	2.2
1	A	1097	TYR	2.2
1	B	712	ALA	2.2
1	E	497	LEU	2.2
1	A	1099	PRO	2.2
1	B	1101	TYR	2.2
1	C	670	GLU	2.2
1	E	485	ALA	2.2
1	A	727	GLU	2.2
1	E	724	ILE	2.2
1	A	710	ASP	2.2
1	C	1045	ALA	2.2
1	E	538	TYR	2.2
1	C	684	GLU	2.2
1	E	506	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	718	PHE	2.2
1	B	1071	ALA	2.2
1	E	824	LEU	2.2
1	E	687	ILE	2.1
1	E	526	MET	2.1
1	A	1109	GLN	2.1
1	C	567	ALA	2.1
1	A	942	VAL	2.1
1	C	739	PRO	2.1
1	B	1151	PHE	2.1
1	C	491	TYR	2.1
1	C	731	LEU	2.1
1	F	2	PRO	2.1
1	B	1097	TYR	2.1
1	A	988	VAL	2.1
1	B	1053	LEU	2.1
1	A	1043	SER	2.1
1	A	1157	ASP	2.1
1	C	606	LEU	2.1
1	E	515	ALA	2.1
1	B	739	PRO	2.0
1	C	798	PHE	2.0
1	E	632	GLU	2.0
1	A	1135	ARG	2.0
1	D	1057	LEU	2.0
1	B	518	MET	2.0
1	B	951	ARG	2.0
1	A	821	VAL	2.0
1	D	1097	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

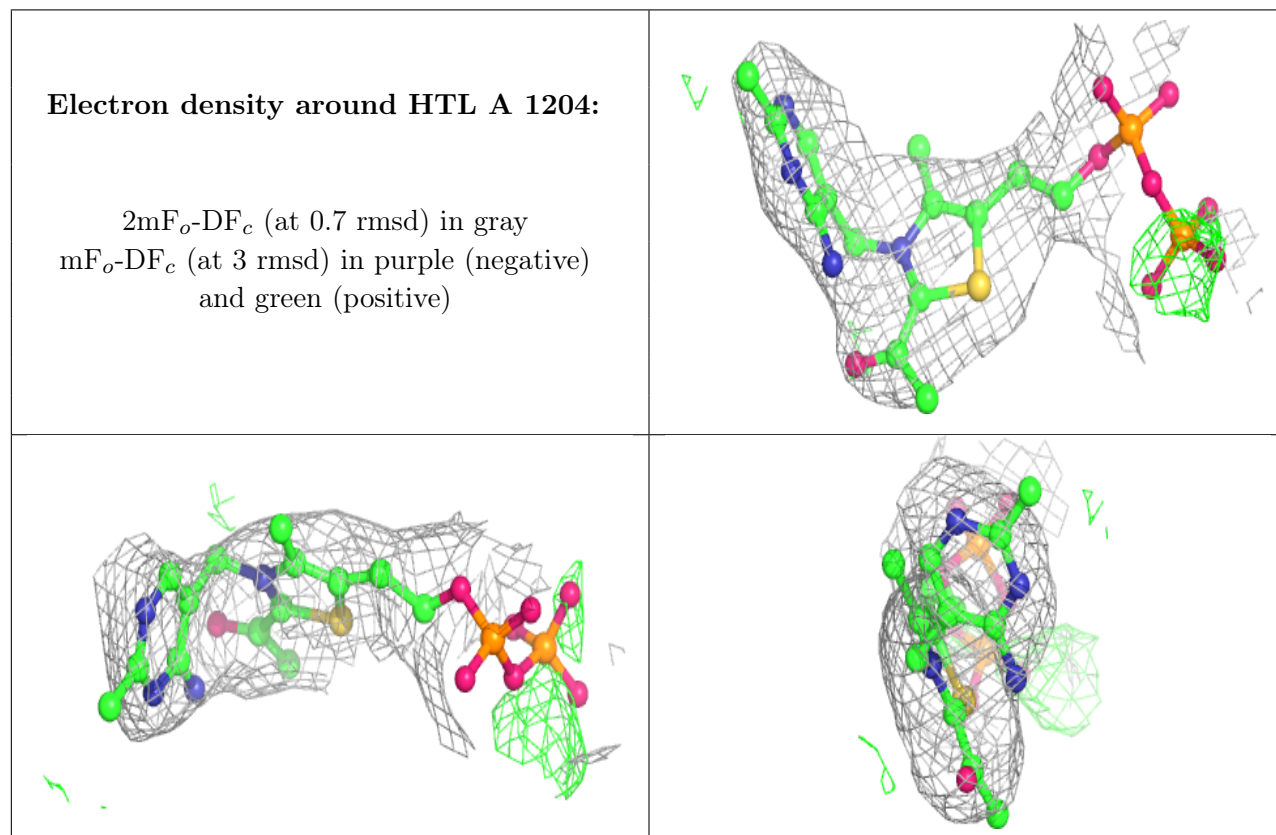
There are no monosaccharides in this entry.

6.4 Ligands i

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

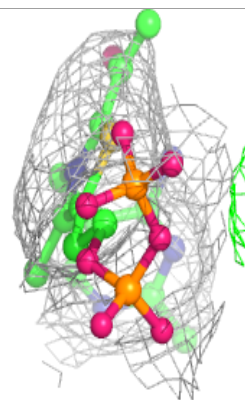
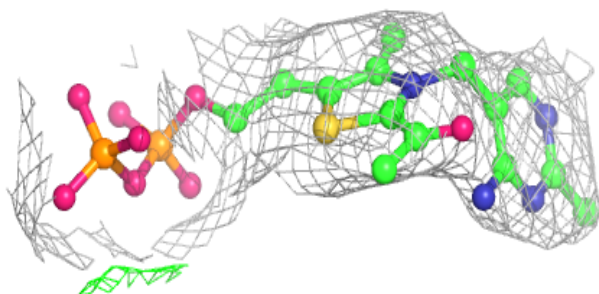
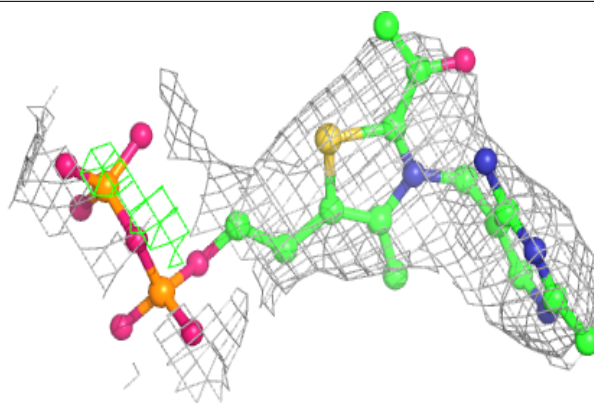
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	E	1206	5/5	0.89	0.15	102,108,110,111	0
4	MG	C	1205	1/1	0.91	0.13	49,49,49,49	0
5	SO4	B	1206	5/5	0.92	0.17	115,122,124,126	0
5	SO4	C	1206	5/5	0.94	0.12	100,107,107,112	0
5	SO4	B	1207	5/5	0.94	0.14	76,95,98,100	0
5	SO4	D	1206	5/5	0.95	0.10	125,127,128,129	0
5	SO4	A	1206	5/5	0.95	0.15	98,99,102,104	0
5	SO4	F	1206	5/5	0.95	0.12	130,130,131,134	0
3	HTL	A	1204	29/29	0.97	0.20	85,99,109,118	0
3	HTL	B	1204	29/29	0.97	0.19	79,107,118,132	0
3	HTL	C	1204	29/29	0.97	0.19	79,88,99,99	0
3	HTL	D	1204	29/29	0.97	0.17	65,82,91,98	0
2	SF4	B	1201	8/8	0.98	0.14	122,135,222,263	0
4	MG	D	1205	1/1	0.98	0.10	36,36,36,36	0
4	MG	F	1205	1/1	0.98	0.13	33,33,33,33	0
2	SF4	B	1202	8/8	0.98	0.19	108,115,203,205	0
2	SF4	C	1203	8/8	0.98	0.14	90,94,133,143	0
2	SF4	F	1203	8/8	0.98	0.28	60,85,105,246	0
3	HTL	E	1204	29/29	0.98	0.16	61,77,88,90	0
3	HTL	F	1204	29/29	0.98	0.18	54,79,94,98	0
4	MG	A	1205	1/1	0.98	0.13	64,64,64,64	0
4	MG	B	1205	1/1	0.98	0.13	66,66,66,66	0
2	SF4	A	1203	8/8	0.99	0.19	73,91,109,122	0
2	SF4	D	1201	8/8	0.99	0.22	98,102,110,122	0
2	SF4	D	1202	8/8	0.99	0.25	83,85,88,91	0
2	SF4	D	1203	8/8	0.99	0.22	71,73,74,101	0
2	SF4	E	1201	8/8	0.99	0.14	88,104,109,134	0
2	SF4	E	1202	8/8	0.99	0.17	70,83,99,130	0
4	MG	E	1205	1/1	0.99	0.10	43,43,43,43	0
2	SF4	E	1203	8/8	0.99	0.16	58,70,82,91	0
2	SF4	F	1201	8/8	0.99	0.24	81,96,107,120	0
2	SF4	F	1202	8/8	0.99	0.22	74,80,86,98	0
2	SF4	A	1201	8/8	0.99	0.16	116,151,193,199	0
2	SF4	A	1202	8/8	0.99	0.19	84,91,97,107	0
2	SF4	B	1203	8/8	0.99	0.20	90,99,120,122	0
2	SF4	C	1201	8/8	0.99	0.13	122,147,207,227	0
2	SF4	C	1202	8/8	0.99	0.16	86,123,210,229	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.

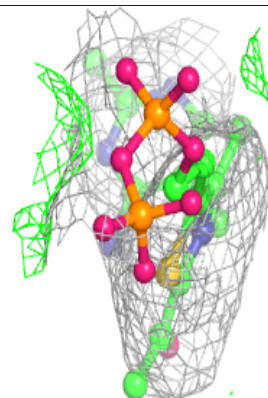
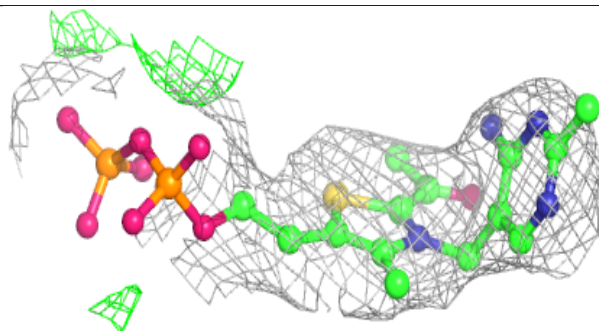
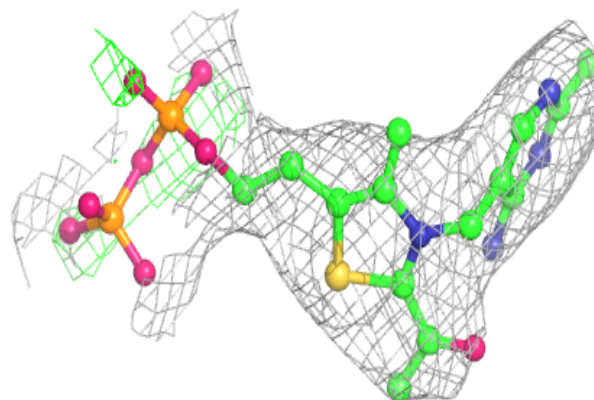


Electron density around HTL B 1204:

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

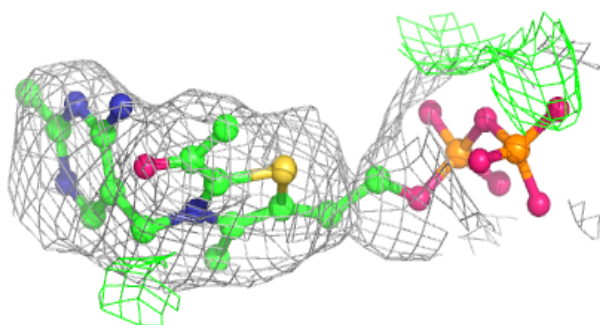
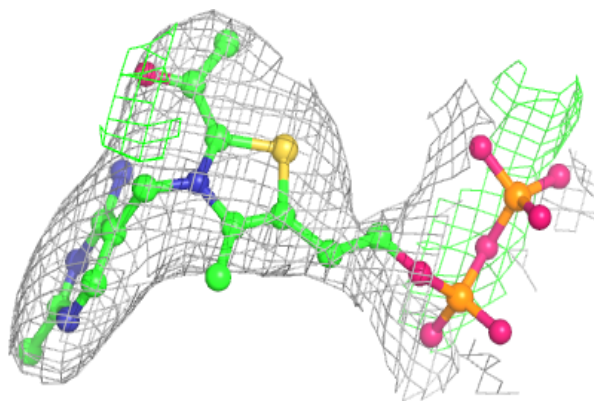
**Electron density around HTL C 1204:**

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

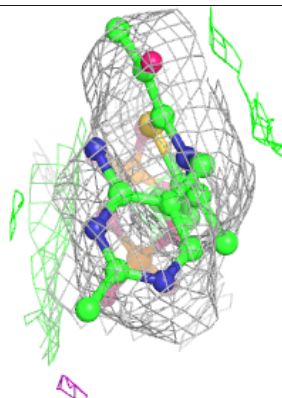
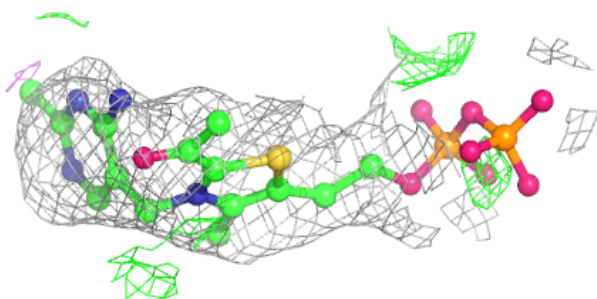
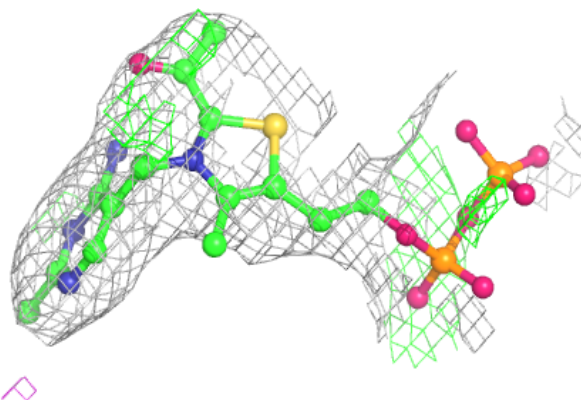


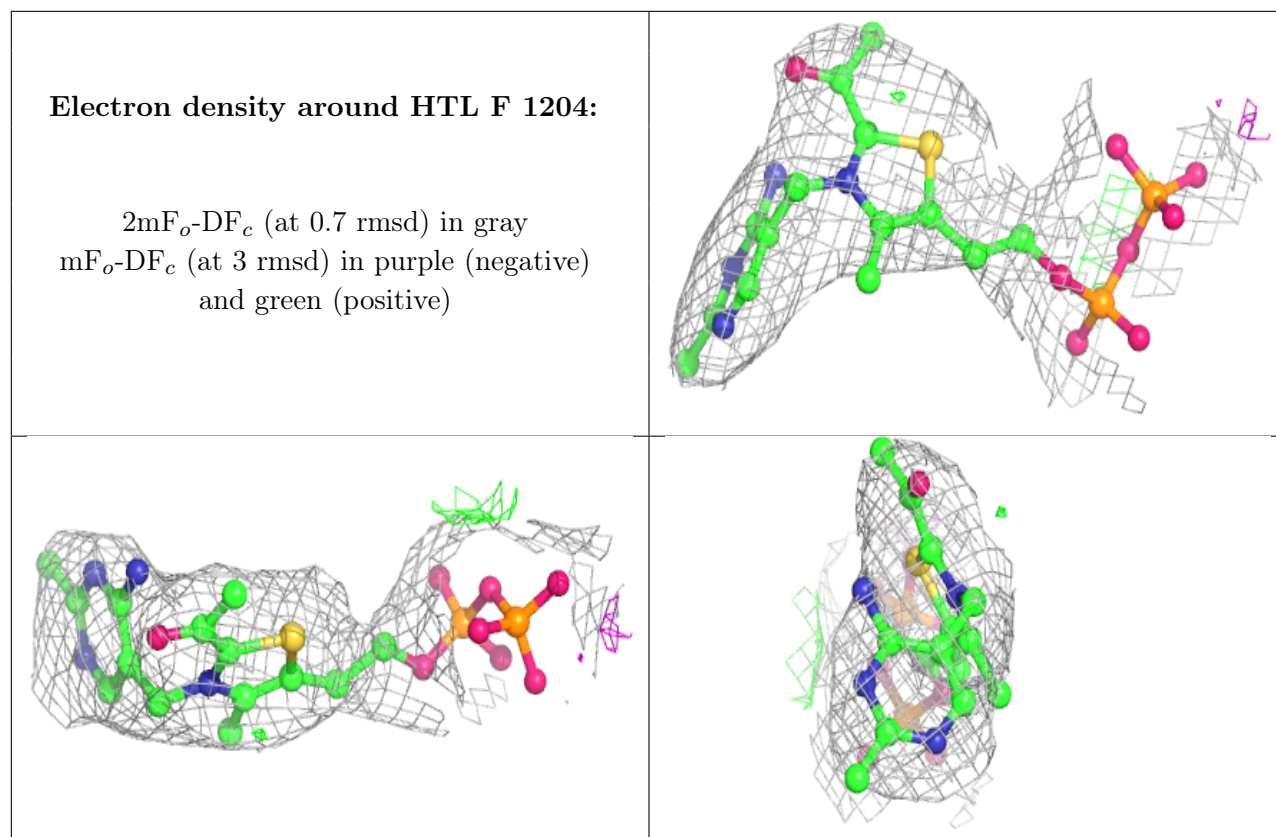
Electron density around HTL D 1204:

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

**Electron density around HTL 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.