



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 02:04 PM EDT

PDB ID : 1B25 / pdb_00001b25
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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

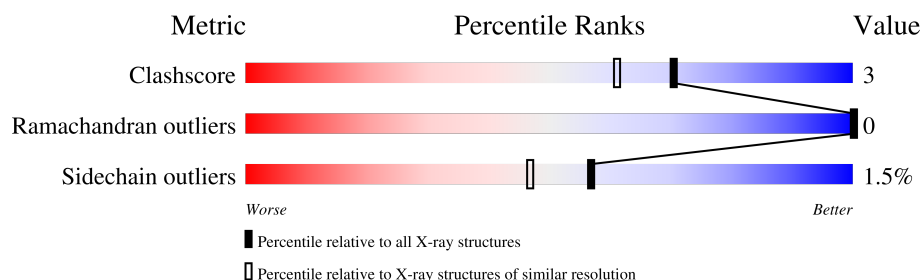
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	619	88% 10% ..
1	B	619	90% 8% ..
1	C	619	87% 10% ..
1	D	619	91% 7% ..

2 Entry composition [i](#)

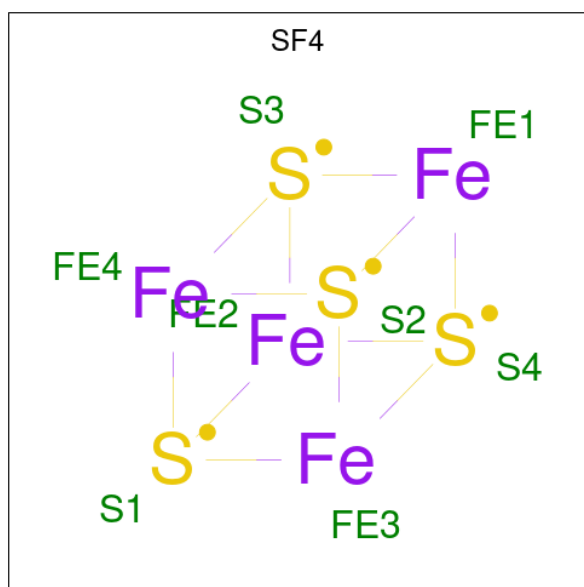
There are 6 unique types of molecules in this entry. The entry contains 20733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SF4) (formula: Fe₄S₄).



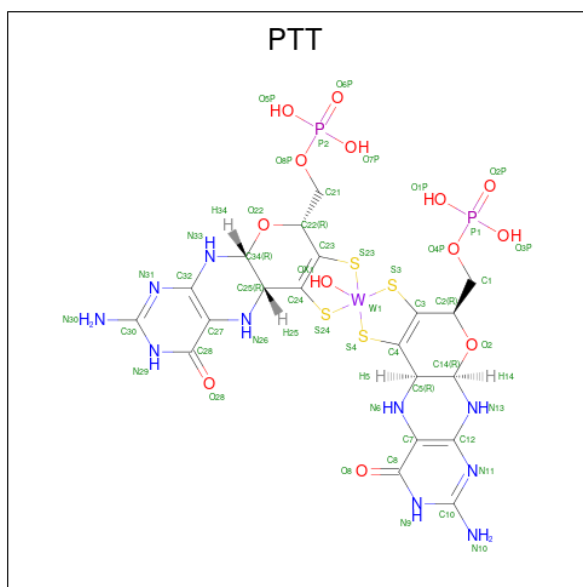
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe S	0	0
			8 4 4			
2	B	1	Total	Fe S	0	0
			8 4 4			

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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 Oxo-tungstopterin cofactor (CCD ID: PTT) (formula: $C_{20}H_{25}N_{10}O_{13}P_2S_4W$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	W	0	0
			50	20	10	13	2	4	1		
3	B	1	Total	C	N	O	P	S	W	0	0
			50	20	10	13	2	4	1		
3	C	1	Total	C	N	O	P	S	W	0	0
			50	20	10	13	2	4	1		
3	D	1	Total	C	N	O	P	S	W	0	0
			50	20	10	13	2	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Mg 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	B	1	Total 1	Ca 1	0	0
5	C	1	Total 1	Ca 1	0	0
5	D	1	Total 1	Ca 1	0	0

- Molecule 6 is water.

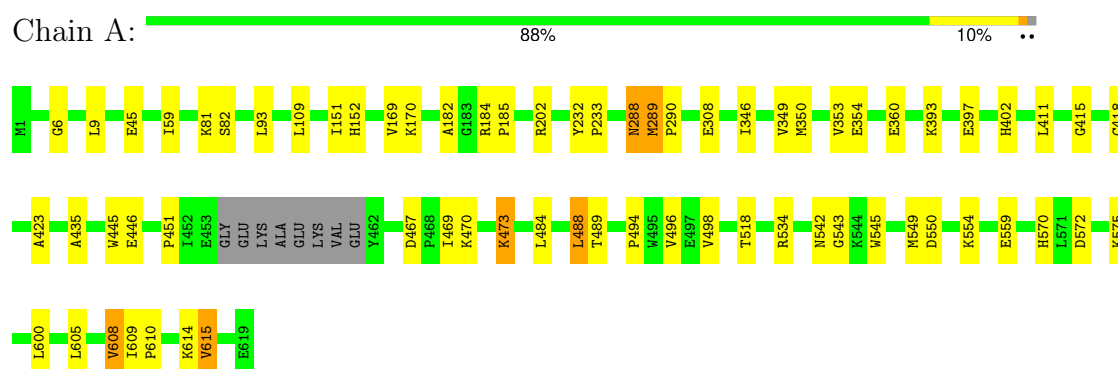
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	288	Total 288	O 288	0	0
6	B	321	Total 321	O 321	0	0
6	C	378	Total 378	O 378	0	0
6	D	362	Total 362	O 362	0	0

3 Residue-property plots

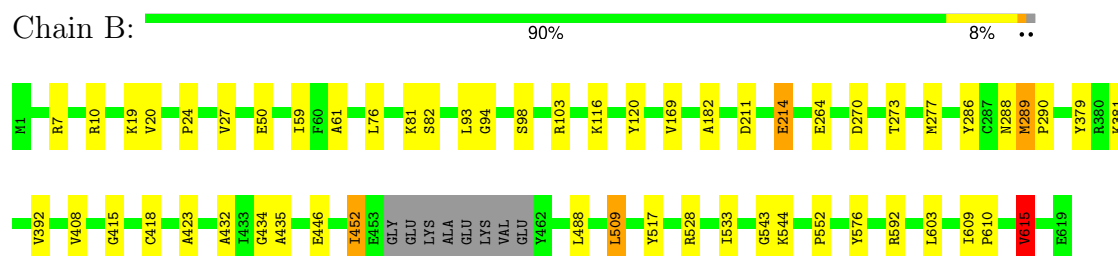
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

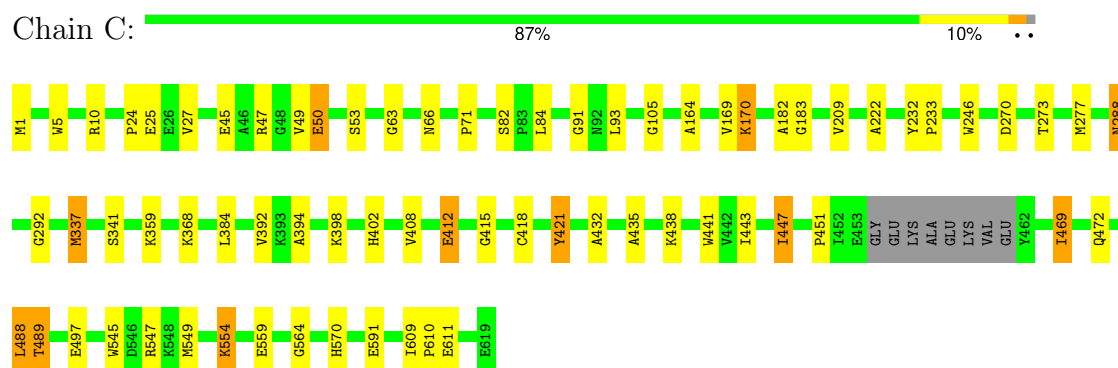
• Molecule 1: PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE)



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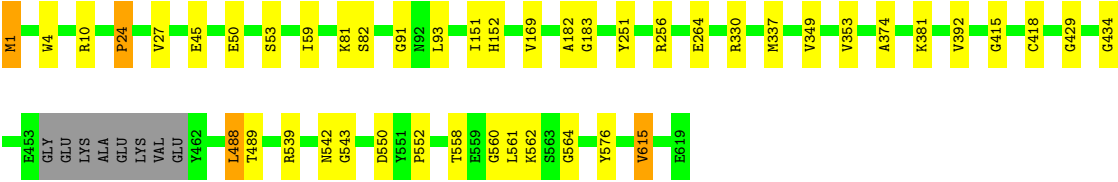


• Molecule 1: PROTEIN (FORMALDEHYDE FERREDOXIN OXIDOREDUCTASE)

Chain D:

91%

7% ..



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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/4896	0.97	15/6619 (0.2%)
1	B	0.57	0/4896	0.99	17/6619 (0.3%)
1	C	0.61	0/4896	0.97	17/6619 (0.3%)
1	D	0.59	0/4896	0.96	14/6619 (0.2%)
All	All	0.59	0/19584	0.97	63/26476 (0.2%)

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 (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	VAL	N-CA-C	8.80	118.87	110.42
1	C	82	SER	N-CA-C	7.62	119.26	109.65
1	B	82	SER	N-CA-C	7.51	119.11	109.65
1	C	418	CYS	N-CA-C	7.46	122.10	112.26
1	A	82	SER	N-CA-C	7.37	118.93	109.65
1	D	82	SER	N-CA-C	7.36	118.93	109.65
1	B	418	CYS	N-CA-C	7.16	121.70	112.26
1	A	488	LEU	N-CA-C	6.97	118.53	111.07
1	C	497	GLU	N-CA-C	6.55	119.39	111.40
1	D	418	CYS	N-CA-C	6.54	120.89	112.26
1	C	564	GLY	CA-C-N	6.53	126.22	119.56
1	C	564	GLY	C-N-CA	6.53	126.22	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	N-CA-C	-6.40	100.72	109.37
1	A	418	CYS	N-CA-C	6.40	119.80	112.57
1	D	392	VAL	N-CA-C	6.40	117.15	110.62
1	A	45	GLU	N-CA-C	6.29	120.99	112.88
1	D	564	GLY	CA-C-N	6.27	125.95	119.56
1	D	564	GLY	C-N-CA	6.27	125.95	119.56
1	B	434	GLY	N-CA-C	-6.18	105.84	112.08
1	C	392	VAL	N-CA-C	6.15	116.89	110.62
1	A	170	LYS	N-CA-C	6.12	118.75	111.71
1	A	152	HIS	N-CA-C	6.08	120.54	113.18
1	C	50	GLU	N-CA-C	-6.02	102.06	109.65
1	B	81	LYS	N-CA-C	-5.99	100.97	109.96
1	D	152	HIS	N-CA-C	5.98	120.42	113.18
1	D	169	VAL	N-CA-C	-5.97	101.31	109.37
1	B	289	MET	CA-C-N	5.89	126.23	119.93
1	B	289	MET	C-N-CA	5.89	126.23	119.93
1	D	81	LYS	N-CA-C	-5.88	101.15	109.96
1	D	434	GLY	N-CA-C	-5.87	106.05	112.04
1	A	518	THR	N-CA-C	-5.83	102.68	110.55
1	A	289	MET	CA-C-N	5.81	126.15	119.93
1	A	289	MET	C-N-CA	5.81	126.15	119.93
1	C	421	TYR	CA-C-N	5.79	125.26	119.24
1	C	421	TYR	C-N-CA	5.79	125.26	119.24
1	B	615	VAL	N-CA-C	5.71	118.67	112.96
1	D	415	GLY	N-CA-C	5.69	126.67	113.18
1	C	488	LEU	N-CA-C	5.67	117.13	111.07
1	C	169	VAL	N-CA-C	-5.59	101.82	109.37
1	B	169	VAL	N-CA-C	-5.59	101.82	109.37
1	C	270	ASP	N-CA-C	5.58	118.52	109.86
1	B	270	ASP	N-CA-C	5.56	118.98	110.36
1	B	615	VAL	CB-CA-C	5.48	115.88	111.06
1	B	59	ILE	N-CA-C	5.47	115.83	108.17
1	A	415	GLY	N-CA-C	5.47	126.14	113.18
1	D	24	PRO	N-CA-C	5.46	119.66	111.14
1	D	59	ILE	N-CA-C	5.44	115.79	108.17
1	B	392	VAL	N-CA-C	5.39	117.82	111.09
1	D	488	LEU	N-CA-C	5.37	116.82	111.07
1	C	415	GLY	N-CA-C	5.33	125.81	113.18
1	B	415	GLY	N-CA-C	5.30	125.75	113.18
1	A	59	ILE	N-CA-C	5.29	115.58	108.17
1	A	81	LYS	N-CA-C	-5.24	102.10	109.96
1	B	488	LEU	N-CA-C	5.22	116.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLY	N-CA-C	-5.21	102.40	111.62
1	C	432	ALA	N-CA-C	5.21	118.42	111.75
1	A	6	GLY	N-CA-C	-5.19	106.91	114.90
1	D	558	THR	N-CA-C	5.15	119.41	113.18
1	C	547	ARG	N-CA-C	5.07	117.55	111.71
1	C	170	LYS	N-CA-C	5.07	117.53	111.71
1	B	61	ALA	N-CA-C	5.06	116.77	108.52
1	C	49	VAL	N-CA-C	5.04	115.55	110.05
1	B	50	GLU	N-CA-C	-5.02	103.32	109.65

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	37	0
1	B	4786	0	4773	27	0
1	C	4786	0	4773	42	0
1	D	4786	0	4773	23	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	50	0	19	2	0
3	B	50	0	19	2	0
3	C	50	0	19	1	0
3	D	50	0	19	2	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
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	288	0	0	4	0
6	B	321	0	0	7	0
6	C	378	0	0	2	0
6	D	362	0	0	4	0
All	All	20733	0	19168	130	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 3.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLY:H	1:C:66:ASN:HD22	1.15	0.93
1:C:554:LYS:HD2	1:C:554:LYS:H	1.36	0.90
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
1:A:93:LEU:HB3	1:A:182:ALA:HB2	1.64	0.78
1:A:423:ALA:HB2	1:A:470:LYS:HG3	1.66	0.78
1:C:554:LYS:H	1:C:554:LYS:CD	1.99	0.76
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:C:50:GLU:HB2	1:C:53:SER:HB3	1.70	0.72
1:C:63:GLY:H	1:C:66:ASN:ND2	1.90	0.67
1:A:610:PRO:O	1:A:614:LYS:HG3	1.96	0.66
1:A:549:MET:HE3	6:A:967:HOH:O	1.96	0.65
1:C:84:LEU:HD13	1:C:170:LYS:HB3	1.79	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:A:451:PRO:HG2	6:A:975:HOH:O	2.04	0.57
1:B:452:ILE:HG13	6:B:950:HOH:O	2.05	0.57
1:C:24:PRO:HG2	1:C:27:VAL:HG23	1.87	0.57
1:D:10:ARG:HH22	1:D:45:GLU:CD	2.13	0.56
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:A:549:MET:HA	1:A:549:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:O	1:A:354:GLU:HG3	2.08	0.54
1:B:93:LEU:HA	3:B:702:PTT:O5P	2.07	0.54
1:B:544:LYS:HE3	6:B:930:HOH:O	2.08	0.53
1:A:308:GLU:HB2	3:A:702: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: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
1:D:24:PRO:HG2	1:D:27:VAL:CG2	2.41	0.51
1:A:93:LEU:HA	3:A:702:PTT:O5P	2.11	0.51
1:C:292:GLY:HA2	6:C:906:HOH:O	2.11	0.51
1:C:359:LYS:HA	1:C:359:LYS:HE2	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:1:MET:HE2	1:D:4:TRP:CE3	2.47	0.50
1:C:91:GLY:HA3	1:C:183:GLY:H	1.76	0.50
1:B:116:LYS:HD3	6:B:906:HOH:O	2.12	0.50
1:A:534:ARG:HH22	1:A:550:ASP:CG	2.21	0.49
1:B:103:ARG:HD2	6:B:855: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	6:B:1090:HOH:O	2.14	0.48
1:C:1:MET:HE2	1:C:25:GLU:HB2	1.95	0.48
1:D:93:LEU:HA	3:D:702:PTT:O5P	2.14	0.47
1:B:288:ASN:C	1:B:290:PRO:HD3	2.40	0.47
1:C:164:ALA:CB	1:C:337:MET:HG2	2.44	0.47
1:C:368:LYS:HG2	6:C:1071:HOH:O	2.15	0.47
1:A:600:LEU:HD13	1:A:608:VAL:HG22	1.97	0.47
1:D:251:TYR:HD1	6:D:891:HOH:O	1.97	0.47
1:A:534:ARG:HH21	1:A:545:TRP:HE1	1.62	0.46
1:C:93:LEU:HA	3:C:702:PTT:O5P	2.14	0.46
1:A:151:ILE:HG13	1:D:151:ILE:HG13	1.96	0.46
1:D:1:MET:HE2	1:D:4:TRP:HE3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:SF4:S4	3:B:702:PTT:H22	2.57	0.45
1:C:402:HIS:CE1	1:C:554:LYS:HD3	2.51	0.45
1:C:545:TRP:CZ3	1:C:549:MET:HE2	2.52	0.45
1:B:103:ARG:HD3	6:B:1045: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: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	6:D:1072: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	6:A:878:HOH:O	2.17	0.43
1:A:402:HIS:CD2	6:A:920: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:D:429:GLY:O	1:D:550:ASP:HA	2.20	0.42
1:A:393:LYS:O	1:A:397:GLU:HG2	2.18	0.42
1:D:337:MET:HE1	1:D:374:ALA:O	2.20	0.42
1:B:423:ALA:HB3	1:B:446:GLU:CD	2.44	0.42
1:D:561:LEU:HD22	6:D:891:HOH:O	2.19	0.42
2:D:701:SF4:S4	3:D:702:PTT:H22	2.59	0.42
1:C:10:ARG:HH22	1:C:45:GLU:CD	2.28	0.42
1:C:441:TRP:HH2	1:C:451:PRO:HD2	1.84	0.42
1:C:50:GLU:HB2	1:C:53:SER:CB	2.45	0.42
1:C:408:VAL:HB	1:C:435:ALA:HB2	2.01	0.42
1:A:346:ILE:O	1:A:350:MET:HG3	2.20	0.42
1:B:211:ASP:CG	1:B:214:GLU:HB2	2.44	0.42
1:C:246:TRP:CH2	1:C:447:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	6:B:848:HOH:O	2.18	0.41
1:D:256:ARG:HD2	6:D:827:HOH:O	2.19	0.41
1:A:559:GLU:O	1:A:570:HIS:HB3	2.19	0.41
1:C:288:ASN:HD22	1:C:288:ASN:H	1.68	0.41
1:D:50:GLU:HB2	1:D:53:SER:HB3	2.02	0.41
1:A:288:ASN:C	1:A:290:PRO:HD3	2.45	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:B:432:ALA:HB1	1:B:533:ILE:HG21	2.03	0.41
1:C:559:GLU:O	1:C:570:HIS:HB3	2.21	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:9:LEU:HD23	1:A:109:LEU:HD13	2.02	0.40
1:A:411:LEU:O	1:A:435:ALA:HB3	2.21	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:A:423:ALA:HB3	1:A:446:GLU:CD	2.47	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	484 (98%)	9 (2%)	51	40
1	B	493/499 (99%)	488 (99%)	5 (1%)	68	60
1	C	493/499 (99%)	482 (98%)	11 (2%)	45	32
1	D	493/499 (99%)	488 (99%)	5 (1%)	68	60
All	All	1972/1996 (99%)	1942 (98%)	30 (2%)	57	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	360	GLU
1	A	469	ILE
1	A	473	LYS
1	A	494	PRO
1	A	498	VAL
1	A	554	LYS
1	A	608	VAL
1	A	615	VAL
1	B	214	GLU
1	B	264	GLU
1	B	452	ILE
1	B	509	LEU
1	B	615	VAL
1	C	209	VAL
1	C	288	ASN

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Mol	Chain	Res	Type
1	C	337	MET
1	C	384	LEU
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	1	MET
1	D	264	GLU
1	D	381	LYS
1	D	539	ARG
1	D	615	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	288	ASN
1	A	293	ASN
1	A	301	GLN
1	A	542	ASN
1	B	228	ASN
1	B	250	ASN
1	B	281	GLN
1	C	66	ASN
1	C	281	GLN
1	C	288	ASN
1	C	372	GLN
1	D	155	ASN
1	D	281	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
3	PTT	B	702	4,5	46,57,57	2.16	11 (23%)	44,94,94	2.77	18 (40%)
2	SF4	C	701	1	0,12,12	-	-	-		
2	SF4	B	701	1	0,12,12	-	-	-		
2	SF4	A	701	1	0,12,12	-	-	-		
3	PTT	D	702	4,5	46,57,57	2.21	11 (23%)	44,94,94	3.31	16 (36%)
3	PTT	A	702	4,5	46,57,57	2.10	12 (26%)	44,94,94	3.25	16 (36%)
3	PTT	C	702	4,5	46,57,57	2.36	12 (26%)	44,94,94	3.14	18 (40%)
2	SF4	D	701	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
3	PTT	B	702	4,5	-	0/12/92/92	0/8/8/8
2	SF4	C	701	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5
2	SF4	A	701	1	-	-	0/6/5/5
3	PTT	D	702	4,5	-	0/12/92/92	0/8/8/8
3	PTT	A	702	4,5	-	0/12/92/92	0/8/8/8
3	PTT	C	702	4,5	-	0/12/92/92	0/8/8/8
2	SF4	D	701	1	-	-	0/6/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	PTT	O28-C28	7.89	1.38	1.23
3	A	702	PTT	O8-C8	7.79	1.38	1.23
3	B	702	PTT	O8-C8	7.78	1.38	1.23
3	D	702	PTT	O28-C28	7.43	1.37	1.23
3	C	702	PTT	O8-C8	7.38	1.37	1.23
3	D	702	PTT	O8-C8	7.22	1.37	1.23
3	B	702	PTT	O28-C28	7.19	1.37	1.23
3	A	702	PTT	O28-C28	6.04	1.35	1.23
3	D	702	PTT	C27-C32	4.65	1.46	1.38
3	C	702	PTT	C34-C25	4.58	1.57	1.53
3	D	702	PTT	C34-C25	4.42	1.57	1.53
3	C	702	PTT	C27-C32	4.30	1.46	1.38
3	C	702	PTT	O2-C14	-3.99	1.37	1.43
3	A	702	PTT	C14-C5	3.89	1.56	1.53
3	B	702	PTT	C34-C25	3.66	1.56	1.53
3	A	702	PTT	C7-C12	3.61	1.44	1.38
3	C	702	PTT	C14-C5	3.46	1.56	1.53
3	B	702	PTT	O2-C14	-3.40	1.38	1.43
3	A	702	PTT	O2-C14	-3.40	1.38	1.43
3	D	702	PTT	C14-C5	3.32	1.56	1.53
3	B	702	PTT	C14-C5	3.25	1.56	1.53
3	B	702	PTT	C27-C32	3.02	1.43	1.38
3	C	702	PTT	P1-O2P	3.01	1.59	1.50
3	A	702	PTT	C27-C32	2.73	1.43	1.38
3	C	702	PTT	C7-C12	2.67	1.43	1.38
3	A	702	PTT	C28-N29	-2.61	1.34	1.38
3	D	702	PTT	C7-C12	2.61	1.43	1.38
3	C	702	PTT	O2-C2	-2.54	1.38	1.43
3	C	702	PTT	C32-N33	-2.51	1.33	1.35
3	C	702	PTT	C1-C2	2.47	1.55	1.51
3	B	702	PTT	C7-C12	2.45	1.42	1.38
3	D	702	PTT	O2-C14	-2.41	1.40	1.43
3	D	702	PTT	C1-C2	2.38	1.55	1.51
3	B	702	PTT	P1-O2P	2.36	1.57	1.50
3	A	702	PTT	O22-C22	-2.36	1.39	1.43
3	A	702	PTT	P1-O2P	2.30	1.57	1.50
3	B	702	PTT	C32-N33	2.26	1.37	1.35
3	A	702	PTT	O22-C34	-2.22	1.40	1.43
3	D	702	PTT	P1-O2P	2.20	1.57	1.50
3	B	702	PTT	O22-C34	-2.20	1.40	1.43
3	D	702	PTT	P2-O7P	-2.18	1.46	1.54
3	A	702	PTT	P2-O6P	2.10	1.57	1.50
3	C	702	PTT	P1-O3P	-2.08	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	PTT	C28-N29	-2.07	1.35	1.38
3	B	702	PTT	C28-N29	-2.03	1.35	1.38
3	A	702	PTT	C34-C25	2.01	1.55	1.53

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	PTT	O22-C34-C25	-14.34	99.40	108.96
3	D	702	PTT	O2-C14-N13	13.50	120.85	108.61
3	C	702	PTT	O2-C14-C5	-11.43	101.34	108.96
3	D	702	PTT	C14-C5-N6	-9.48	98.55	107.87
3	C	702	PTT	O22-C34-C25	-9.18	102.84	108.96
3	A	702	PTT	O22-C34-N33	9.12	116.88	108.61
3	B	702	PTT	O22-C34-C25	-7.21	104.15	108.96
3	D	702	PTT	O22-C34-C25	7.12	113.71	108.96
3	C	702	PTT	C14-C5-N6	6.71	114.46	107.87
3	B	702	PTT	C30-N31-C32	5.57	123.18	113.36
3	B	702	PTT	C34-C25-N26	5.51	113.28	107.87
3	B	702	PTT	O2-C14-C5	5.30	112.50	108.96
3	D	702	PTT	O2-C14-C5	5.23	112.45	108.96
3	C	702	PTT	C10-N11-C12	5.20	122.53	113.36
3	B	702	PTT	O22-C34-N33	4.97	113.12	108.61
3	A	702	PTT	O28-C28-C27	-4.66	116.02	127.26
3	B	702	PTT	C10-N11-C12	4.56	121.41	113.36
3	D	702	PTT	C10-N11-C12	4.33	121.00	113.36
3	C	702	PTT	C34-C25-N26	4.22	112.02	107.87
3	B	702	PTT	O2-C2-C3	4.06	114.82	109.09
3	B	702	PTT	C27-C28-N29	3.97	123.04	112.13
3	A	702	PTT	O3P-P1-O4P	3.97	117.02	106.67
3	D	702	PTT	O22-C34-N33	-3.92	105.05	108.61
3	A	702	PTT	C30-N31-C32	3.91	120.27	113.36
3	B	702	PTT	C3-C4-S4	3.89	125.28	119.62
3	A	702	PTT	C3-C4-S4	3.84	125.20	119.62
3	B	702	PTT	O28-C28-C27	-3.79	118.12	127.26
3	A	702	PTT	C10-N11-C12	3.77	120.01	113.36
3	B	702	PTT	O2-C14-N13	-3.60	105.34	108.61
3	C	702	PTT	C23-C24-S24	3.57	124.80	119.62
3	A	702	PTT	O22-C22-C23	-3.48	104.17	109.09
3	B	702	PTT	O8-C8-C7	-3.44	118.96	127.26
3	C	702	PTT	O28-C28-C27	-3.41	119.05	127.26
3	D	702	PTT	O28-C28-C27	-3.18	119.59	127.26
3	C	702	PTT	O8-C8-C7	-3.15	119.67	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	PTT	O8-C8-C7	-3.11	119.75	127.26
3	C	702	PTT	N10-C10-N9	3.02	123.13	116.76
3	C	702	PTT	C3-C4-S4	2.96	123.93	119.62
3	D	702	PTT	C8-C7-N6	2.95	124.31	116.27
3	D	702	PTT	N10-C10-N9	2.94	122.96	116.76
3	A	702	PTT	O8-C8-C7	-2.79	120.53	127.26
3	B	702	PTT	C7-C8-N9	2.78	119.77	112.13
3	D	702	PTT	C30-N31-C32	2.76	118.23	113.36
3	C	702	PTT	C7-C8-N9	2.68	119.50	112.13
3	C	702	PTT	C30-N31-C32	2.68	118.08	113.36
3	B	702	PTT	C28-C27-N26	2.68	123.57	116.27
3	B	702	PTT	N29-C30-N31	-2.67	118.44	123.32
3	A	702	PTT	O2-C14-C5	-2.66	107.19	108.96
3	A	702	PTT	C7-C8-N9	2.58	119.22	112.13
3	A	702	PTT	C27-C28-N29	2.55	119.14	112.13
3	D	702	PTT	N9-C10-N11	-2.55	118.65	123.32
3	D	702	PTT	C27-C28-N29	2.54	119.11	112.13
3	C	702	PTT	O8P-C21-C22	-2.54	102.31	108.58
3	C	702	PTT	C8-C7-N6	2.54	123.18	116.27
3	D	702	PTT	C28-C27-N26	2.53	123.16	116.27
3	A	702	PTT	O28-C28-N29	2.50	124.81	120.11
3	A	702	PTT	C23-C24-S24	2.47	123.21	119.62
3	D	702	PTT	C7-C8-N9	2.37	118.64	112.13
3	C	702	PTT	C27-C28-N29	2.37	118.64	112.13
3	A	702	PTT	N30-C30-N29	2.26	121.53	116.76
3	D	702	PTT	C3-C4-S4	2.26	122.90	119.62
3	B	702	PTT	N10-C10-N9	2.24	121.49	116.76
3	C	702	PTT	N9-C10-N11	-2.18	119.33	123.32
3	B	702	PTT	C8-C7-N6	2.14	122.09	116.27
3	B	702	PTT	N9-C10-N11	-2.12	119.44	123.32
3	C	702	PTT	C28-C27-N26	2.10	122.00	116.27
3	C	702	PTT	C10-N9-C8	-2.06	121.38	125.11
3	A	702	PTT	C8-C7-N6	2.01	121.76	116.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

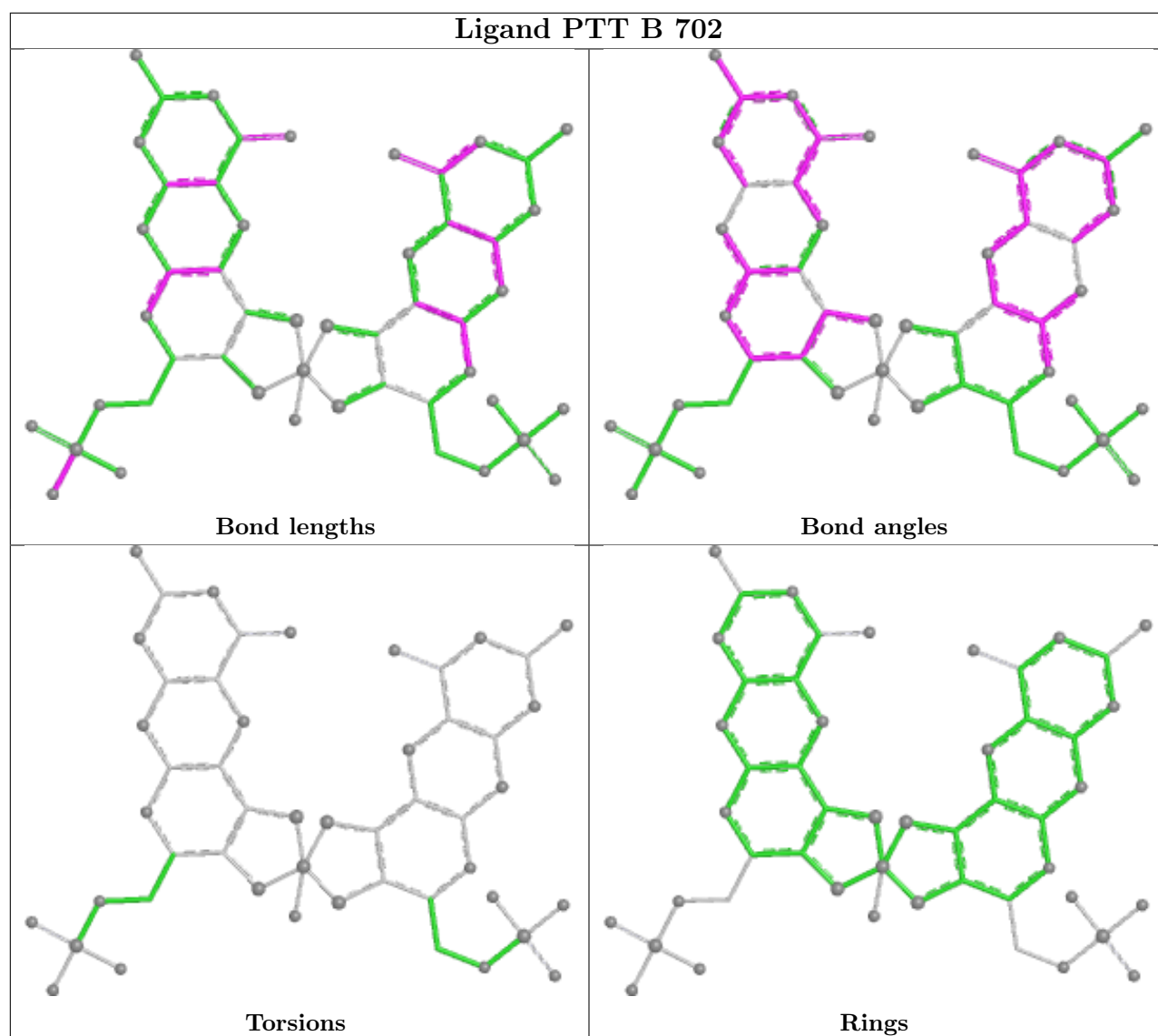
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	PTT	2	0

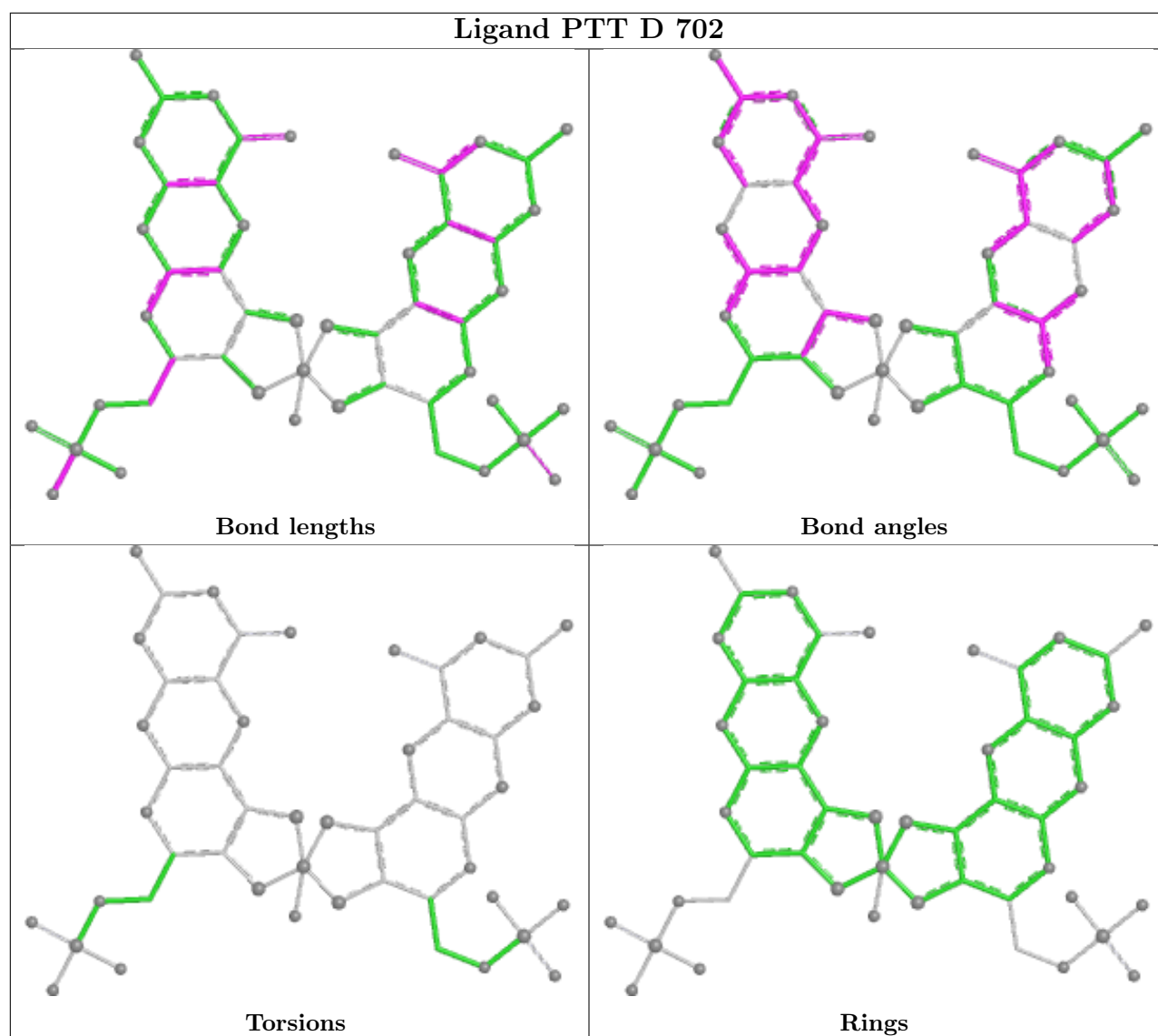
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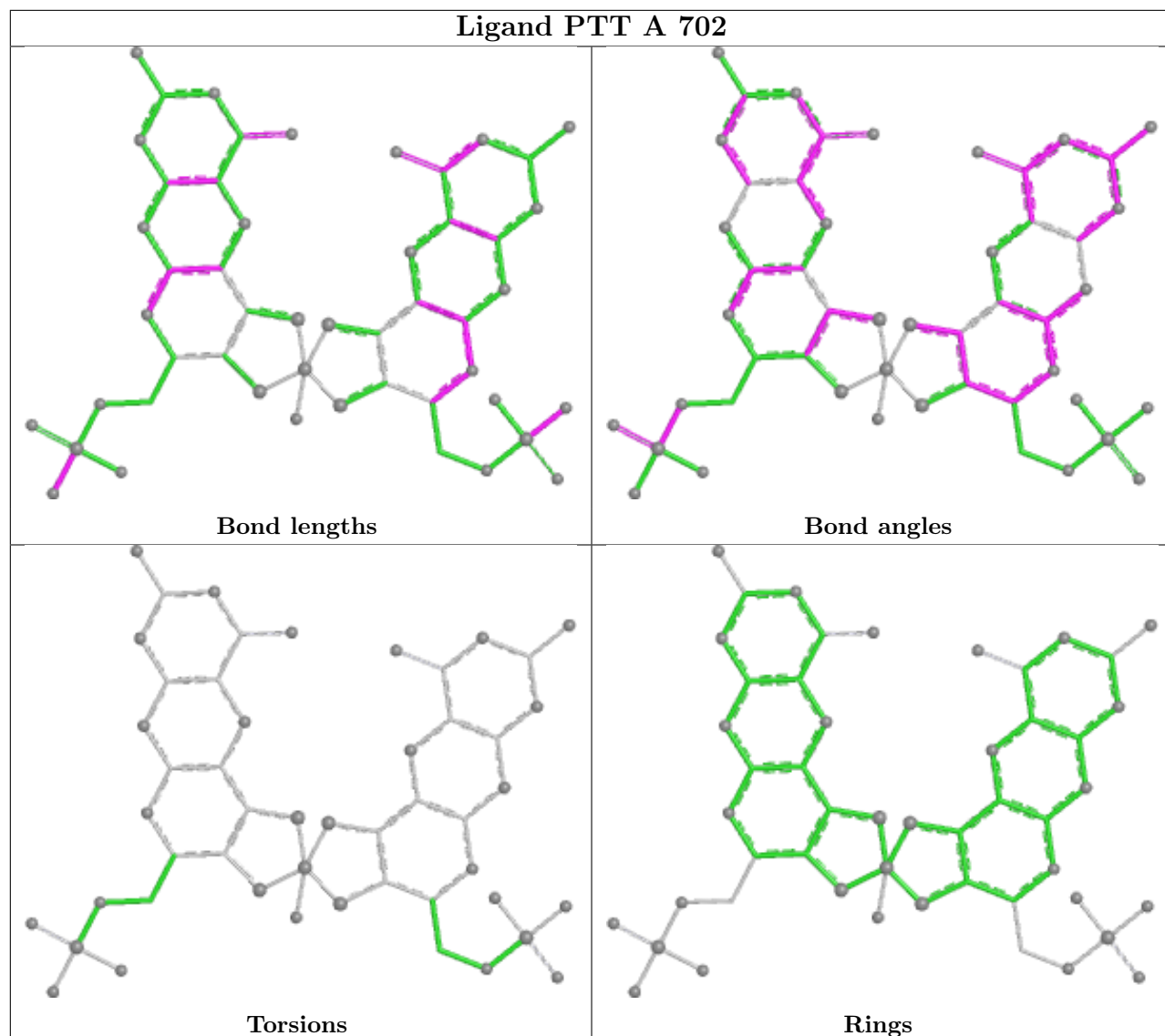
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	SF4	1	0
3	D	702	PTT	2	0
3	A	702	PTT	2	0
3	C	702	PTT	1	0
2	D	701	SF4	1	0

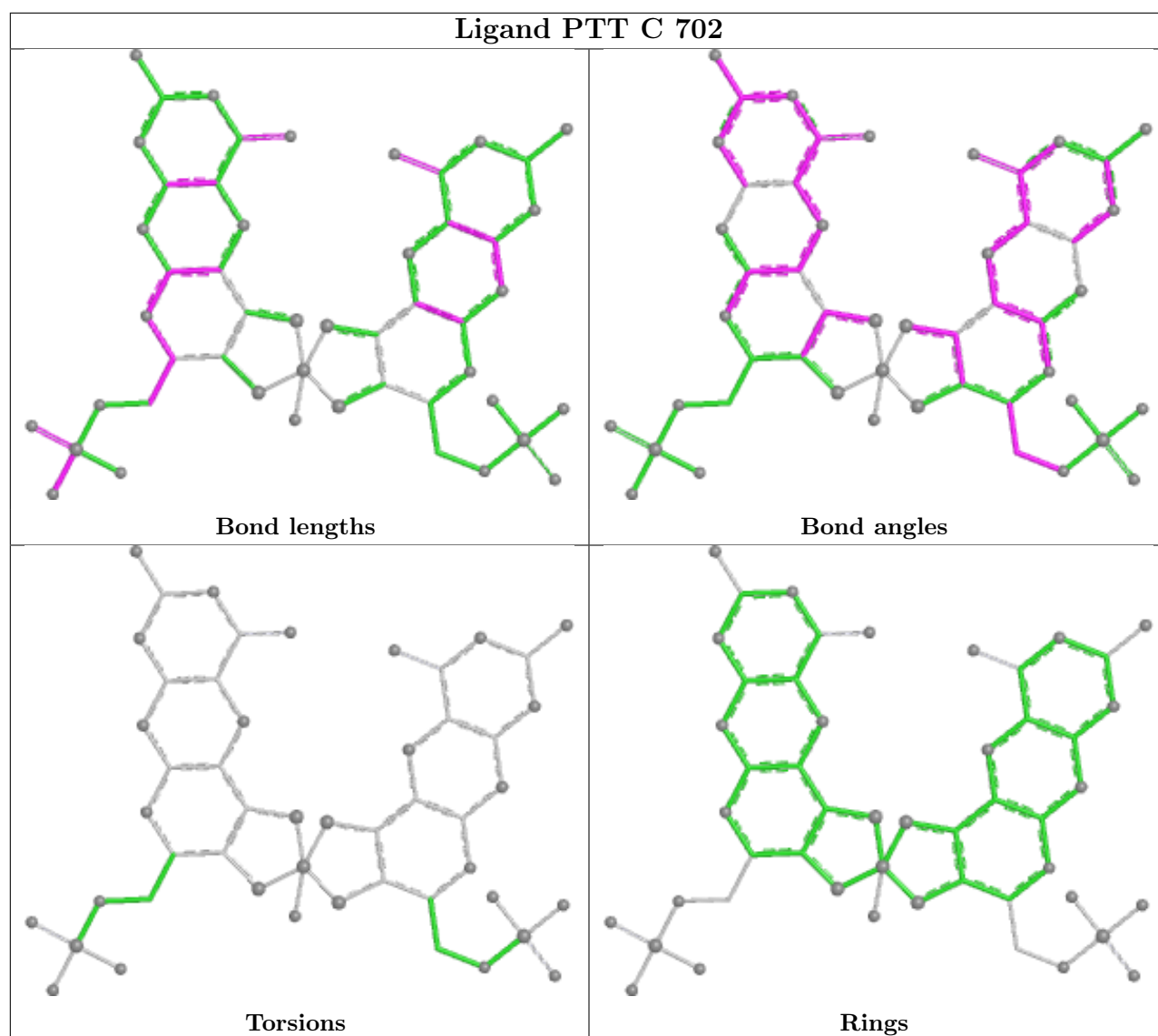
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand PTT A 702





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.