



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 07:34 am BST

PDB ID : 1B25
Title : FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE FROM PYRO-
COCCUS FURIOSUS
Authors : Hu, Y.L.; Faham, S.; Roy, R.; Adams, M.W.W.; Rees, D.C.
Deposited on : 1998-12-04
Resolution : 1.85 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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

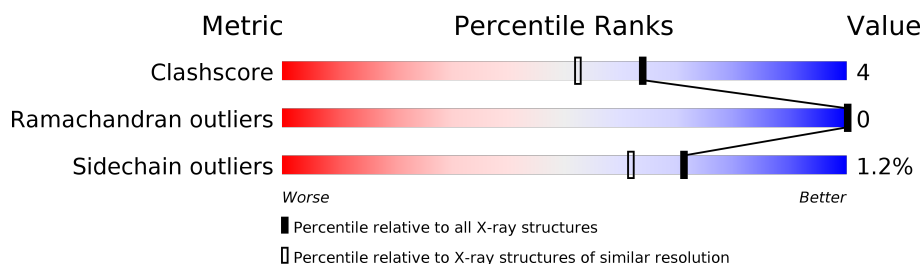
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	619	
1	B	619	
1	C	619	
1	D	619	

2 Entry composition [i](#)

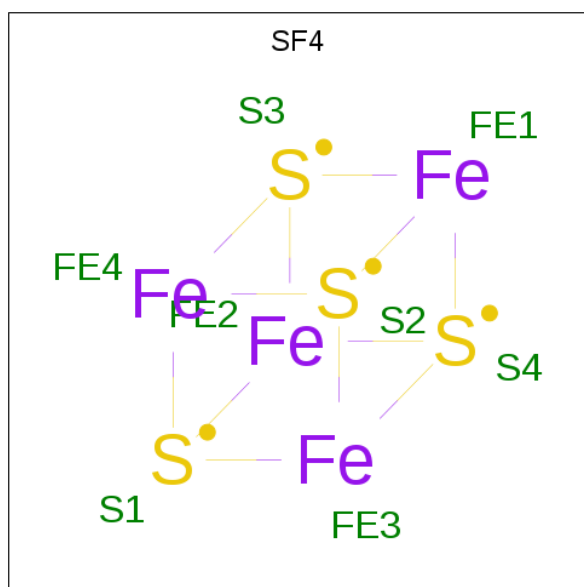
There are 4 unique types of molecules in this entry. The entry contains 20733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	B	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	C	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			
1	D	611	Total	C	N	O	S	0	0	0
			4786	3067	809	888	22			

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



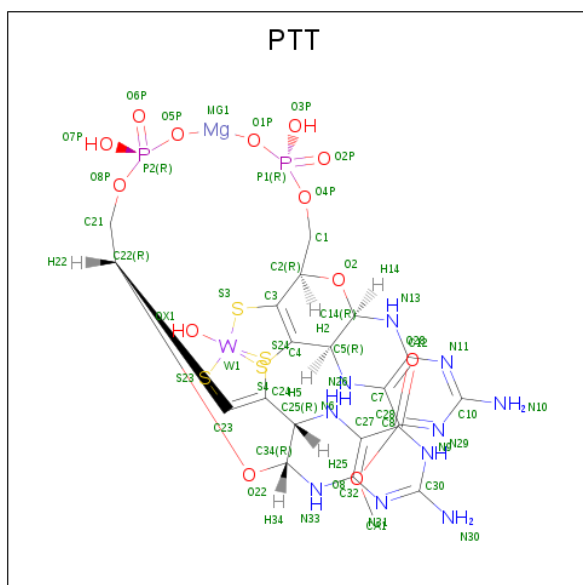
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is TUNGSTOPTERIN (three-letter code: PTT) (formula: $C_{21}H_{25}MgN_{10}O_{13}P_2S_4W$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	A	1	Total	C	Mg	N	O	P	S	W	0	0
			52	21	1	10	13	2	4	1		
3	B	1	Total	C	Mg	N	O	P	S	W	0	0
			52	21	1	10	13	2	4	1		
3	C	1	Total	C	Mg	N	O	P	S	W	0	0
			52	21	1	10	13	2	4	1		
3	D	1	Total	C	Mg	N	O	P	S	W	0	0
			52	21	1	10	13	2	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total	O	0	0
			285	285		
4	B	318	Total	O	0	0
			318	318		
4	C	393	Total	O	0	0
			393	393		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	353	Total	O	0	0
			353	353		

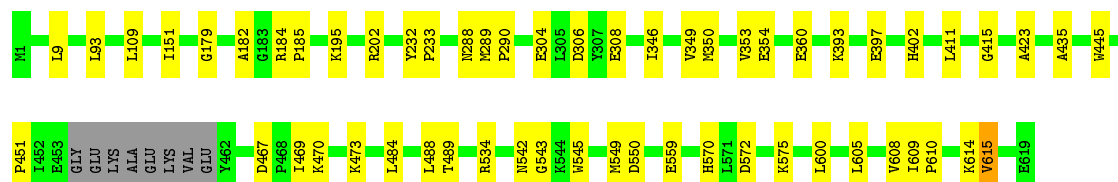
3 Residue-property plots [i](#)

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

Note EDS was not executed.

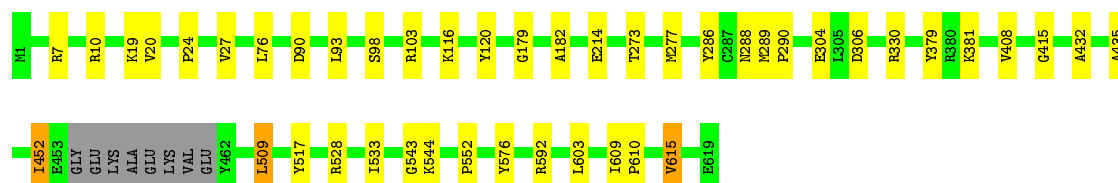
- Molecule 1: PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE)

Chain A: 




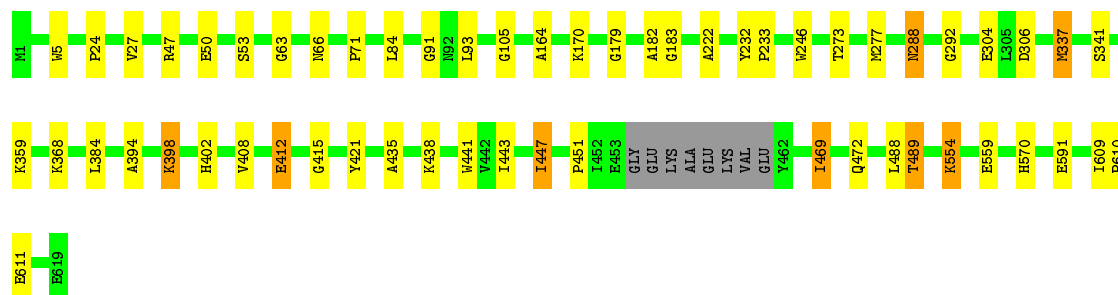
- Molecule 1: PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE)

Chain B: 



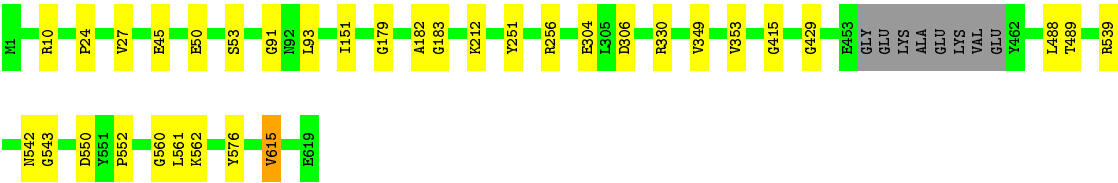
- Molecule 1: PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE)

Chain C: 



- Molecule 1: PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE)

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.34Å 170.85Å 180.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85	Depositor
% Data completeness (in resolution range)	91.4 (20.00-1.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.174 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20733	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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: SF4, PTT

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	0.49	0/4896	0.68	1/6619 (0.0%)
1	B	0.48	0/4896	0.69	2/6619 (0.0%)
1	C	0.52	0/4896	0.70	1/6619 (0.0%)
1	D	0.51	0/4896	0.69	2/6619 (0.0%)
All	All	0.50	0/19584	0.69	6/26476 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	539	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	D	415	GLY	N-CA-C	5.43	126.67	113.10
1	A	415	GLY	N-CA-C	5.22	126.14	113.10
1	C	415	GLY	N-CA-C	5.09	125.81	113.10
1	B	415	GLY	N-CA-C	5.06	125.75	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	TYR	Sidechain

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	4786	0	4773	39	0
1	B	4786	0	4773	30	0
1	C	4786	0	4773	44	0
1	D	4786	0	4773	26	0
2	A	8	0	0	0	0
2	B	8	0	0	1	0
2	C	8	0	0	0	0
2	D	8	0	0	1	0
3	A	52	0	22	12	0
3	B	52	0	22	12	0
3	C	52	0	22	11	0
3	D	52	0	22	13	0
4	A	285	0	0	8	0
4	B	318	0	0	11	0
4	C	393	0	0	6	0
4	D	353	0	0	8	0
All	All	20733	0	19180	160	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 (160) 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:D:179:GLY:O	3:D:803:PTT:HA12	1.43	1.17
1:C:179:GLY:O	3:C:802:PTT:HA12	1.46	1.13
1:B:179:GLY:O	3:B:801:PTT:HA12	1.46	1.12
1:A:179:GLY:O	3:A:800:PTT:HA12	1.50	1.11
3:A:800:PTT:HA13	4:A:1084:HOH:O	1.57	1.04
3:D:803:PTT:HA11	4:D:1156:HOH:O	1.57	1.02
3:C:802:PTT:HA13	4:C:1194:HOH:O	1.60	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:802:PTT:CA1	3:C:802:PTT:O8	2.12	0.97
3:D:803:PTT:O8	3:D:803:PTT:CA1	2.11	0.97
3:A:800:PTT:CA1	3:A:800:PTT:O8	2.13	0.95
3:B:801:PTT:CA1	3:B:801:PTT:O8	2.14	0.94
3:B:801:PTT:HA13	4:B:1118:HOH:O	1.68	0.94
1:C:63:GLY:H	1:C:66:ASN:HD22	1.15	0.93
3:B:801:PTT:HA11	4:B:1119:HOH:O	1.69	0.91
1:C:554:LYS:HD2	1:C:554:LYS:H	1.36	0.90
3:D:803:PTT:HA13	4:D:1155:HOH:O	1.74	0.87
1:C:306:ASP:OD2	3:C:802:PTT:CA1	2.27	0.83
1:D:93:LEU:HB3	1:D:182:ALA:HB2	1.61	0.82
1:B:379:TYR:HB2	1:B:381:LYS:HE2	1.61	0.81
3:A:800:PTT:HA11	4:A:1085:HOH:O	1.82	0.80
1:C:306:ASP:OD2	3:C:802:PTT:HA11	1.81	0.79
1:A:93:LEU:HB3	1:A:182:ALA:HB2	1.64	0.78
1:D:179:GLY:O	3:D:803:PTT:CA1	2.28	0.78
1:D:306:ASP:OD2	3:D:803:PTT:CA1	2.30	0.78
1:A:423:ALA:HB2	1:A:470:LYS:HG3	1.66	0.78
3:C:802:PTT:HA11	4:C:1195:HOH:O	1.85	0.77
1:B:179:GLY:O	3:B:801:PTT:CA1	2.32	0.77
1:B:306:ASP:OD2	3:B:801:PTT:CA1	2.33	0.76
1:C:554:LYS:H	1:C:554:LYS:CD	1.99	0.76
1:A:179:GLY:O	3:A:800:PTT:CA1	2.32	0.76
1:C:179:GLY:O	3:C:802:PTT:CA1	2.30	0.74
1:C:93:LEU:HB3	1:C:182:ALA:HB2	1.71	0.73
1:B:93:LEU:HB3	1:B:182:ALA:HB2	1.70	0.73
1:A:306:ASP:OD2	3:A:800:PTT:CA1	2.36	0.73
1:C:50:GLU:HB2	1:C:53:SER:HB3	1.70	0.72
3:D:803:PTT:CA1	4:D:1155:HOH:O	2.33	0.70
1:A:306:ASP:OD2	3:A:800:PTT:HA11	1.91	0.70
3:A:800:PTT:CA1	4:A:1085:HOH:O	2.38	0.69
3:B:801:PTT:CA1	4:B:1119:HOH:O	2.34	0.68
1:C:63:GLY:H	1:C:66:ASN:ND2	1.90	0.67
3:C:802:PTT:CA1	4:C:1195:HOH:O	2.40	0.66
1:A:610:PRO:O	1:A:614:LYS:HG3	1.96	0.66
1:B:306:ASP:OD2	3:B:801:PTT:HA11	1.95	0.65
1:C:84:LEU:HD13	1:C:170:LYS:HB3	1.79	0.64
1:D:306:ASP:OD2	3:D:803:PTT:HA13	1.96	0.64
1:B:528:ARG:HD3	1:B:603:LEU:O	2.01	0.60
1:C:443:ILE:O	1:C:447:ILE:HG12	2.00	0.60
1:B:304:GLU:OE1	3:B:801:PTT:CA1	2.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:PRO:HG2	4:A:882:HOH:O	2.04	0.57
1:B:452:ILE:HG13	4:B:960:HOH:O	2.05	0.57
1:C:24:PRO:HG2	1:C:27:VAL:HG23	1.87	0.57
1:B:543:GLY:CA	1:B:615:VAL:HG13	2.35	0.56
1:B:7:ARG:NH1	1:B:20:VAL:HG11	2.20	0.55
1:D:543:GLY:CA	1:D:615:VAL:HG13	2.36	0.55
1:A:605:LEU:O	1:A:608:VAL:HG13	2.06	0.54
1:D:24:PRO:HG2	1:D:27:VAL:HG23	1.89	0.54
1:A:350:MET:O	1:A:354:GLU:HG3	2.08	0.54
1:A:549:MET:HE2	4:A:958:HOH:O	2.06	0.54
1:B:93:LEU:HA	3:B:801:PTT:O5P	2.07	0.54
1:A:304:GLU:OE1	3:A:800:PTT:CA1	2.56	0.54
1:B:544:LYS:HE3	4:B:948:HOH:O	2.08	0.53
1:A:308:GLU:HB2	3:A:800:PTT:S4	2.50	0.52
1:D:349:VAL:O	1:D:353:VAL:HG23	2.08	0.52
1:A:423:ALA:HB2	1:A:470:LYS:CG	2.37	0.52
1:B:509:LEU:HD13	1:B:517:TYR:CD1	2.45	0.52
1:D:10:ARG:HH22	1:D:45:GLU:CD	2.13	0.52
1:C:341:SER:OG	1:C:412:GLU:HG2	2.10	0.52
1:C:63:GLY:N	1:C:66:ASN:HD22	1.95	0.51
3:A:800:PTT:CA1	4:A:1084:HOH:O	2.36	0.51
1:D:24:PRO:HG2	1:D:27:VAL:CG2	2.41	0.51
1:A:93:LEU:HA	3:A:800:PTT:O5P	2.11	0.51
1:C:292:GLY:HA2	4:C:1064:HOH:O	2.11	0.51
1:C:359:LYS:HE2	1:C:359:LYS:HA	1.92	0.51
1:C:341:SER:HA	1:C:412:GLU:CG	2.41	0.50
1:D:91:GLY:HA3	1:D:183:GLY:H	1.75	0.50
1:A:572:ASP:OD2	1:A:575:LYS:HG3	2.12	0.50
1:D:304:GLU:OE1	3:D:803:PTT:CA1	2.60	0.50
1:C:304:GLU:OE1	3:C:802:PTT:CA1	2.60	0.50
1:C:91:GLY:HA3	1:C:183:GLY:H	1.76	0.50
1:B:116:LYS:HD3	4:B:935:HOH:O	2.12	0.50
1:B:103:ARG:HD2	4:B:1103:HOH:O	2.12	0.48
1:A:542:ASN:HA	1:A:615:VAL:HG21	1.96	0.48
1:B:103:ARG:NH2	1:B:286:TYR:OH	2.46	0.48
1:B:24:PRO:HG2	1:B:27:VAL:HG23	1.95	0.48
1:C:421:TYR:HE1	1:C:447:ILE:HG23	1.78	0.48
1:B:452:ILE:HD11	4:B:1006:HOH:O	2.14	0.48
1:D:93:LEU:HA	3:D:803:PTT:O5P	2.14	0.47
1:C:164:ALA:CB	1:C:337:MET:HG2	2.44	0.47
1:C:368:LYS:HG2	4:C:976:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:HD13	1:A:608:VAL:HG22	1.97	0.47
1:D:251:TYR:HD1	4:D:1096:HOH:O	1.97	0.47
3:C:802:PTT:CA1	4:C:1194:HOH:O	2.37	0.47
1:A:534:ARG:HH21	1:A:545:TRP:HE1	1.62	0.46
1:C:93:LEU:HA	3:C:802:PTT:O5P	2.14	0.46
1:A:151:ILE:HG13	1:D:151:ILE:HG13	1.96	0.46
1:D:552:PRO:HD3	1:D:576:TYR:CZ	2.50	0.46
1:D:10:ARG:NH2	1:D:45:GLU:OE2	2.48	0.46
1:B:609:ILE:HB	1:B:610:PRO:HD3	1.98	0.45
1:C:341:SER:HA	1:C:412:GLU:HG2	1.98	0.45
2:B:701:SF4:S4	3:B:801:PTT:H22	2.57	0.45
1:C:402:HIS:CE1	1:C:554:LYS:HD3	2.51	0.45
3:B:801:PTT:CA1	4:B:1118:HOH:O	2.41	0.45
1:B:103:ARG:HD3	4:B:979:HOH:O	2.16	0.45
1:C:609:ILE:HB	1:C:610:PRO:HD3	1.98	0.45
1:C:341:SER:HA	1:C:412:GLU:HG3	2.00	0.44
1:A:349:VAL:O	1:A:353:VAL:HG23	2.18	0.44
1:A:534:ARG:HH22	1:A:550:ASP:CG	2.21	0.44
1:A:609:ILE:HB	1:A:610:PRO:HD3	1.99	0.44
1:B:552:PRO:HD3	1:B:576:TYR:CZ	2.52	0.44
1:D:330:ARG:HD3	4:D:1132:HOH:O	2.18	0.44
1:A:534:ARG:NH2	1:A:550:ASP:OD2	2.51	0.44
1:D:542:ASN:HA	1:D:615:VAL:HG21	2.00	0.44
1:A:467:ASP:O	1:A:470:LYS:HB2	2.18	0.44
1:A:445:TRP:CE2	1:A:473:LYS:HG3	2.53	0.43
1:C:232:TYR:HB3	1:C:233:PRO:HD3	2.00	0.43
1:D:488:LEU:N	1:D:489:THR:HA	2.33	0.43
1:C:394:ALA:O	1:C:398:LYS:HE2	2.18	0.43
1:A:202:ARG:HD2	4:A:910:HOH:O	2.17	0.43
1:A:402:HIS:CD2	4:A:855:HOH:O	2.71	0.43
1:B:76:LEU:HB2	1:B:98:SER:HB2	1.99	0.43
1:C:273:THR:O	1:C:277:MET:HG2	2.18	0.43
1:C:421:TYR:CE1	1:C:447:ILE:HG23	2.53	0.43
1:D:560:GLY:O	1:D:562:LYS:HE3	2.19	0.43
1:A:184:ARG:HB2	1:A:185:PRO:HD3	2.01	0.43
1:C:488:LEU:N	1:C:489:THR:HA	2.34	0.43
1:B:10:ARG:HB2	1:B:19:LYS:HG3	2.01	0.43
1:A:543:GLY:CA	1:A:615:VAL:HG13	2.49	0.43
1:A:289:MET:N	1:A:290:PRO:HD3	2.34	0.42
1:B:288:ASN:C	1:B:290:PRO:HD3	2.40	0.42
1:D:429:GLY:O	1:D:550:ASP:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LYS:O	1:A:397:GLU:HG2	2.18	0.42
1:D:561:LEU:HD22	4:D:1096:HOH:O	2.19	0.42
2:D:703:SF4:S4	3:D:803:PTT:H22	2.59	0.42
1:C:441:TRP:HH2	1:C:451:PRO:HD2	1.84	0.42
1:C:408:VAL:HB	1:C:435:ALA:HB2	2.01	0.42
1:C:50:GLU:HB2	1:C:53:SER:CB	2.45	0.42
1:A:346:ILE:O	1:A:350:MET:HG3	2.20	0.42
1:C:246:TRP:CH2	1:C:447:ILE:HD11	2.54	0.42
1:C:469:ILE:HD13	1:C:472:GLN:HB3	2.02	0.42
1:A:484:LEU:O	1:A:488:LEU:HG	2.20	0.41
1:A:488:LEU:N	1:A:489:THR:HA	2.35	0.41
1:B:592:ARG:HD2	4:B:1065:HOH:O	2.18	0.41
1:D:256:ARG:HD2	4:D:968:HOH:O	2.19	0.41
1:D:306:ASP:OD2	3:D:803:PTT:HA11	2.16	0.41
1:A:559:GLU:O	1:A:570:HIS:HB3	2.19	0.41
1:C:288:ASN:H	1:C:288:ASN:HD22	1.68	0.41
1:D:50:GLU:HB2	1:D:53:SER:HB3	2.02	0.41
3:D:803:PTT:CA1	4:D:1156:HOH:O	2.38	0.41
1:B:273:THR:O	1:B:277:MET:HG2	2.21	0.41
1:B:289:MET:N	1:B:290:PRO:HD3	2.36	0.41
1:C:559:GLU:O	1:C:570:HIS:HB3	2.21	0.41
1:B:432:ALA:HB1	1:B:533:ILE:HG21	2.03	0.41
1:A:232:TYR:HB3	1:A:233:PRO:HD3	2.03	0.41
1:C:71:PRO:HG2	1:C:222:ALA:HB3	2.03	0.41
1:C:47:ARG:NH1	1:C:611:GLU:OE2	2.54	0.40
1:A:411:LEU:O	1:A:435:ALA:HB3	2.21	0.40
1:A:9:LEU:HD23	1:A:109:LEU:HD13	2.02	0.40
1:B:408:VAL:HB	1:B:435:ALA:HB2	2.03	0.40
1:C:66:ASN:HD21	1:C:489:THR:HG22	1.85	0.40
1:C:5:TRP:CE2	1:C:105:GLY:HA2	2.57	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	607/619 (98%)	588 (97%)	19 (3%)	0	100	100
1	B	607/619 (98%)	588 (97%)	19 (3%)	0	100	100
1	C	607/619 (98%)	588 (97%)	19 (3%)	0	100	100
1	D	607/619 (98%)	591 (97%)	16 (3%)	0	100	100
All	All	2428/2476 (98%)	2355 (97%)	73 (3%)	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	493/499 (99%)	488 (99%)	5 (1%)	76	69
1	B	493/499 (99%)	488 (99%)	5 (1%)	76	69
1	C	493/499 (99%)	482 (98%)	11 (2%)	52	36
1	D	493/499 (99%)	491 (100%)	2 (0%)	91	89
All	All	1972/1996 (99%)	1949 (99%)	23 (1%)	71	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LYS
1	A	288	ASN
1	A	360	GLU
1	A	469	ILE
1	A	615	VAL
1	B	214	GLU
1	B	330	ARG
1	B	452	ILE
1	B	509	LEU
1	B	615	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	288	ASN
1	C	337	MET
1	C	384	LEU
1	C	398	LYS
1	C	412	GLU
1	C	438	LYS
1	C	447	ILE
1	C	469	ILE
1	C	489	THR
1	C	554	LYS
1	C	591	GLU
1	D	212	LYS
1	D	615	VAL

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

Mol	Chain	Res	Type
1	A	288	ASN
1	A	542	ASN
1	C	66	ASN
1	C	288	ASN
1	C	372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	$\# Z > 2$
3	PTT	C	802	1,4	48,60,60	4.79	17 (35%)	38,98,98	8.27	18 (47%)
2	SF4	D	703	1	0,12,12	0.00	-	-		
2	SF4	C	702	1	0,12,12	0.00	-	-		
2	SF4	B	701	1	0,12,12	0.00	-	-		
3	PTT	A	800	1,4	48,60,60	4.57	16 (33%)	38,98,98	8.63	16 (42%)
3	PTT	B	801	1,4	48,60,60	4.58	16 (33%)	38,98,98	8.33	17 (44%)
2	SF4	A	700	1	0,12,12	0.00	-	-		
3	PTT	D	803	1,4	48,60,60	4.30	16 (33%)	38,98,98	7.89	16 (42%)

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	PTT	C	802	1,4	-	0/14/102/102	-
2	SF4	D	703	1	-	-	0/6/5/5
2	SF4	C	702	1	-	-	0/6/5/5
3	PTT	D	803	1,4	-	1/14/102/102	-
3	PTT	A	800	1,4	-	0/14/102/102	-
3	PTT	B	801	1,4	-	0/14/102/102	-
2	SF4	A	700	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	PTT	O8-CA1	23.97	2.14	1.42
3	A	800	PTT	O8-CA1	23.63	2.13	1.42
3	C	802	PTT	O8-CA1	23.12	2.12	1.42
3	D	803	PTT	O8-CA1	22.79	2.11	1.42
3	C	802	PTT	W1-S23	10.79	2.54	2.33
3	A	800	PTT	W1-S3	10.31	2.53	2.33
3	C	802	PTT	W1-S24	9.97	2.52	2.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	PTT	W1-S24	9.57	2.52	2.33
3	A	800	PTT	W1-S4	9.29	2.51	2.33
3	C	802	PTT	W1-S3	9.15	2.51	2.33
3	B	801	PTT	W1-S23	8.78	2.50	2.33
3	D	803	PTT	W1-S23	8.73	2.50	2.33
3	C	802	PTT	W1-S4	8.57	2.50	2.33
3	A	800	PTT	W1-S23	8.41	2.49	2.33
3	B	801	PTT	W1-S4	8.06	2.49	2.33
3	D	803	PTT	W1-S3	7.07	2.47	2.33
3	D	803	PTT	W1-S4	6.76	2.46	2.33
3	D	803	PTT	W1-S24	6.29	2.45	2.33
3	B	801	PTT	W1-S3	5.88	2.44	2.33
3	C	802	PTT	O28-C28	5.56	1.38	1.24
3	D	803	PTT	O28-C28	5.21	1.37	1.24
3	A	800	PTT	P1-O1P	5.13	1.58	1.50
3	C	802	PTT	P2-O5P	5.11	1.58	1.50
3	B	801	PTT	O28-C28	5.03	1.37	1.24
3	B	801	PTT	P1-O1P	4.74	1.58	1.50
3	A	800	PTT	P2-O5P	4.67	1.58	1.50
3	A	800	PTT	W1-S24	4.59	2.42	2.33
3	C	802	PTT	C34-C25	4.58	1.57	1.53
3	B	801	PTT	P2-O5P	4.47	1.57	1.50
3	D	803	PTT	C34-C25	4.42	1.57	1.53
3	C	802	PTT	O2-C14	-4.17	1.37	1.43
3	A	800	PTT	O28-C28	4.16	1.35	1.24
3	C	802	PTT	P1-O1P	4.09	1.57	1.50
3	D	803	PTT	P1-O1P	3.94	1.56	1.50
3	A	800	PTT	C14-C5	3.89	1.56	1.53
3	C	802	PTT	O2-C2	-3.77	1.38	1.43
3	B	801	PTT	C34-C25	3.66	1.56	1.53
3	B	801	PTT	O2-C14	-3.56	1.38	1.43
3	A	800	PTT	O2-C14	-3.56	1.38	1.43
3	A	800	PTT	O22-C22	-3.51	1.39	1.43
3	C	802	PTT	C14-C5	3.46	1.56	1.53
3	D	803	PTT	P2-O5P	3.33	1.55	1.50
3	D	803	PTT	C14-C5	3.32	1.56	1.53
3	B	801	PTT	C14-C5	3.25	1.56	1.53
3	D	803	PTT	O2-C2	-2.95	1.39	1.43
3	A	800	PTT	O2-C2	-2.89	1.39	1.43
3	C	802	PTT	O22-C22	-2.84	1.39	1.43
3	D	803	PTT	C27-C32	2.73	1.46	1.41
3	B	801	PTT	O22-C22	-2.69	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	803	PTT	O2-C14	-2.53	1.40	1.43
3	C	802	PTT	P1-O2P	2.52	1.59	1.50
3	C	802	PTT	C1-C2	2.44	1.55	1.52
3	C	802	PTT	C27-C32	2.42	1.46	1.41
3	B	801	PTT	O2-C2	-2.38	1.40	1.43
3	C	802	PTT	C8-N9	2.34	1.35	1.32
3	D	803	PTT	C1-C2	2.34	1.55	1.52
3	A	800	PTT	O22-C34	-2.33	1.40	1.43
3	B	801	PTT	O22-C34	-2.31	1.40	1.43
3	B	801	PTT	C8-N9	2.29	1.35	1.32
3	D	803	PTT	C8-N9	2.28	1.35	1.32
3	A	800	PTT	C8-N9	2.27	1.35	1.32
3	D	803	PTT	O22-C22	-2.19	1.40	1.43
3	A	800	PTT	O8-C8	2.08	1.38	1.35
3	B	801	PTT	O8-C8	2.07	1.38	1.35
3	A	800	PTT	C34-C25	2.01	1.55	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	PTT	CA1-O8-C8	48.95	165.72	117.21
3	B	801	PTT	CA1-O8-C8	48.35	165.12	117.21
3	C	802	PTT	CA1-O8-C8	46.92	163.70	117.21
3	D	803	PTT	CA1-O8-C8	44.10	160.91	117.21
3	A	800	PTT	O22-C34-C25	-14.34	99.40	108.96
3	D	803	PTT	O2-C14-N13	11.96	120.85	108.57
3	C	802	PTT	O2-C14-C5	-11.43	101.34	108.96
3	C	802	PTT	O22-C34-C25	-9.18	102.84	108.96
3	A	800	PTT	O22-C34-N33	8.09	116.88	108.57
3	B	801	PTT	O22-C34-C25	-7.21	104.15	108.96
3	D	803	PTT	O22-C34-C25	7.12	113.71	108.96
3	B	801	PTT	O2-C14-C5	5.30	112.50	108.96
3	B	801	PTT	C28-C27-N26	5.30	123.57	119.12
3	D	803	PTT	O2-C14-C5	5.23	112.45	108.96
3	D	803	PTT	C28-N29-C30	5.14	124.10	115.93
3	D	803	PTT	C10-N9-C8	4.97	123.82	115.93
3	D	803	PTT	C28-C27-N26	4.82	123.16	119.12
3	B	801	PTT	N29-C30-N31	-4.45	118.44	125.42
3	B	801	PTT	O22-C34-N33	4.43	113.12	108.57
3	A	800	PTT	C10-N9-C8	4.39	122.90	115.93
3	D	803	PTT	C7-C8-N9	-4.38	118.64	124.51
3	C	802	PTT	C28-N29-C30	4.38	122.88	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	PTT	N11-C10-N9	-4.31	118.65	125.42
3	A	800	PTT	C28-N29-C30	4.15	122.53	115.93
3	A	800	PTT	C7-C8-N9	-3.95	119.22	124.51
3	B	801	PTT	C3-C4-S4	3.89	125.28	119.62
3	C	802	PTT	N11-C10-N9	-3.88	119.33	125.42
3	B	801	PTT	C30-N31-C32	3.86	123.18	114.54
3	A	800	PTT	C3-C4-S4	3.84	125.20	119.62
3	B	801	PTT	N11-C10-N9	-3.81	119.44	125.42
3	B	801	PTT	C10-N9-C8	3.78	121.94	115.93
3	C	802	PTT	N10-C10-N9	3.78	123.13	117.25
3	C	802	PTT	C7-C8-N9	-3.74	119.50	124.51
3	B	801	PTT	C28-N29-C30	3.67	121.77	115.93
3	D	803	PTT	N10-C10-N9	3.67	122.96	117.25
3	C	802	PTT	C23-C24-S24	3.57	124.80	119.62
3	C	802	PTT	C10-N11-C12	3.56	122.53	114.54
3	B	801	PTT	C7-C8-N9	-3.54	119.77	124.51
3	A	800	PTT	N11-C10-N9	-3.48	119.96	125.42
3	C	802	PTT	C28-C27-N26	3.43	122.00	119.12
3	C	802	PTT	C10-N9-C8	3.43	121.38	115.93
3	D	803	PTT	O22-C34-N33	-3.43	105.05	108.57
3	A	800	PTT	N29-C30-N31	-3.40	120.09	125.42
3	D	803	PTT	N29-C30-N31	-3.36	120.15	125.42
3	B	801	PTT	N30-C30-N31	3.34	122.44	117.25
3	B	801	PTT	O2-C14-N13	-3.14	105.34	108.57
3	C	802	PTT	N29-C30-N31	-3.11	120.55	125.42
3	B	801	PTT	C10-N11-C12	3.07	121.41	114.54
3	C	802	PTT	C27-C32-N33	3.01	120.89	118.13
3	C	802	PTT	C3-C4-S4	2.96	123.93	119.62
3	D	803	PTT	C10-N11-C12	2.88	121.00	114.54
3	D	803	PTT	N30-C30-N31	2.86	121.70	117.25
3	A	800	PTT	C28-C27-C32	2.84	117.10	114.57
3	A	800	PTT	N30-C30-N29	2.75	121.53	117.25
3	B	801	PTT	N10-C10-N9	2.73	121.49	117.25
3	A	800	PTT	O2-C14-C5	-2.66	107.19	108.96
3	B	801	PTT	C12-N13-C14	-2.60	118.59	123.67
3	C	802	PTT	C7-C12-N13	2.57	120.48	118.13
3	A	800	PTT	C30-N31-C32	2.56	120.27	114.54
3	A	800	PTT	C23-C24-S24	2.47	123.21	119.62
3	C	802	PTT	C32-N33-C34	-2.46	118.86	123.67
3	A	800	PTT	C10-N11-C12	2.44	120.01	114.54
3	C	802	PTT	C27-N26-C25	-2.30	111.64	120.00
3	D	803	PTT	C3-C4-S4	2.26	122.90	119.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	PTT	C27-N26-C25	-2.22	111.93	120.00
3	C	802	PTT	N30-C30-N31	2.04	120.42	117.25
3	A	800	PTT	N10-C10-N11	2.03	120.41	117.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	803	PTT	N9-C8-O8-CA1

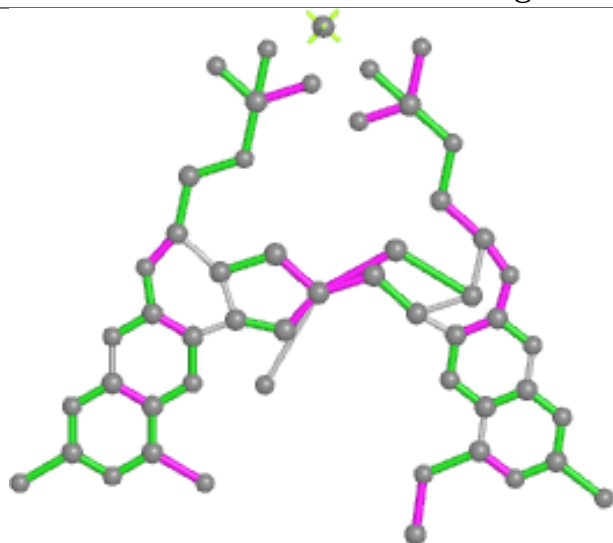
There are no ring outliers.

6 monomers are involved in 48 short contacts:

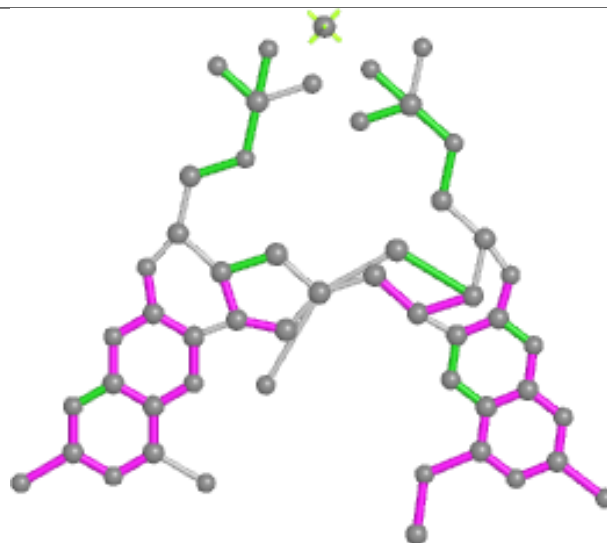
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	PTT	11	0
2	D	703	SF4	1	0
2	B	701	SF4	1	0
3	A	800	PTT	12	0
3	B	801	PTT	12	0
3	D	803	PTT	13	0

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

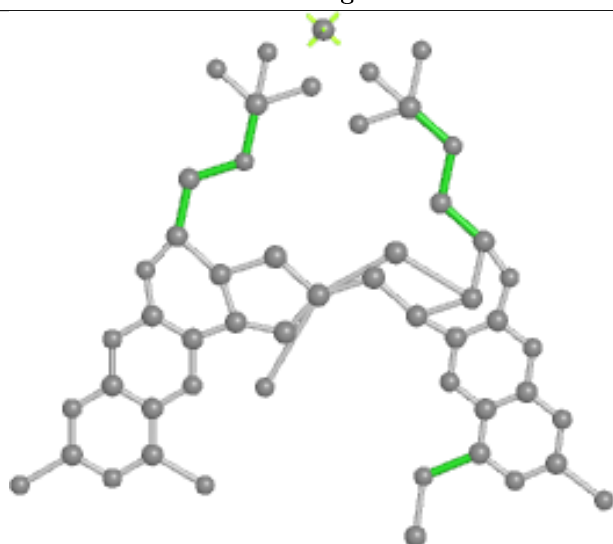
Ligand PTT C 802



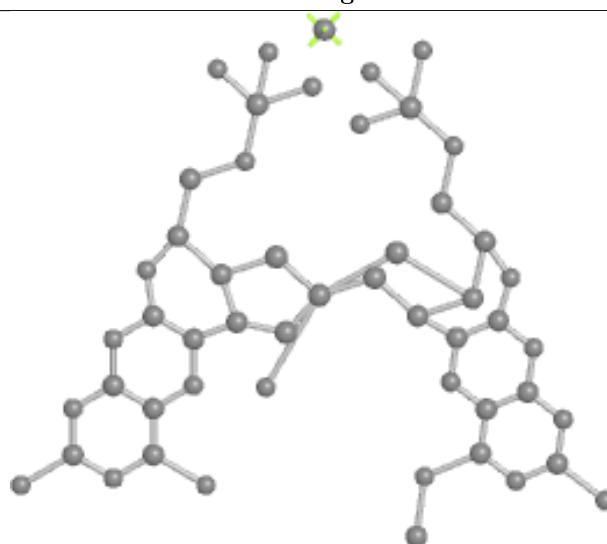
Bond lengths



Bond angles

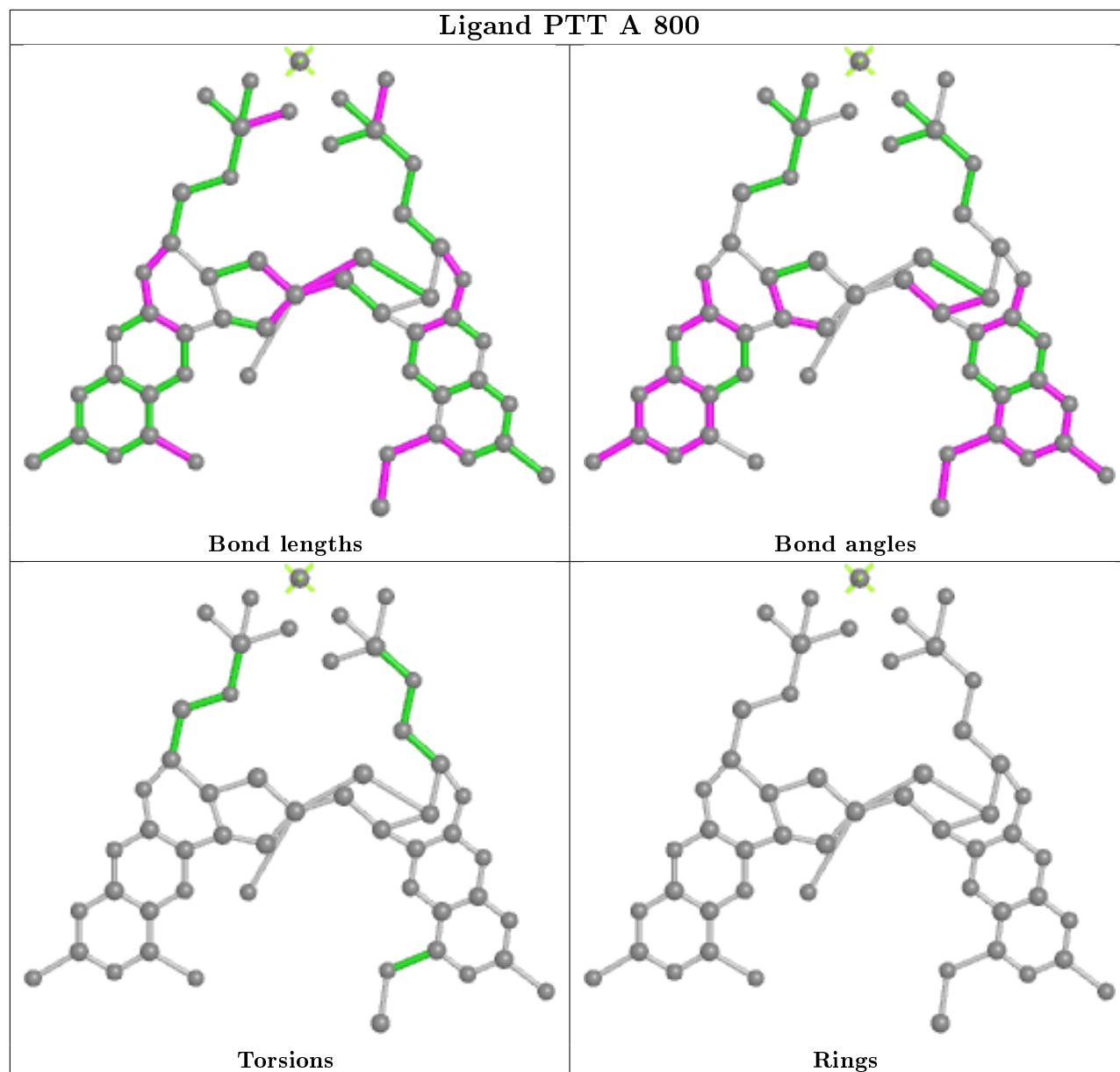


Torsions

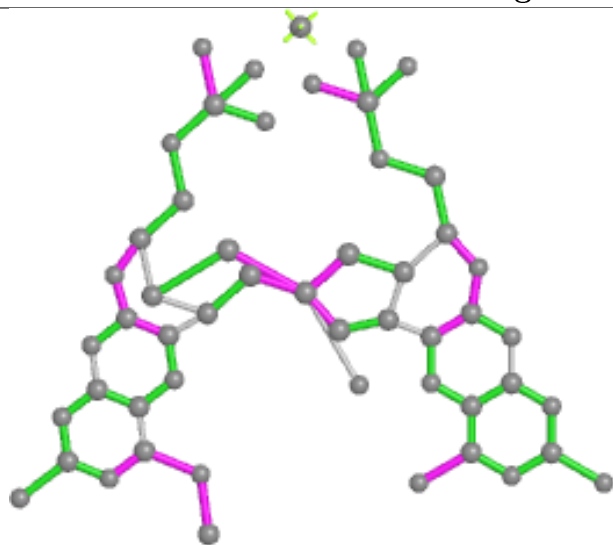


Rings

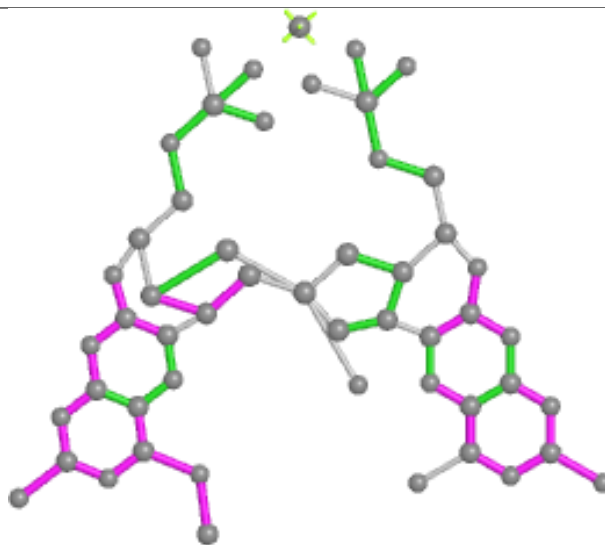
Ligand PTT A 800



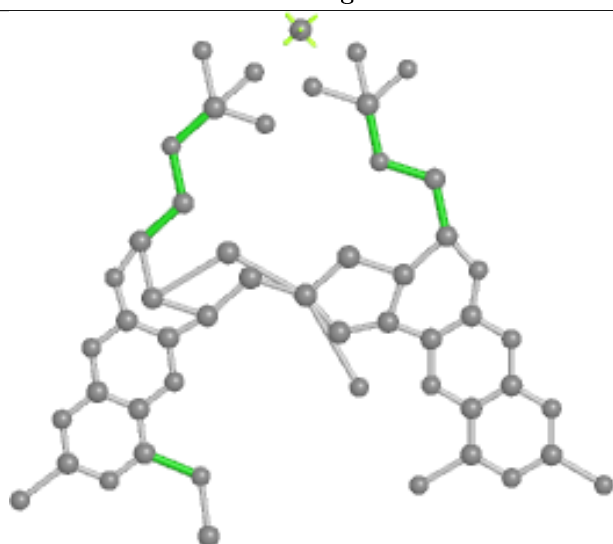
Ligand PTT B 801



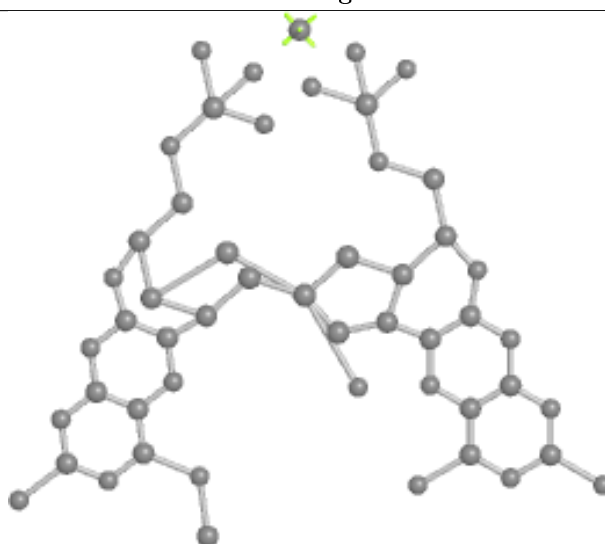
Bond lengths



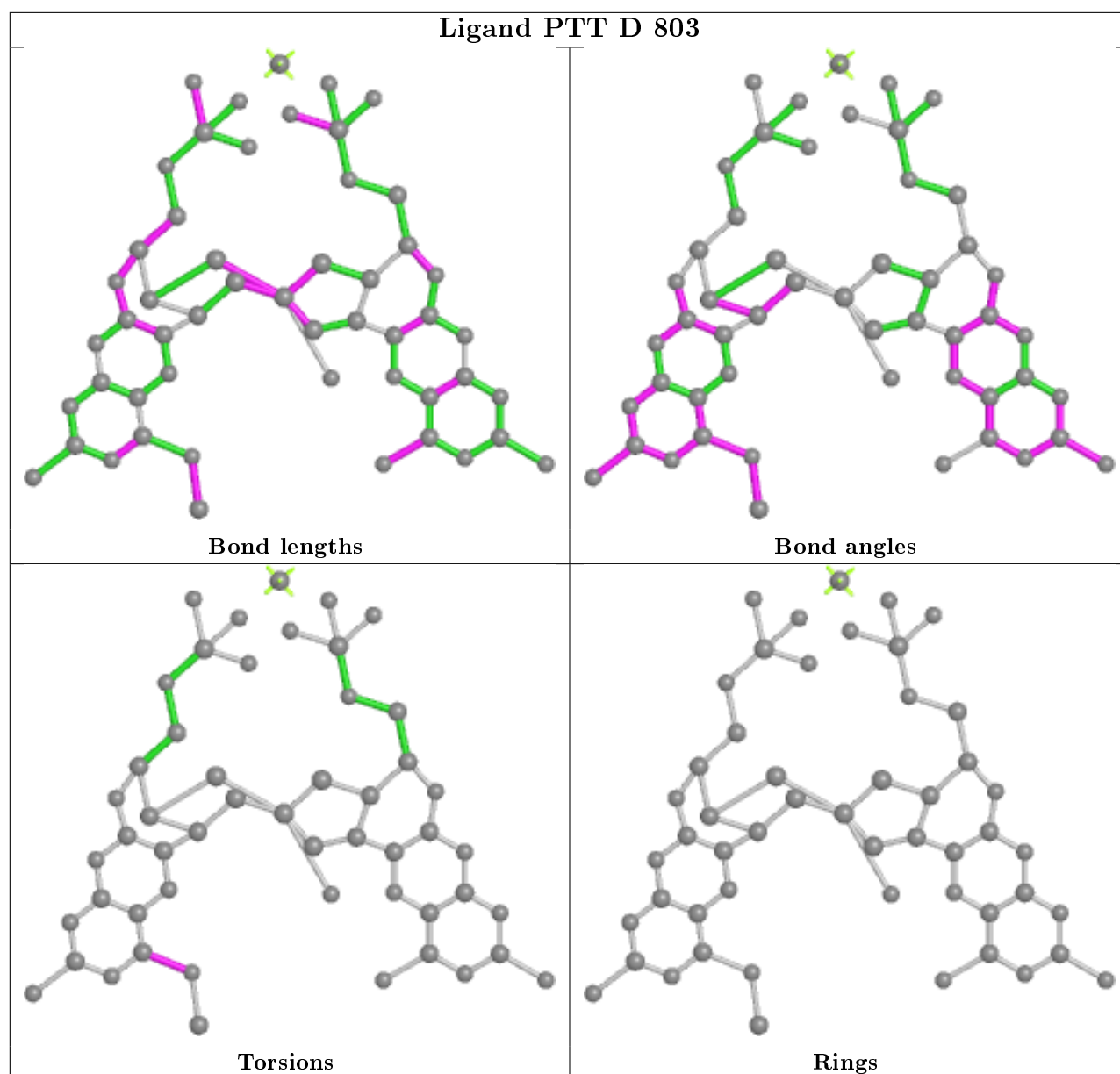
Bond angles



Torsions



Rings



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.