



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:09 PM UTC

PDB ID : 6CIQ / pdb_00006ciq
Title : Pyruvate:ferredoxin oxidoreductase from Moorella thermoacetica with coenzyme A bound
Authors : Chen, P.Y.-T.; Drennan, C.L.
Deposited on : 2018-02-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

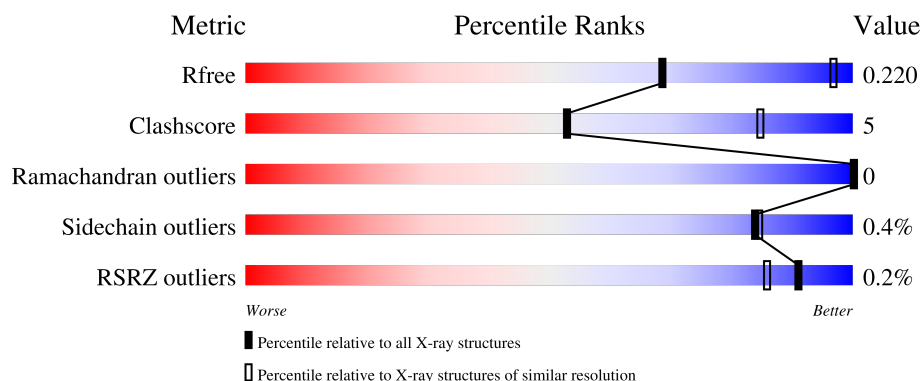
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	 88% 12%
1	B	1171	 86% 14%
1	C	1171	 86% 13%

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
2	SF4	B	1201	-	-	X	-

2 Entry composition [i](#)

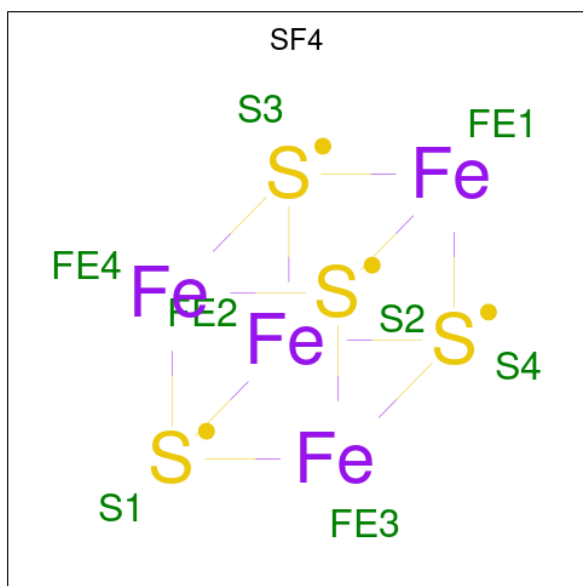
There are 6 unique types of molecules in this entry. The entry contains 26915 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1169	Total	C	N	O	S	0	0	0
			8893	5659	1509	1682	43			
1	B	1166	Total	C	N	O	S	0	0	0
			8860	5643	1506	1668	43			
1	C	1161	Total	C	N	O	S	0	0	0
			8836	5628	1499	1665	44			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



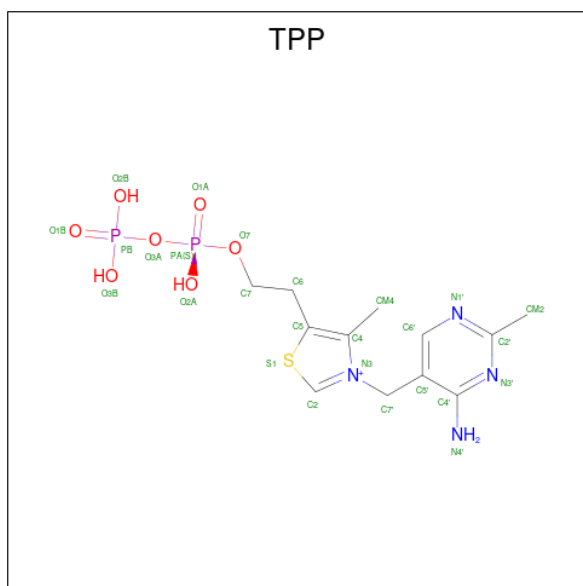
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

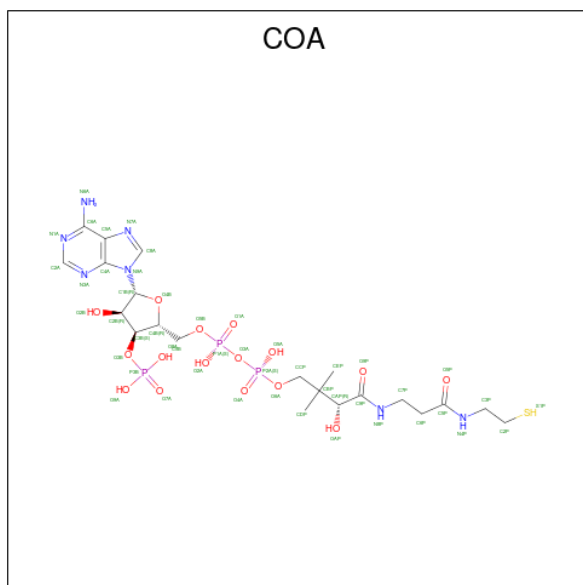


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

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

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
5	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
5	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	9	Total O 9 9	0	0
6	C	8	Total O 8 8	0	0

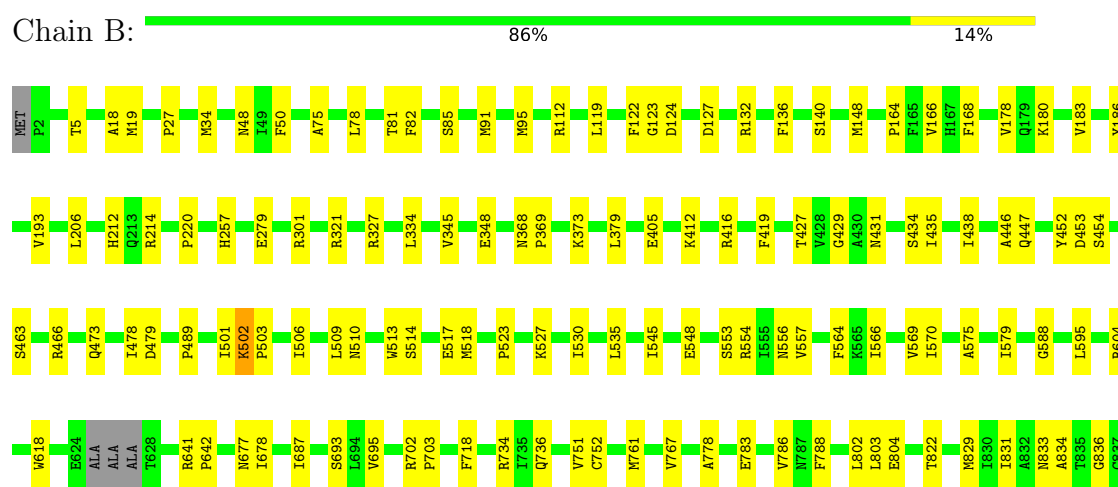
3 Residue-property plots

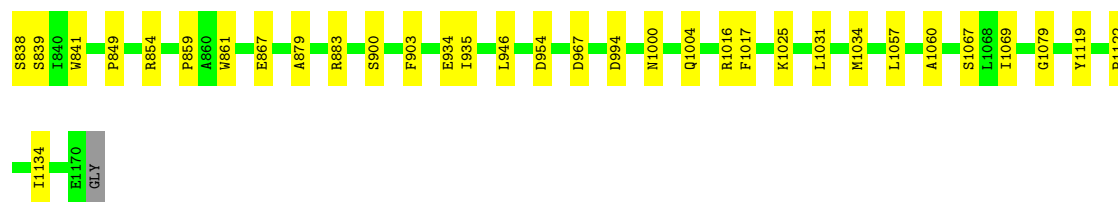
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

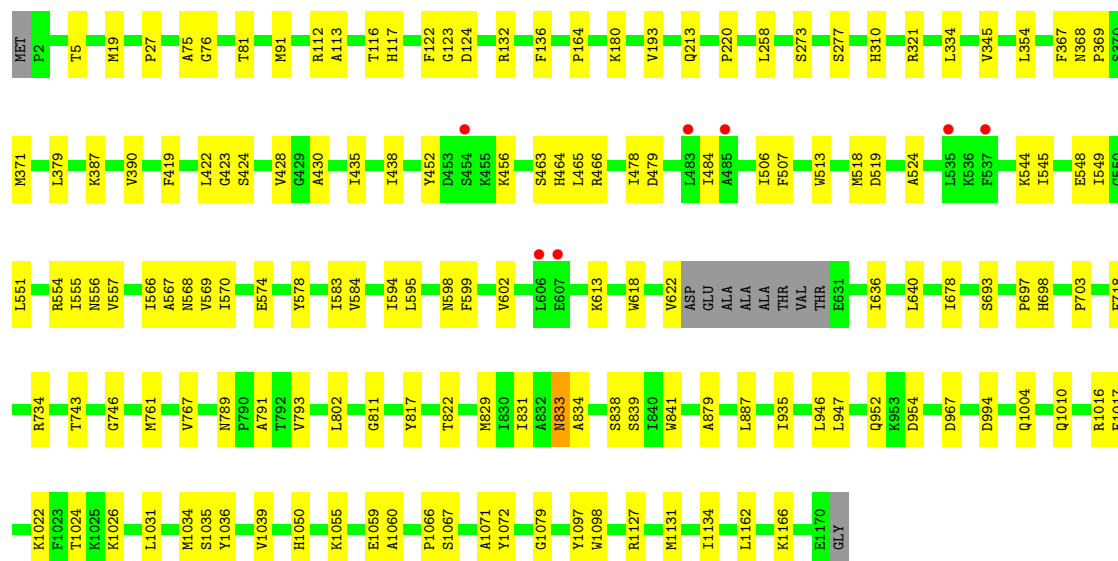
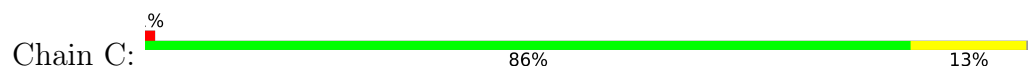


• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





• Molecule 1: PYRUVATE-FERREDONIN OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	337.71Å 106.99Å 120.47Å 90.00° 109.85° 90.00°	Depositor
Resolution (Å)	80.25 – 3.30 80.25 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (80.25-3.30) 96.5 (80.25-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.184 , 0.223 (Not available) , 0.220	Depositor DCC
R_{free} test set	2952 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26915	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/9086	0.32	0/12325
1	B	0.13	0/9054	0.32	0/12283
1	C	0.14	0/9030	0.33	0/12251
All	All	0.14	0/27170	0.33	0/36859

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	8893	0	8795	82	0
1	B	8860	0	8740	99	0
1	C	8836	0	8726	94	0
2	A	24	0	0	0	0
2	B	24	0	0	2	0
2	C	24	0	0	0	0
3	A	26	0	16	0	0
3	B	26	0	16	2	0
3	C	26	0	16	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	48	0	32	2	0
5	B	48	0	32	2	0
5	C	48	0	32	5	0
6	A	12	0	0	0	0
6	B	9	0	0	1	0
6	C	8	0	0	0	0
All	All	26915	0	26405	265	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 5.

All (265) 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:A:81:THR:HG21	1:A:91:MET:HE1	1.64	0.79
1:B:81:THR:HG21	1:B:91:MET:HE1	1.65	0.79
1:A:802:LEU:HB2	1:A:822:THR:HB	1.68	0.75
1:C:81:THR:HG21	1:C:91:MET:HE1	1.69	0.73
1:C:430:ALA:HB2	1:C:556:ASN:HB2	1.69	0.72
1:C:746:GLY:HA2	1:C:761:MET:HE3	1.70	0.72
1:C:802:LEU:HB2	1:C:822:THR:HB	1.73	0.71
1:C:419:PHE:HB2	1:C:463:SER:HB2	1.73	0.69
1:B:419:PHE:HB2	1:B:463:SER:HB2	1.74	0.68
1:B:345:VAL:HB	1:C:334:LEU:HD21	1.75	0.68
1:B:427:THR:O	1:B:431:ASN:ND2	2.27	0.67
1:B:802:LEU:HB2	1:B:822:THR:HB	1.77	0.65
1:A:746:GLY:HA2	1:A:761:MET:HE3	1.79	0.65
1:C:793:VAL:HG21	1:C:1050:HIS:HB3	1.80	0.64
1:B:348:GLU:OE1	1:C:387:LYS:NZ	2.32	0.62
1:B:588:GLY:HA2	1:B:595:LEU:HD21	1.82	0.62
1:A:290:GLU:OE2	1:B:412:LYS:HD3	2.01	0.61
1:A:1079:GLY:HA3	1:A:1134:ILE:HB	1.84	0.60
1:C:1055:LYS:HE2	1:C:1059:GLU:OE2	2.01	0.60
1:C:569:VAL:HG12	1:C:570:ILE:HG13	1.83	0.60
1:C:479:ASP:OD1	1:C:479:ASP:N	2.35	0.60
1:C:435:ILE:HD11	1:C:465:LEU:HB3	1.85	0.59
1:A:1076:ILE:HA	1:A:1082:MET:HE3	1.85	0.58
1:C:428:VAL:HG11	1:C:452:TYR:HE1	1.70	0.57
1:B:967:ASP:HB3	1:B:994:ASP:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:LYS:NZ	1:A:1024:THR:O	2.33	0.57
1:A:282:GLU:OE2	1:A:473:GLN:NE2	2.36	0.56
1:B:702:ARG:NH2	1:B:804:GLU:OE1	2.34	0.56
1:B:900:SER:OG	1:B:934:GLU:OE2	2.18	0.56
1:B:479:ASP:OD1	1:B:479:ASP:N	2.36	0.55
1:B:1031:LEU:HA	1:B:1034:MET:HE3	1.89	0.55
1:C:368:ASN:HB2	1:C:369:PRO:HD2	1.89	0.55
1:B:553:SER:OG	1:B:554:ARG:NH1	2.39	0.55
1:B:1060:ALA:HB1	1:B:1067:SER:HB3	1.88	0.55
1:B:570:ILE:HG23	1:B:575:ALA:HB2	1.89	0.55
1:A:967:ASP:HB3	1:A:994:ASP:HA	1.87	0.54
1:A:141:SER:HG	1:A:167:HIS:HE2	1.54	0.54
1:C:466:ARG:NH1	1:C:478:ILE:HA	2.23	0.54
1:B:513:TRP:HA	1:B:517:GLU:OE2	2.06	0.54
1:B:883:ARG:NH1	1:C:76:GLY:O	2.41	0.54
1:A:19:MET:HE1	1:A:193:VAL:HG22	1.88	0.54
1:B:509:LEU:HD23	1:B:518:MET:HE2	1.89	0.54
1:C:5:THR:HG22	1:C:180:LYS:HB2	1.90	0.54
1:C:438:ILE:HD12	1:C:569:VAL:HG11	1.90	0.54
1:A:1060:ALA:HB1	1:A:1067:SER:HB3	1.91	0.53
1:B:678:ILE:HD11	1:B:767:VAL:HG23	1.91	0.53
1:B:368:ASN:HB2	1:B:369:PRO:HD2	1.89	0.53
1:B:734:ARG:NH1	1:B:736:GLN:OE1	2.40	0.52
1:A:112:ARG:HH21	1:A:119:LEU:HD11	1.73	0.52
1:A:1031:LEU:HA	1:A:1034:MET:HE3	1.90	0.52
1:C:321:ARG:HB3	1:C:379:LEU:HD22	1.91	0.52
1:C:1022:LYS:NZ	1:C:1024:THR:O	2.42	0.52
1:B:502:LYS:HG2	1:B:503:PRO:HD2	1.92	0.52
1:C:697:PRO:HG2	1:C:811:GLY:HA2	1.92	0.52
1:B:695:VAL:HG11	1:B:751:VAL:HG21	1.92	0.52
1:C:1004:GLN:HG2	1:C:1017:PHE:CE2	2.44	0.52
1:B:18:ALA:HB2	1:B:186:TYR:CZ	2.45	0.51
1:C:935:ILE:HD13	1:C:947:LEU:HD23	1.93	0.51
1:B:879:ALA:HB3	1:C:75:ALA:HB3	1.92	0.51
1:A:479:ASP:N	1:A:479:ASP:OD1	2.42	0.51
1:C:599:PHE:O	1:C:602:VAL:HG22	2.11	0.51
1:C:1060:ALA:HB1	1:C:1067:SER:HB3	1.93	0.51
1:B:556:ASN:OD1	1:B:557:VAL:N	2.43	0.51
1:C:1026:LYS:HZ3	1:C:1098:TRP:HZ3	1.58	0.51
1:B:1004:GLN:HG2	1:B:1017:PHE:CE2	2.46	0.50
1:C:321:ARG:HG2	1:C:354:LEU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:HG	1:C:277:SER:HG	1.57	0.50
1:A:793:VAL:HG21	1:A:1050:HIS:HB3	1.94	0.50
1:B:212:HIS:NE2	1:B:214:ARG:NH1	2.55	0.50
1:C:967:ASP:HB3	1:C:994:ASP:HA	1.93	0.50
1:A:482:ASP:OD1	1:A:502:LYS:HE2	2.11	0.50
1:A:576:ILE:HD13	1:A:606:LEU:HD11	1.94	0.50
1:B:140:SER:HB2	1:B:168:PHE:CZ	2.47	0.49
1:C:513:TRP:HB2	1:C:518:MET:HE2	1.94	0.49
1:A:1113:ASN:ND2	1:A:1115:PHE:H	2.10	0.49
1:B:1031:LEU:HD23	1:C:1035:SER:HB2	1.94	0.49
1:C:464:HIS:HB3	1:C:478:ILE:HG13	1.94	0.49
1:A:838:SER:HA	1:A:841:TRP:CE2	2.47	0.49
1:B:112:ARG:HA	1:B:123:GLY:HA2	1.93	0.49
1:B:545:ILE:HG23	1:B:604:ARG:HD2	1.94	0.49
1:A:802:LEU:HD13	1:A:859:PRO:HD3	1.94	0.49
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	1.95	0.49
1:C:1079:GLY:HA3	1:C:1134:ILE:HB	1.95	0.48
1:B:18:ALA:HB2	1:B:186:TYR:CE1	2.48	0.48
1:C:1039:VAL:HG22	1:C:1066:PRO:HG2	1.95	0.48
1:A:887:LEU:HD13	1:A:952:GLN:HB2	1.94	0.48
1:C:574:GLU:HB3	1:C:578:TYR:CE2	2.49	0.48
1:A:112:ARG:NH2	1:A:119:LEU:HD11	2.28	0.48
1:B:693:SER:HB2	1:B:703:PRO:HD3	1.96	0.48
1:A:146:GLU:OE1	1:A:301:ARG:NH2	2.47	0.47
1:B:112:ARG:NH2	1:B:119:LEU:HD11	2.29	0.47
1:B:334:LEU:HD21	1:C:345:VAL:HB	1.96	0.47
1:C:551:LEU:O	1:C:554:ARG:HG2	2.13	0.47
1:B:1000:ASN:OD1	5:B:1206:COA:H21	2.14	0.47
1:A:583:ILE:HG22	1:A:595:LEU:HD22	1.96	0.47
1:A:85:SER:HB2	1:A:112:ARG:HB3	1.97	0.47
1:C:1031:LEU:HA	1:C:1034:MET:HE3	1.96	0.47
1:A:141:SER:HB2	1:A:169:PHE:HB3	1.96	0.47
1:A:326:ASP:CG	1:A:336:GLU:HB3	2.38	0.47
1:A:1004:GLN:HG2	1:A:1017:PHE:CE2	2.50	0.47
1:B:527:LYS:HD2	1:B:618:TRP:CE2	2.49	0.47
1:A:570:ILE:HG13	1:A:575:ALA:HB2	1.97	0.47
1:B:838:SER:HA	1:B:841:TRP:CE2	2.50	0.47
1:C:545:ILE:O	1:C:549:ILE:HG13	2.15	0.47
1:B:802:LEU:HD13	1:B:859:PRO:HD3	1.96	0.46
1:C:1072:TYR:HB2	1:C:1098:TRP:CE2	2.50	0.46
1:A:283:GLU:OE2	1:A:476:TYR:OH	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PRO:HB3	1:B:1017:PHE:HE2	1.80	0.46
1:B:321:ARG:HB3	1:B:379:LEU:HD22	1.97	0.46
1:C:554:ARG:HD2	5:C:1206:COA:C4A	2.46	0.46
1:C:678:ILE:HD11	1:C:767:VAL:HG23	1.96	0.46
5:C:1206:COA:H8A	5:C:1206:COA:H52A	1.97	0.46
1:A:189:MET:O	1:A:193:VAL:HG23	2.16	0.46
1:A:453:ASP:OD1	1:A:454:SER:N	2.48	0.46
1:B:416:ARG:HG2	1:B:466:ARG:HG2	1.98	0.46
1:B:641:ARG:HB2	1:B:642:PRO:HD3	1.98	0.46
1:C:556:ASN:OD1	1:C:557:VAL:N	2.48	0.46
1:A:263:GLY:HA3	1:A:296:GLY:HA2	1.98	0.46
1:B:279:GLU:OE1	1:B:473:GLN:HG2	2.16	0.46
1:B:453:ASP:OD1	1:B:454:SER:N	2.48	0.46
1:C:506:ILE:HG21	1:C:566:ILE:HG21	1.96	0.46
1:B:373:LYS:HE2	1:B:405:GLU:OE2	2.16	0.46
1:B:903:PHE:HB2	1:B:934:GLU:OE2	2.15	0.46
1:B:220:PRO:HD3	1:C:122:PHE:CE2	2.52	0.45
1:C:554:ARG:HD2	5:C:1206:COA:C5A	2.46	0.45
1:A:594:ILE:O	1:A:598:ASN:ND2	2.45	0.45
3:B:1204:TPP:H2	6:B:1308:HOH:O	2.15	0.45
1:A:424:SER:N	5:A:1206:COA:O4A	2.50	0.45
1:B:677:ASN:HB2	1:B:761:MET:HE3	1.99	0.45
1:C:584:VAL:HA	1:C:595:LEU:HD11	1.98	0.45
1:B:206:LEU:HD23	1:B:212:HIS:CE1	2.52	0.45
1:A:1002:GLY:HA3	1:A:1016:ARG:NH1	2.32	0.45
1:B:501:ILE:HD13	1:B:535:LEU:HD13	1.98	0.45
1:B:506:ILE:HG21	1:B:566:ILE:HD12	1.97	0.45
1:B:435:ILE:HG23	1:B:446:ALA:HB1	1.96	0.45
1:C:484:ILE:O	1:C:507:PHE:HA	2.17	0.45
1:C:838:SER:HA	1:C:841:TRP:CE2	2.52	0.45
1:C:1127:ARG:O	1:C:1131:MET:HG2	2.17	0.45
1:B:75:ALA:HB3	1:C:879:ALA:HB3	1.99	0.45
1:B:836:GLY:HA2	3:B:1204:TPP:S1	2.57	0.45
1:A:422:LEU:N	1:A:425:ASP:OD2	2.49	0.45
1:B:514:SER:H	1:B:517:GLU:HG2	1.82	0.45
1:A:681:TRP:CD1	1:A:735:ILE:HB	2.52	0.44
1:B:91:MET:O	1:B:95:MET:HG3	2.17	0.44
1:B:834:ALA:O	1:B:839:SER:HB3	2.17	0.44
1:A:545:ILE:HB	1:A:558:ILE:HD13	1.98	0.44
1:B:718:PHE:HE1	1:B:778:ALA:HB2	1.82	0.44
1:C:113:ALA:HB2	1:C:124:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASP:OD1	1:A:527:LYS:NZ	2.50	0.44
1:A:18:ALA:HB2	1:A:186:TYR:CE1	2.53	0.44
1:A:419:PHE:HB2	1:A:463:SER:HB2	1.99	0.44
1:B:132:ARG:HH11	1:C:132:ARG:HH11	1.66	0.44
1:B:257:HIS:O	1:B:301:ARG:HG3	2.17	0.44
1:B:564:PHE:CD2	1:B:579:ILE:HD11	2.53	0.44
1:C:698:HIS:CE1	1:C:743:THR:HG21	2.52	0.44
1:C:834:ALA:O	1:C:839:SER:HB3	2.17	0.44
1:A:85:SER:HA	1:A:127:ASP:HB3	2.00	0.44
1:A:556:ASN:OD1	1:A:557:VAL:N	2.50	0.44
1:C:116:THR:OG1	1:C:117:HIS:N	2.51	0.44
1:A:128:VAL:HG21	1:A:168:PHE:CD2	2.52	0.44
1:A:659:ASP:OD1	1:A:659:ASP:N	2.51	0.44
1:C:466:ARG:HH11	1:C:478:ILE:HA	1.83	0.44
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	2.00	0.43
1:A:206:LEU:HD23	1:A:212:HIS:CE1	2.53	0.43
1:B:136:PHE:CE2	1:B:164:PRO:HB2	2.54	0.43
1:C:567:ALA:O	1:C:568:ASN:ND2	2.51	0.43
1:C:636:ILE:HA	1:C:640:LEU:HB3	2.00	0.43
1:A:556:ASN:ND2	1:A:587:TYR:OH	2.51	0.43
1:B:783:GLU:HB2	1:B:854:ARG:HD2	2.00	0.43
1:B:829:MET:HE2	1:B:831:ILE:HD11	1.99	0.43
1:C:19:MET:HE1	1:C:193:VAL:HG22	2.00	0.43
1:A:430:ALA:HB2	1:A:556:ASN:HB2	2.01	0.43
1:A:1139:LEU:HD21	1:A:1150:LEU:HD12	2.00	0.43
1:C:954:ASP:OD1	1:C:954:ASP:N	2.52	0.43
1:A:954:ASP:OD1	1:A:954:ASP:N	2.52	0.43
1:C:613:LYS:HA	1:C:613:LYS:HD3	1.76	0.43
1:C:1004:GLN:HG3	1:C:1016:ARG:HB2	2.00	0.43
1:C:829:MET:HE2	1:C:831:ILE:HD11	2.01	0.43
1:A:32:SER:O	1:A:36:GLU:HG3	2.19	0.43
1:B:18:ALA:O	1:B:48:ASN:HB2	2.19	0.43
1:C:594:ILE:O	1:C:598:ASN:ND2	2.49	0.43
1:A:427:THR:O	1:A:431:ASN:ND2	2.52	0.43
1:A:136:PHE:CD2	1:A:166:VAL:HG23	2.54	0.43
1:B:122:PHE:CE2	1:C:220:PRO:HD3	2.53	0.43
1:C:371:MET:HB3	1:C:390:VAL:HG11	2.00	0.43
1:C:718:PHE:CZ	1:C:734:ARG:HD3	2.54	0.43
1:C:112:ARG:HA	1:C:123:GLY:HA2	2.00	0.43
1:A:514:SER:O	1:A:518:MET:HG2	2.19	0.42
1:B:530:ILE:HA	1:B:535:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:GLU:OE1	1:B:867:GLU:N	2.50	0.42
5:A:1206:COA:C8A	5:A:1206:COA:H51A	2.49	0.42
1:B:50:PHE:CZ	1:B:78:LEU:HD12	2.54	0.42
1:B:489:PRO:HG3	1:B:510:ASN:O	2.20	0.42
1:B:523:PRO:O	1:B:527:LYS:HG3	2.19	0.42
1:B:687:ILE:HG12	2:B:1201:SF4:S3	2.59	0.42
1:C:422:LEU:HG	1:C:423:GLY:N	2.34	0.42
1:C:519:ASP:CG	1:C:618:TRP:HE1	2.27	0.42
1:C:817:TYR:CZ	1:C:1071:ALA:HB1	2.54	0.42
1:A:998:TYR:CE1	1:A:1006:SER:HB2	2.54	0.42
1:A:781:LEU:O	1:A:854:ARG:NH2	2.52	0.42
1:C:693:SER:HB2	1:C:703:PRO:HD3	2.01	0.42
1:A:604:ARG:HA	1:A:607:GLU:CD	2.44	0.42
1:A:464:HIS:CE1	1:A:477:LEU:HD22	2.55	0.42
1:C:887:LEU:HD13	1:C:952:GLN:HB2	2.00	0.42
1:A:694:LEU:HD22	1:A:793:VAL:HG13	2.01	0.42
1:A:1004:GLN:HG3	1:A:1016:ARG:HB2	2.01	0.42
1:A:1119:TYR:HE2	1:A:1122:PRO:HA	1.85	0.42
1:C:789:ASN:OD1	1:C:791:ALA:HB3	2.19	0.42
1:C:1162:LEU:HG	1:C:1166:LYS:HE3	2.01	0.42
1:A:113:ALA:HB2	1:A:124:ASP:OD2	2.20	0.42
1:B:124:ASP:HA	1:B:327:ARG:HD3	2.01	0.42
1:B:178:VAL:O	1:B:447:GLN:HA	2.20	0.42
1:C:544:LYS:O	1:C:548:GLU:HG2	2.19	0.42
1:A:678:ILE:HD11	1:A:767:VAL:HG23	2.03	0.41
1:A:704:TYR:CE1	1:A:736:GLN:HB3	2.55	0.41
1:B:19:MET:HE1	1:B:193:VAL:HG22	2.01	0.41
1:C:428:VAL:HG11	1:C:452:TYR:CE1	2.52	0.41
1:A:416:ARG:HG2	1:A:466:ARG:HG2	2.02	0.41
1:B:752:CYS:HA	2:B:1201:SF4:S1	2.61	0.41
1:B:1025:LYS:NZ	1:C:1036:TYR:O	2.44	0.41
1:B:935:ILE:HG12	1:B:946:LEU:HB3	2.01	0.41
1:C:136:PHE:CE2	1:C:164:PRO:HB2	2.55	0.41
1:A:136:PHE:CE2	1:A:164:PRO:HB2	2.55	0.41
1:C:371:MET:HB3	1:C:390:VAL:CG1	2.50	0.41
1:C:1010:GLN:HG3	1:C:1097:TYR:CZ	2.55	0.41
1:A:1079:GLY:O	1:A:1134:ILE:HG13	2.20	0.41
1:C:456:LYS:O	5:C:1206:COA:OAP	2.26	0.41
1:C:583:ILE:HD13	1:C:598:ASN:HB3	2.02	0.41
1:A:416:ARG:HB3	1:A:478:ILE:HD12	2.01	0.41
1:A:480:GLN:HA	1:A:500:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:GLN:HG3	1:B:1016:ARG:HB2	2.01	0.41
1:B:1057:LEU:HD23	1:B:1069:ILE:HD13	2.03	0.41
1:A:803:LEU:HD12	1:A:849:PRO:HB2	2.02	0.41
1:B:695:VAL:HG21	1:B:751:VAL:HG21	2.03	0.41
1:C:258:LEU:HD12	1:C:310:HIS:CG	2.56	0.41
1:A:422:LEU:HG	1:A:423:GLY:N	2.36	0.41
1:C:27:PRO:HB3	1:C:1017:PHE:HE2	1.84	0.41
1:B:34:MET:HE3	1:B:82:PHE:HB3	2.03	0.41
1:B:416:ARG:HB3	1:B:478:ILE:HD13	2.03	0.41
1:B:429:GLY:N	5:B:1206:COA:O1A	2.46	0.41
1:B:434:SER:O	1:B:438:ILE:HG13	2.21	0.41
1:B:548:GLU:OE1	1:B:604:ARG:NH1	2.54	0.41
1:C:1072:TYR:HB2	1:C:1098:TRP:CD2	2.56	0.41
1:A:257:HIS:O	1:A:301:ARG:HG3	2.21	0.41
1:A:641:ARG:HB2	1:A:642:PRO:HD3	2.02	0.40
1:B:5:THR:HG22	1:B:180:LYS:HB2	2.02	0.40
1:B:1119:TYR:HE2	1:B:1122:PRO:HA	1.86	0.40
1:A:667:THR:HG22	1:A:847:ALA:HB1	2.03	0.40
1:B:148:MET:HE3	1:B:183:VAL:HA	2.03	0.40
1:B:861:TRP:HE3	1:C:213:GLN:HG3	1.86	0.40
1:C:524:ALA:HB1	1:C:622:VAL:HA	2.04	0.40
1:C:1010:GLN:HG3	1:C:1097:TYR:OH	2.20	0.40
1:A:790:PRO:HG3	1:A:799:ARG:NH2	2.37	0.40
1:A:903:PHE:HB2	1:A:934:GLU:OE2	2.21	0.40
1:B:786:VAL:HG13	1:B:788:PHE:H	1.85	0.40
1:B:954:ASP:OD1	1:B:954:ASP:N	2.49	0.40
1:A:112:ARG:HA	1:A:123:GLY:HA2	2.03	0.40
1:A:783:GLU:HB2	1:A:854:ARG:HD2	2.03	0.40
1:A:1080:ILE:HD13	1:A:1088:GLU:HG2	2.03	0.40
1:B:85:SER:HA	1:B:127:ASP:HB3	2.04	0.40
1:B:803:LEU:HD12	1:B:849:PRO:HB2	2.03	0.40
1:C:367:PHE:HA	1:C:371:MET:SD	2.61	0.40
1:C:424:SER:N	5:C:1206:COA:O5A	2.50	0.40
1:B:136:PHE:CD2	1:B:166:VAL:HG23	2.56	0.40
1:C:833:ASN:HD22	1:C:834:ALA:N	2.20	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	1167/1171 (100%)	1143 (98%)	24 (2%)	0	100	100
1	B	1162/1171 (99%)	1135 (98%)	27 (2%)	0	100	100
1	C	1157/1171 (99%)	1136 (98%)	21 (2%)	0	100	100
All	All	3486/3513 (99%)	3414 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	918/932 (98%)	914 (100%)	4 (0%)	84	84
1	B	911/932 (98%)	907 (100%)	4 (0%)	84	84
1	C	912/932 (98%)	909 (100%)	3 (0%)	86	86
All	All	2741/2796 (98%)	2730 (100%)	11 (0%)	84	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	TYR
1	A	460	VAL
1	A	719	VAL
1	A	833	ASN
1	B	452	TYR

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Mol	Chain	Res	Type
1	B	502	LYS
1	B	569	VAL
1	B	833	ASN
1	C	555	ILE
1	C	833	ASN
1	C	946	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	431	ASN
1	A	797	GLN
1	A	823	GLN
1	A	1113	ASN
1	A	1142	GLN
1	B	255	HIS
1	B	398	HIS
1	B	406	HIS
1	B	431	ASN
1	B	441	HIS
1	B	470	GLN
1	B	560	GLN
1	B	680	GLN
1	B	682	GLN
1	B	833	ASN
1	B	952	GLN
1	B	1113	ASN
1	C	55	GLN
1	C	247	GLN
1	C	255	HIS
1	C	433	ASN
1	C	480	GLN
1	C	547	GLN
1	C	560	GLN
1	C	568	ASN
1	C	682	GLN
1	C	833	ASN
1	C	952	GLN
1	C	1050	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	C	1201	1	0,12,12	-	-	-		
2	SF4	C	1203	1	0,12,12	-	-	-		
5	COA	A	1206	-	47,50,50	1.19	5 (10%)	69,75,75	1.72	12 (17%)
5	COA	B	1206	-	47,50,50	1.22	5 (10%)	69,75,75	1.72	14 (20%)
3	TPP	C	1204	4	26,27,27	1.89	8 (30%)	38,40,40	1.92	11 (28%)
2	SF4	B	1202	1	0,12,12	-	-	-		
5	COA	C	1206	-	47,50,50	1.22	5 (10%)	69,75,75	1.65	11 (15%)
2	SF4	B	1201	1	0,12,12	-	-	-		
2	SF4	A	1201	1	0,12,12	-	-	-		
3	TPP	A	1204	4	26,27,27	1.87	8 (30%)	38,40,40	1.85	10 (26%)
2	SF4	A	1202	1	0,12,12	-	-	-		
2	SF4	C	1202	1	0,12,12	-	-	-		
3	TPP	B	1204	4	26,27,27	1.86	7 (26%)	38,40,40	1.79	9 (23%)
2	SF4	A	1203	1	0,12,12	-	-	-		
2	SF4	B	1203	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	1201	1	-	-	0/6/5/5
2	SF4	C	1203	1	-	-	0/6/5/5
5	COA	A	1206	-	-	11/48/64/64	0/3/3/3
5	COA	B	1206	-	-	3/48/64/64	0/3/3/3
3	TPP	C	1204	4	-	3/17/17/17	0/2/2/2
2	SF4	B	1202	1	-	-	0/6/5/5
5	COA	C	1206	-	-	11/48/64/64	0/3/3/3
3	TPP	A	1204	4	-	4/17/17/17	0/2/2/2
2	SF4	A	1201	1	-	-	0/6/5/5
2	SF4	B	1201	1	-	-	0/6/5/5
2	SF4	A	1202	1	-	-	0/6/5/5
2	SF4	C	1202	1	-	-	0/6/5/5
3	TPP	B	1204	4	-	3/17/17/17	0/2/2/2
2	SF4	A	1203	1	-	-	0/6/5/5
2	SF4	B	1203	1	-	-	0/6/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1206	COA	C8A-N9A	5.05	1.46	1.37
5	C	1206	COA	C8A-N9A	4.91	1.45	1.37
5	B	1206	COA	C8A-N9A	4.86	1.45	1.37
3	A	1204	TPP	C7'-C5'	3.65	1.57	1.51
3	C	1204	TPP	C4'-N4'	3.65	1.43	1.34
3	A	1204	TPP	C4'-N4'	3.63	1.43	1.34
3	B	1204	TPP	C5-S1	-3.63	1.63	1.72
3	B	1204	TPP	C4'-N4'	3.62	1.43	1.34
3	B	1204	TPP	C7'-C5'	3.61	1.57	1.51
3	A	1204	TPP	C5-S1	-3.58	1.63	1.72
3	C	1204	TPP	C7'-C5'	3.54	1.57	1.51
3	C	1204	TPP	C5-S1	-3.49	1.63	1.72
3	C	1204	TPP	C2-N3	3.19	1.40	1.32
3	A	1204	TPP	C2-N3	3.07	1.39	1.32
5	B	1206	COA	P2A-O3A	2.97	1.62	1.59
3	B	1204	TPP	C2-N3	2.96	1.39	1.32
5	C	1206	COA	P2A-O3A	2.82	1.62	1.59
3	B	1204	TPP	C7'-N3	-2.80	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1206	COA	P2A-O6A	2.80	1.70	1.59
3	C	1204	TPP	C7'-N3	-2.75	1.42	1.48
3	A	1204	TPP	C7'-N3	-2.72	1.42	1.48
5	B	1206	COA	P2A-O6A	2.69	1.69	1.59
5	C	1206	COA	P2A-O6A	2.61	1.69	1.59
5	C	1206	COA	P1A-O3A	2.60	1.62	1.59
5	B	1206	COA	C8A-N7A	2.52	1.36	1.31
5	B	1206	COA	P1A-O3A	2.49	1.62	1.59
5	C	1206	COA	C8A-N7A	2.49	1.36	1.31
3	C	1204	TPP	C5-C4	2.45	1.40	1.35
5	A	1206	COA	P2A-O3A	2.43	1.62	1.59
5	A	1206	COA	C8A-N7A	2.43	1.36	1.31
3	C	1204	TPP	C6'-C5'	2.38	1.42	1.37
3	B	1204	TPP	C5-C4	2.36	1.40	1.35
3	A	1204	TPP	C6'-C5'	2.32	1.42	1.37
3	B	1204	TPP	C6'-C5'	2.29	1.42	1.37
3	C	1204	TPP	C4-N3	-2.25	1.35	1.39
3	A	1204	TPP	C5-C4	2.24	1.39	1.35
5	A	1206	COA	P1A-O3A	2.13	1.61	1.59
3	A	1204	TPP	C4-N3	-2.11	1.35	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1206	COA	N3A-C2A-N1A	-4.68	121.49	128.58
5	A	1206	COA	N3A-C2A-N1A	-4.61	121.61	128.58
3	C	1204	TPP	C2-S1-C5	-4.56	88.19	91.22
5	A	1206	COA	O4B-C1B-N9A	4.48	116.70	108.09
5	C	1206	COA	N9A-C8A-N7A	-4.48	107.58	113.94
5	B	1206	COA	N3A-C2A-N1A	-4.45	121.84	128.58
5	C	1206	COA	O4B-C1B-N9A	4.38	116.50	108.09
5	B	1206	COA	C1B-N9A-C8A	-4.37	117.39	127.09
5	B	1206	COA	C5A-C4A-N9A	4.30	110.50	105.81
5	B	1206	COA	N9A-C8A-N7A	-4.26	107.89	113.94
5	A	1206	COA	N9A-C8A-N7A	-4.26	107.90	113.94
5	A	1206	COA	C5A-C4A-N9A	4.23	110.43	105.81
3	B	1204	TPP	C2-N3-C4	-4.20	108.39	114.06
3	A	1204	TPP	C2-N3-C4	-4.16	108.44	114.06
5	C	1206	COA	C5A-N7A-C8A	4.14	109.95	103.45
5	B	1206	COA	O4B-C1B-N9A	4.12	116.01	108.09
3	C	1204	TPP	C2-N3-C4	-4.11	108.51	114.06
5	C	1206	COA	C5A-C4A-N9A	4.09	110.26	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1206	COA	C5A-N7A-C8A	4.07	109.84	103.45
5	A	1206	COA	C5A-N7A-C8A	3.96	109.67	103.45
3	B	1204	TPP	C2-S1-C5	-3.94	88.61	91.22
3	A	1204	TPP	C2-S1-C5	-3.79	88.71	91.22
5	B	1206	COA	C5A-C4A-N3A	-3.77	121.53	126.72
3	B	1204	TPP	S1-C2-N3	3.76	117.06	112.30
3	C	1204	TPP	S1-C2-N3	3.74	117.03	112.30
5	A	1206	COA	C5A-C4A-N3A	-3.70	121.62	126.72
5	A	1206	COA	C1B-N9A-C8A	-3.64	119.03	127.09
3	C	1204	TPP	C4-C5-S1	3.53	116.07	110.56
3	A	1204	TPP	S1-C2-N3	3.52	116.76	112.30
5	C	1206	COA	C5A-C4A-N3A	-3.51	121.88	126.72
3	C	1204	TPP	N4'-C4'-N3'	3.46	121.69	117.03
3	B	1204	TPP	C4-C5-S1	3.39	115.85	110.56
5	C	1206	COA	C1B-N9A-C8A	-3.33	119.70	127.09
3	A	1204	TPP	C4-C5-S1	3.22	115.59	110.56
3	B	1204	TPP	C6'-N1'-C2'	3.21	121.34	116.07
5	B	1206	COA	C3P-N4P-C5P	3.20	128.78	122.82
3	A	1204	TPP	N4'-C4'-N3'	3.16	121.29	117.03
5	A	1206	COA	C7P-N8P-C9P	3.15	128.20	122.55
3	C	1204	TPP	C6'-N1'-C2'	3.10	121.16	116.07
3	A	1204	TPP	C6'-N1'-C2'	3.08	121.12	116.07
3	B	1204	TPP	C5'-C6'-N1'	-2.89	119.14	123.83
3	A	1204	TPP	C5'-C6'-N1'	-2.84	119.21	123.83
3	C	1204	TPP	C5'-C6'-N1'	-2.81	119.27	123.83
5	A	1206	COA	C2A-N3A-C4A	2.56	118.09	111.83
5	B	1206	COA	C4A-C5A-N7A	-2.53	107.68	110.58
5	A	1206	COA	C3P-N4P-C5P	2.52	127.52	122.82
5	A	1206	COA	C3B-C2B-C1B	2.52	105.43	99.89
5	C	1206	COA	C2A-N3A-C4A	2.52	117.98	111.83
5	B	1206	COA	C2A-N3A-C4A	2.51	117.95	111.83
5	C	1206	COA	C4A-C5A-N7A	-2.49	107.74	110.58
5	A	1206	COA	C4A-C5A-N7A	-2.33	107.91	110.58
3	B	1204	TPP	N4'-C4'-N3'	2.33	120.17	117.03
5	B	1206	COA	C7P-N8P-C9P	2.31	126.70	122.55
3	C	1204	TPP	C5'-C4'-N4'	-2.29	119.05	122.14
3	B	1204	TPP	CM4-C4-N3	2.28	125.84	120.57
5	C	1206	COA	C3P-N4P-C5P	2.26	127.03	122.82
3	C	1204	TPP	C6-C5-C4	-2.20	122.66	128.17
5	B	1206	COA	CDP-CBP-CAP	2.19	112.50	108.77
5	B	1206	COA	O6A-CCP-CBP	-2.17	107.06	110.55
3	A	1204	TPP	C6-C5-C4	-2.14	122.80	128.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1206	COA	CEP-CBP-CAP	2.14	112.41	108.77
3	B	1204	TPP	N1'-C2'-N3'	-2.13	122.00	125.53
3	C	1204	TPP	N1'-C2'-N3'	-2.10	122.03	125.53
5	B	1206	COA	CEP-CBP-CAP	2.09	112.34	108.77
3	A	1204	TPP	N1'-C2'-N3'	-2.08	122.06	125.53
3	C	1204	TPP	C7'-N3-C2	2.05	127.76	123.48
3	A	1204	TPP	CM4-C4-N3	2.04	125.27	120.57

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1206	COA	C5B-O5B-P1A-O3A
5	A	1206	COA	CCP-O6A-P2A-O3A
5	A	1206	COA	CCP-O6A-P2A-O4A
5	A	1206	COA	S1P-C2P-C3P-N4P
5	C	1206	COA	CCP-O6A-P2A-O3A
5	C	1206	COA	CCP-O6A-P2A-O4A
5	C	1206	COA	CCP-O6A-P2A-O5A
5	A	1206	COA	C3B-C4B-C5B-O5B
5	A	1206	COA	O4B-C4B-C5B-O5B
5	A	1206	COA	O5P-C5P-C6P-C7P
3	C	1204	TPP	PB-O3A-PA-O7
5	C	1206	COA	P2A-O3A-P1A-O5B
5	C	1206	COA	P1A-O3A-P2A-O6A
5	A	1206	COA	C2B-C1B-N9A-C8A
5	C	1206	COA	S1P-C2P-C3P-N4P
3	A	1204	TPP	C7-O7-PA-O1A
3	B	1204	TPP	C7-O7-PA-O1A
3	C	1204	TPP	C7-O7-PA-O1A
5	A	1206	COA	C5B-O5B-P1A-O1A
5	A	1206	COA	CCP-O6A-P2A-O5A
5	C	1206	COA	C3B-O3B-P3B-O8A
5	A	1206	COA	N4P-C5P-C6P-C7P
3	A	1204	TPP	PA-O3A-PB-O1B
3	A	1204	TPP	S1-C5-C6-C7
3	B	1204	TPP	S1-C5-C6-C7
5	C	1206	COA	C3B-O3B-P3B-O7A
5	C	1206	COA	P1A-O3A-P2A-O4A
3	C	1204	TPP	S1-C5-C6-C7
3	A	1204	TPP	C4-C5-C6-C7
3	B	1204	TPP	C4-C5-C6-C7

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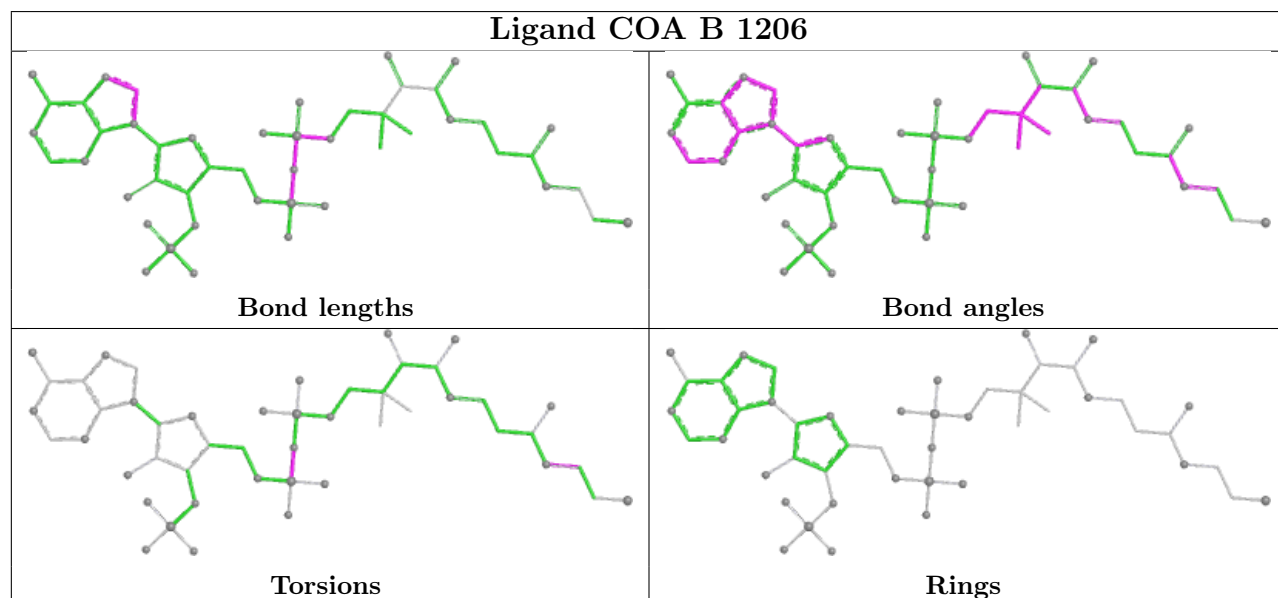
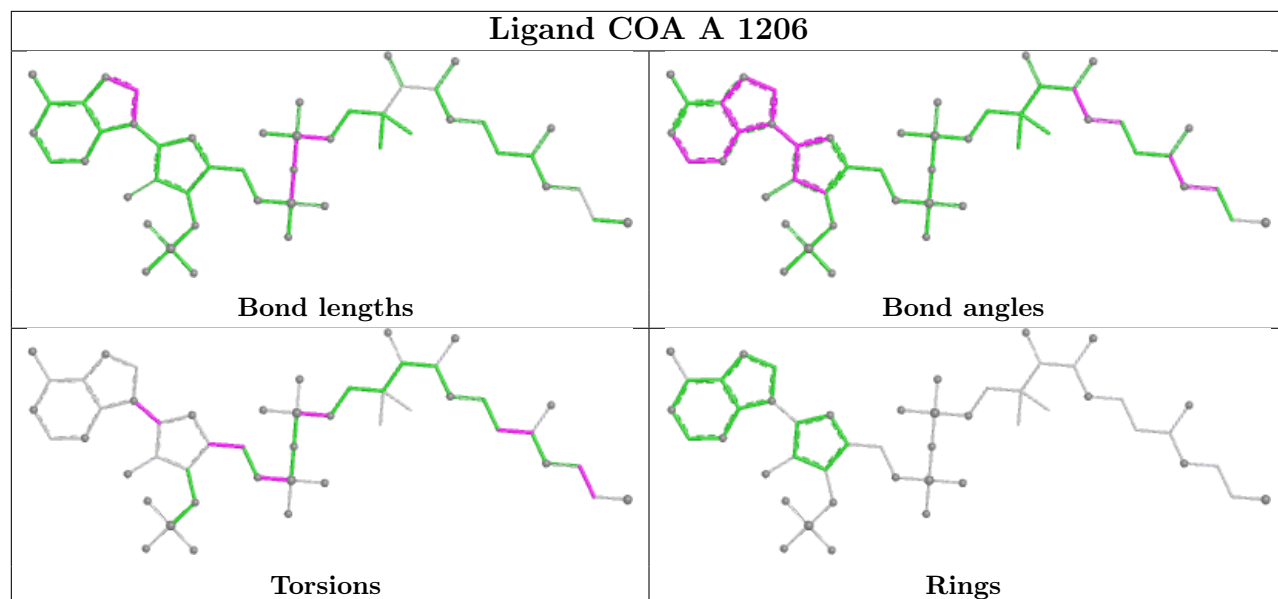
Mol	Chain	Res	Type	Atoms
5	B	1206	COA	C2P-C3P-N4P-C5P
5	B	1206	COA	P2A-O3A-P1A-O2A
5	C	1206	COA	C3B-O3B-P3B-O9A
5	C	1206	COA	C6P-C7P-N8P-C9P
5	B	1206	COA	P2A-O3A-P1A-O1A

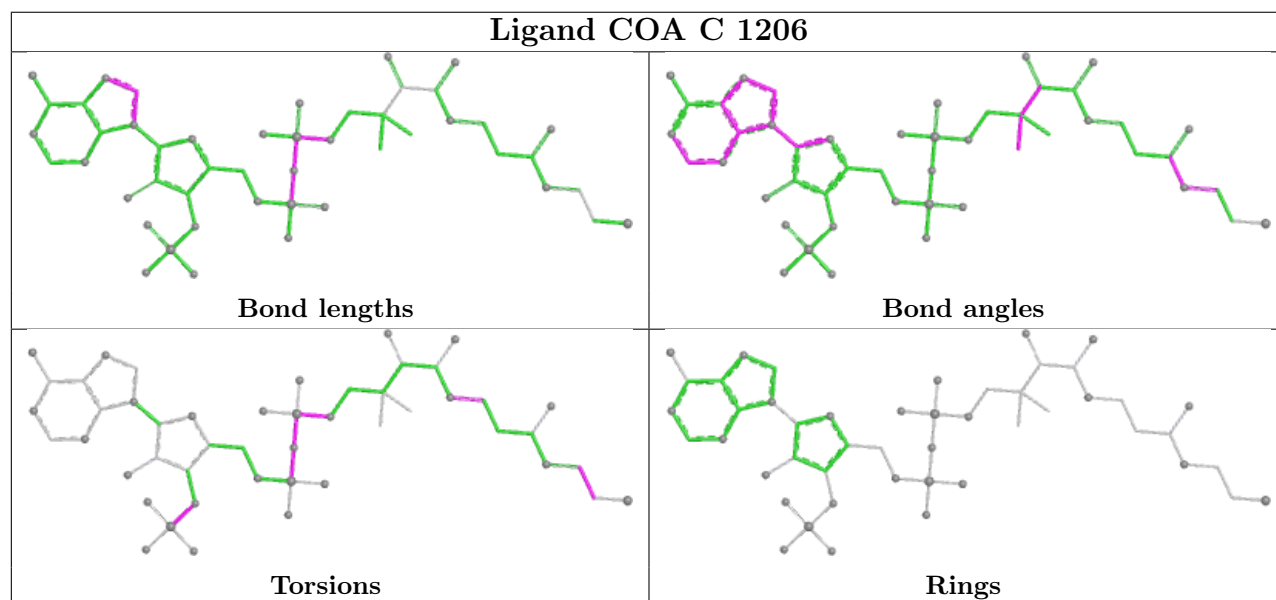
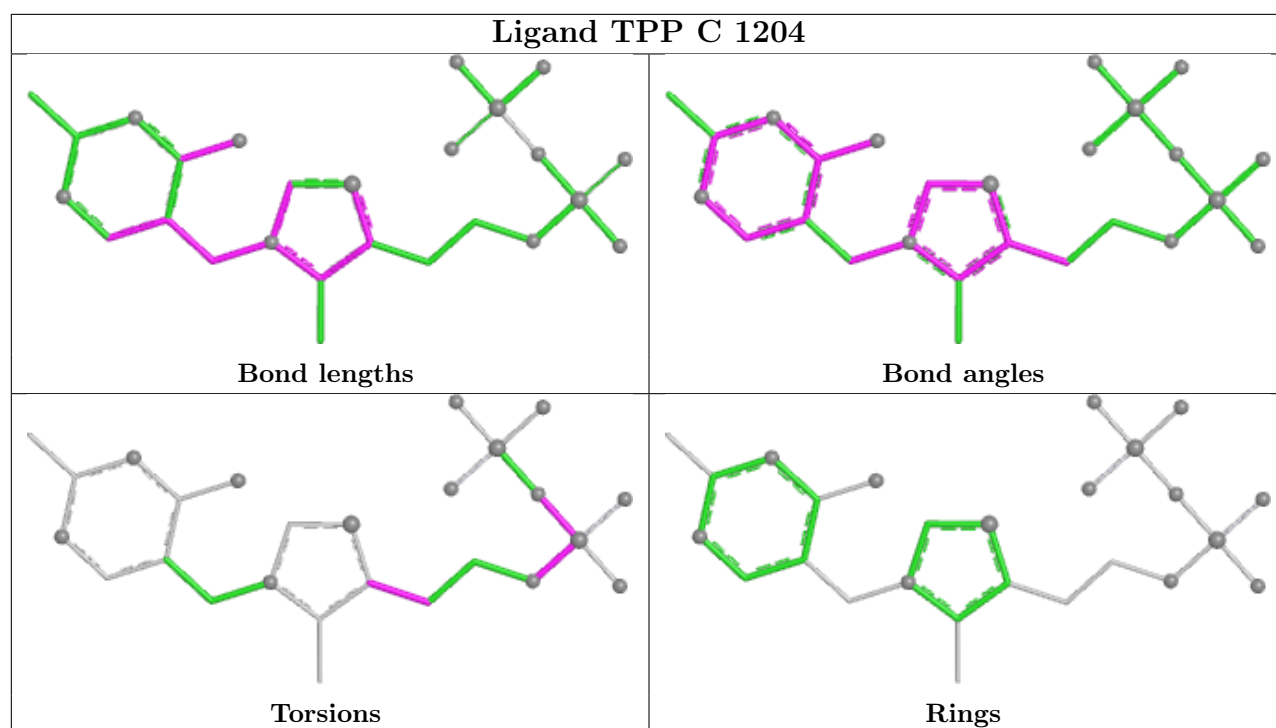
There are no ring outliers.

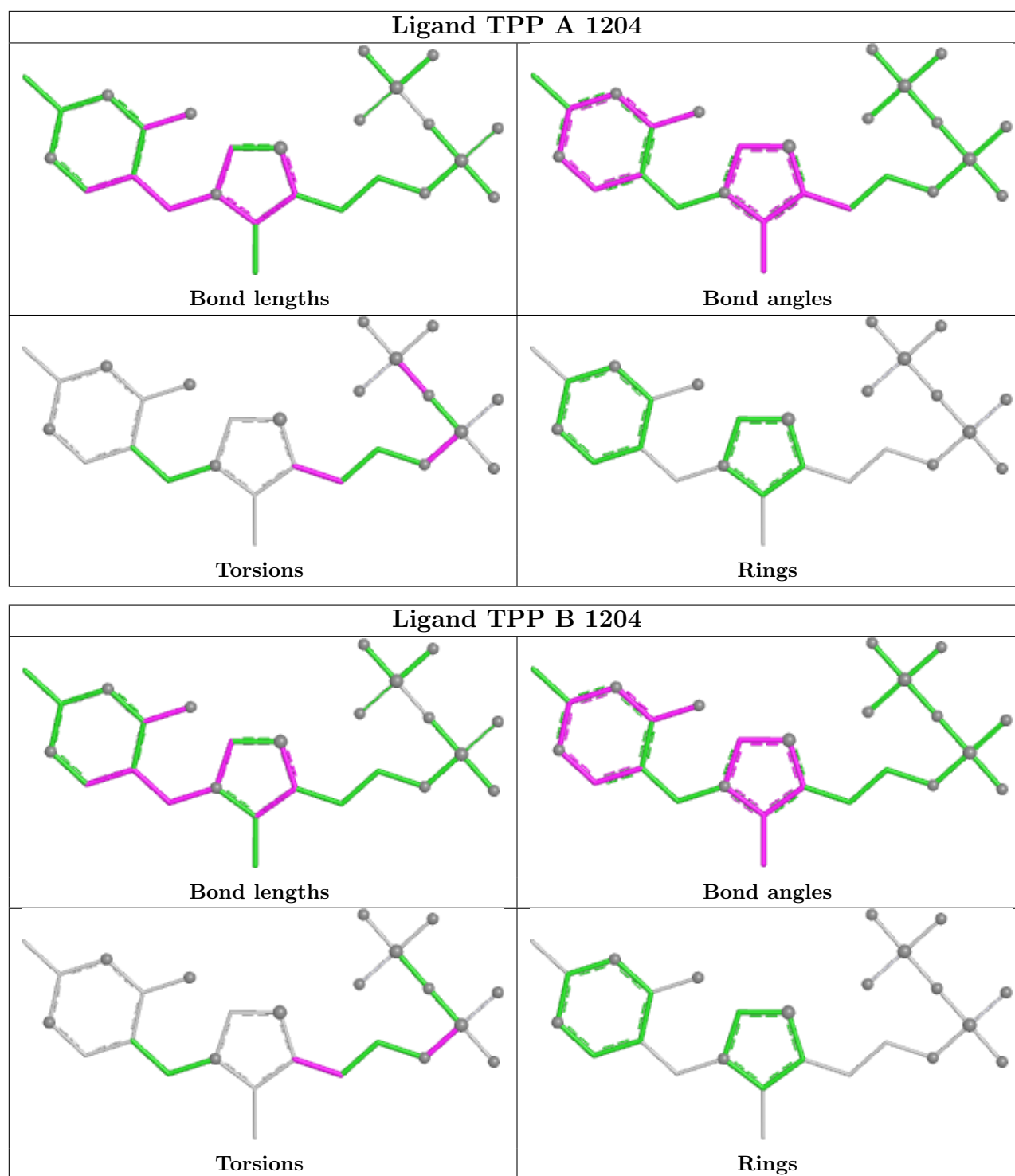
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1206	COA	2	0
5	B	1206	COA	2	0
5	C	1206	COA	5	0
2	B	1201	SF4	2	0
3	B	1204	TPP	2	0

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1169/1171 (99%)	-0.49	1 (0%) 92 90	40, 79, 150, 187	0
1	B	1166/1171 (99%)	-0.42	0 100 100	36, 90, 178, 253	0
1	C	1161/1171 (99%)	-0.39	7 (0%) 85 73	48, 89, 172, 259	0
All	All	3496/3513 (99%)	-0.44	8 (0%) 91 86	36, 86, 169, 259	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	SER	5.6
1	C	537	PHE	2.4
1	C	607	GLU	2.4
1	C	485	ALA	2.3
1	C	483	LEU	2.1
1	C	535	LEU	2.1
1	C	606	LEU	2.0
1	A	458	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

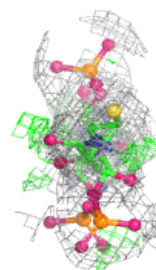
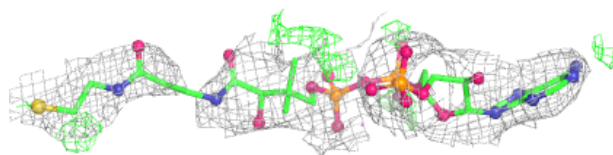
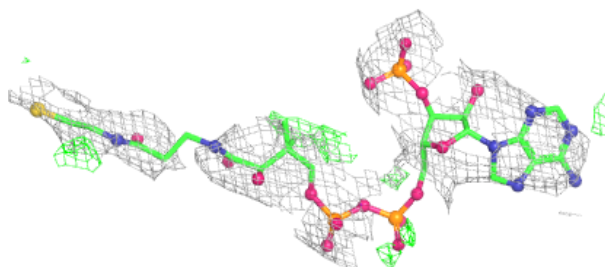
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	COA	B	1206	48/48	0.82	0.10	118,130,138,138	0
5	COA	C	1206	48/48	0.83	0.10	102,112,136,137	0
5	COA	A	1206	48/48	0.85	0.10	123,131,141,141	0
3	TPP	C	1204	26/26	0.96	0.07	54,63,67,71	0
3	TPP	A	1204	26/26	0.96	0.07	68,74,79,82	0
3	TPP	B	1204	26/26	0.97	0.05	53,63,65,70	0
2	SF4	B	1201	8/8	0.98	0.04	126,156,197,211	0
2	SF4	C	1202	8/8	0.99	0.03	70,72,74,98	0
2	SF4	A	1202	8/8	0.99	0.03	74,81,107,115	0
2	SF4	A	1203	8/8	0.99	0.02	60,73,84,89	0
2	SF4	A	1201	8/8	0.99	0.03	91,110,112,126	0
4	MG	A	1205	1/1	0.99	0.05	35,35,35,35	0
2	SF4	B	1202	8/8	0.99	0.03	97,107,117,169	0
2	SF4	B	1203	8/8	0.99	0.03	63,78,80,97	0
2	SF4	C	1201	8/8	0.99	0.03	81,85,96,104	0
2	SF4	C	1203	8/8	1.00	0.02	61,63,65,65	0
4	MG	B	1205	1/1	1.00	0.03	30,30,30,30	0
4	MG	C	1205	1/1	1.00	0.07	19,19,19,19	0

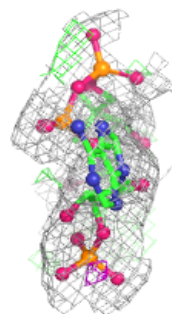
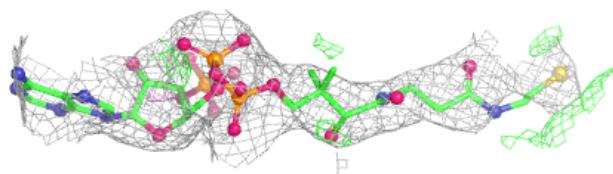
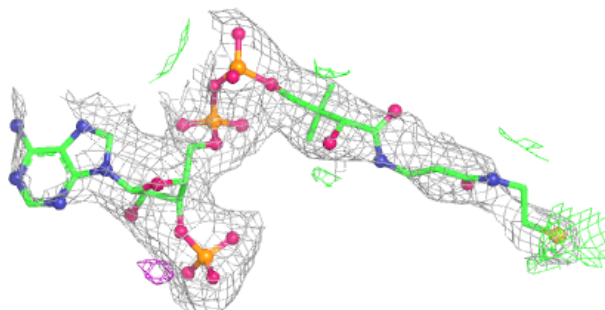
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA B 1206:

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

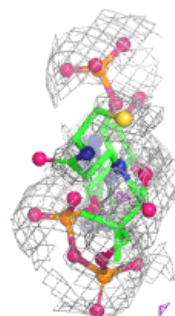
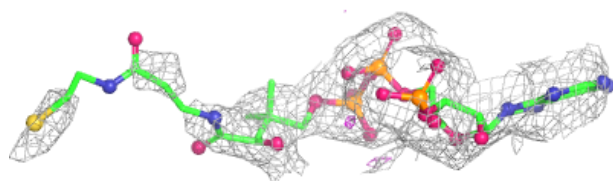
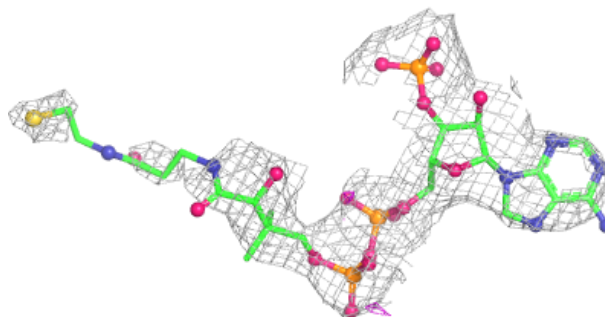
**Electron density around COA C 1206:**

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

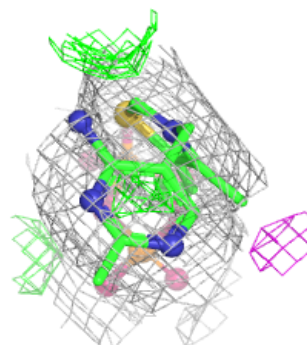
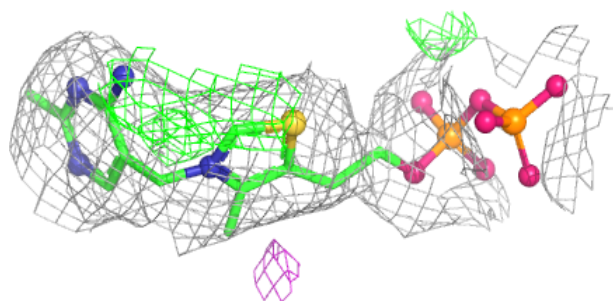
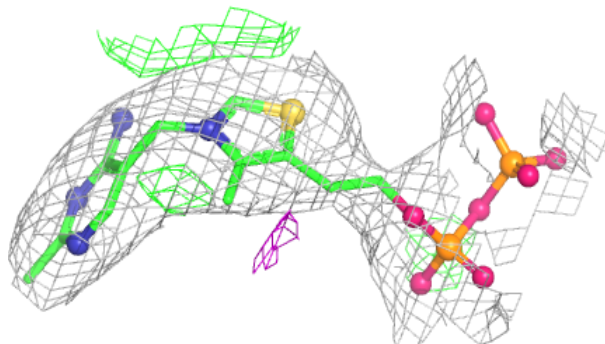


Electron density around COA A 1206:

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

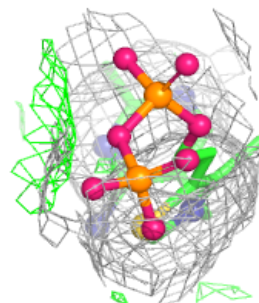
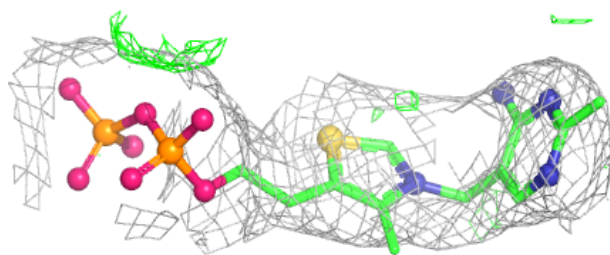
**Electron density around TPP C 1204:**

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

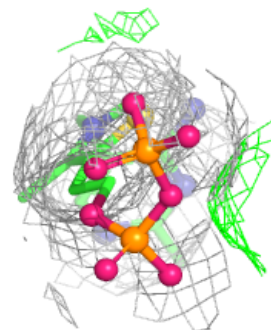
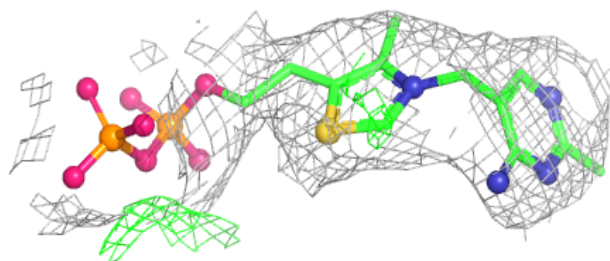
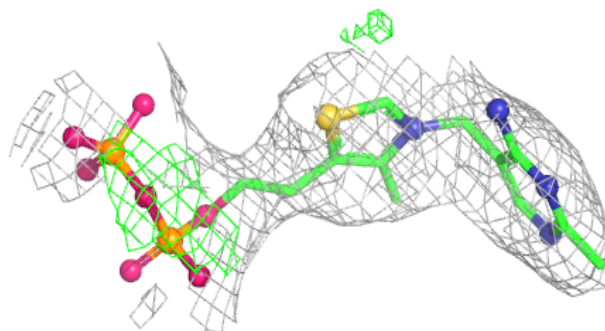


Electron density around TPP A 1204:

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

**Electron density around TPP B 1204:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.