



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:22 PM UTC

PDB ID : 1H5N / pdb_00001h5n
Title : DMSO REDUCTASE MODIFIED BY THE PRESENCE OF DMS AND AIR
Authors : Bailey, S.; Adams, B.; Smith, A.T.; Richards, R.L.; Lowe, D.J.; Bray, R.C.
Deposited on : 2001-05-22
Resolution : 2.00 Å(reported)

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

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

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

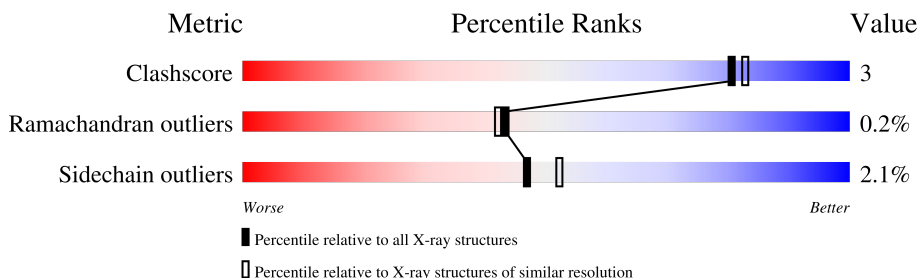
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	823	
1	C	823	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13178 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 Dimethyl sulfoxide/trimethylamine N-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			5867	3730	994	1116	27			
1	C	766	Total	C	N	O	S	0	0	0
			5877	3737	995	1118	27			

There are 28 discrepancies between the modelled and reference sequences:

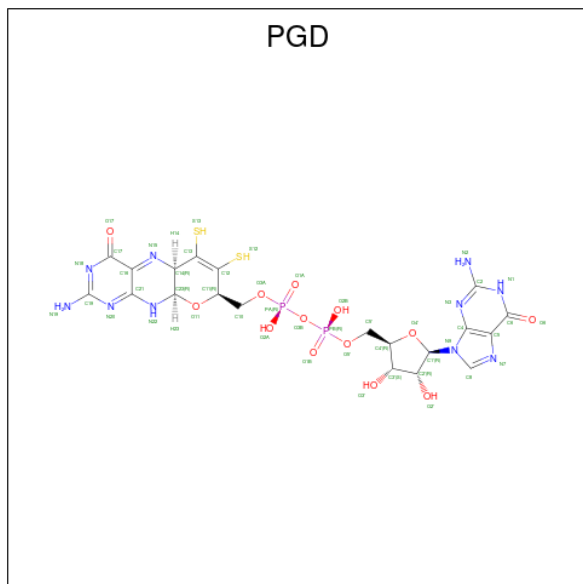
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	THR	conflict	UNP Q52675
A	43	ALA	GLU	conflict	UNP Q52675
A	107	GLU	GLN	conflict	UNP Q52675
A	234	GLU	ASP	conflict	UNP Q52675
A	236	ILE	VAL	conflict	UNP Q52675
A	280	ASP	MET	conflict	UNP Q52675
A	294	GLU	SER	conflict	UNP Q52675
A	295	GLY	ASP	conflict	UNP Q52675
A	312	GLU	ILE	conflict	UNP Q52675
A	374	ALA	SER	conflict	UNP Q52675
A	456	VAL	ILE	conflict	UNP Q52675
A	526	ALA	LYS	conflict	UNP Q52675
A	552	ALA	GLY	conflict	UNP Q52675
A	555	GLN	GLU	conflict	UNP Q52675
C	39	SER	THR	conflict	UNP Q52675
C	43	ALA	GLU	conflict	UNP Q52675
C	107	GLU	GLN	conflict	UNP Q52675
C	234	GLU	ASP	conflict	UNP Q52675
C	236	ILE	VAL	conflict	UNP Q52675
C	280	ASP	MET	conflict	UNP Q52675
C	294	GLU	SER	conflict	UNP Q52675
C	295	GLY	ASP	conflict	UNP Q52675
C	312	GLU	ILE	conflict	UNP Q52675
C	374	ALA	SER	conflict	UNP Q52675
C	456	VAL	ILE	conflict	UNP Q52675

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Chain	Residue	Modelled	Actual	Comment	Reference
C	526	ALA	LYS	conflict	UNP Q52675
C	552	ALA	GLY	conflict	UNP Q52675
C	555	GLN	GLU	conflict	UNP Q52675

- Molecule 2 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: PGD) (formula: C₂₀H₂₄N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
2	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
2	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
2	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 3 is MOLYBDENUM(VI) ION (CCD ID: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mo	0	0
			1	1		
3	C	1	Total	Mo	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	652	Total	O	0	0
			652	652		
5	C	582	Total	O	0	0
			582	582		

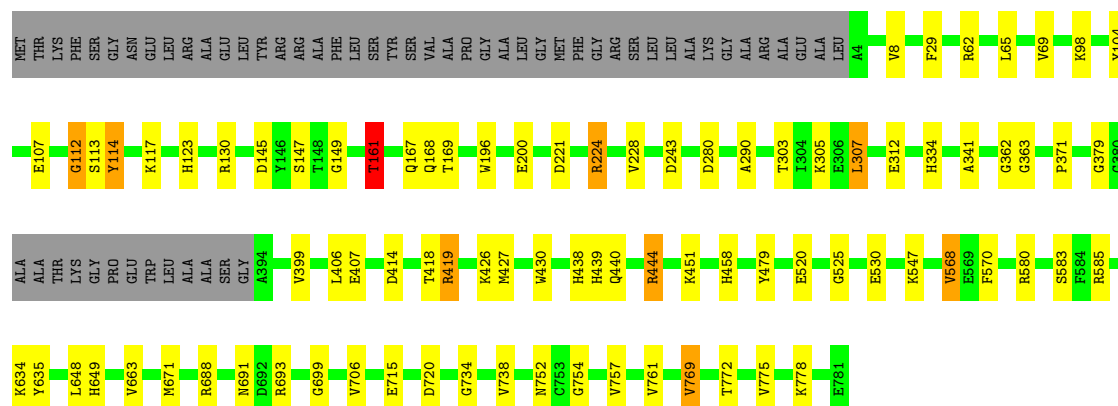
3 Residue-property plots

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.

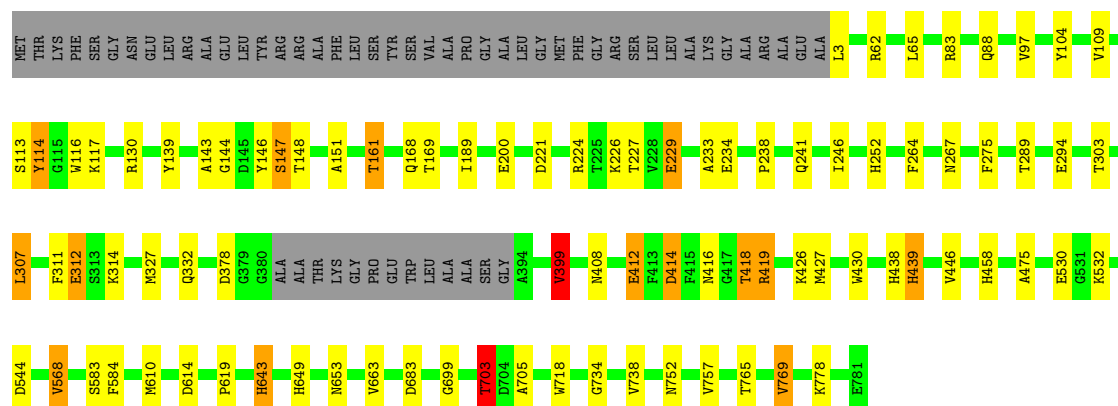
- Molecule 1: Dimethyl sulfoxide/trimethylamine N-oxide reductase

Chain A: 



- Molecule 1: Dimethyl sulfoxide/trimethylamine N-oxide reductase

Chain C: 



4 Data and refinement statistics

Xtrriage (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	68.80Å 116.10Å 230.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	83.7 (20.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.209	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13178	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: SO4, PGD, 6MO

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	0.83	1/6024 (0.0%)	1.57	60/8198 (0.7%)
1	C	0.79	0/6034	1.57	59/8213 (0.7%)
All	All	0.81	1/12058 (0.0%)	1.57	119/16411 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLU	CD-OE1	-5.78	1.14	1.25

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ARG	CD-NE-CZ	10.70	139.38	124.40
1	A	568	VAL	CB-CA-C	-10.68	94.74	110.33
1	A	568	VAL	N-CA-CB	10.52	126.88	111.52
1	C	62	ARG	NE-CZ-NH2	-10.49	109.75	119.20
1	C	568	VAL	N-CA-CB	9.98	125.19	111.41
1	C	130	ARG	NE-CZ-NH1	-9.77	111.73	121.50
1	A	769	VAL	N-CA-CB	-9.70	95.55	111.45
1	C	568	VAL	CB-CA-C	-9.30	96.86	110.63
1	A	458	HIS	CA-CB-CG	9.24	123.04	113.80
1	A	224	ARG	NE-CZ-NH2	8.98	127.28	119.20
1	C	703	THR	CB-CA-C	-8.98	91.89	109.68
1	A	752	ASN	OD1-CG-ND2	8.97	131.57	122.60
1	C	114	TYR	O-C-N	8.42	133.16	123.06
1	C	130	ARG	NE-CZ-NH2	8.17	126.55	119.20
1	A	419	ARG	CD-NE-CZ	8.05	135.67	124.40
1	A	688	ARG	CD-NE-CZ	7.97	135.56	124.40
1	A	312	GLU	CG-CD-OE2	7.90	136.58	118.40
1	C	584	PHE	CA-CB-CG	7.77	121.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	TYR	CA-C-O	-7.26	113.21	121.19
1	A	568	VAL	CA-C-O	-7.24	112.69	120.36
1	C	643	HIS	CA-CB-CG	-7.18	106.62	113.80
1	C	378	ASP	CA-CB-CG	7.09	119.69	112.60
1	C	568	VAL	CA-C-O	-7.08	112.96	120.39
1	C	752	ASN	OD1-CG-ND2	7.07	129.67	122.60
1	A	114	TYR	O-C-N	6.91	131.36	122.87
1	C	88	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	C	161	THR	CB-CA-C	-6.86	95.38	110.67
1	A	62	ARG	NE-CZ-NH2	-6.63	113.23	119.20
1	A	221	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	161	THR	CA-CB-OG1	6.59	119.49	109.60
1	C	458	HIS	CA-CB-CG	6.57	120.37	113.80
1	A	568	VAL	CA-CB-CG2	6.42	121.32	110.40
1	A	754	GLY	N-CA-C	6.38	121.48	114.40
1	C	83	ARG	NE-CZ-NH1	6.35	127.85	121.50
1	C	294	GLU	CB-CG-CD	6.32	123.34	112.60
1	C	114	TYR	CA-C-O	-6.30	114.10	120.96
1	C	416	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	A	379	GLY	CA-C-O	-6.26	113.00	119.20
1	A	196	TRP	N-CA-C	-6.21	104.43	111.14
1	C	233	ALA	N-CA-C	6.20	119.24	110.50
1	C	649	HIS	CB-CA-C	-6.19	108.81	117.23
1	A	243	ASP	CA-CB-CG	-6.18	106.42	112.60
1	C	312	GLU	CG-CD-OE2	6.17	132.60	118.40
1	C	267	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	C	544	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	419	ARG	CB-CA-C	-6.03	99.29	109.72
1	A	29	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	757	VAL	CB-CA-C	-6.03	101.92	110.12
1	A	112	GLY	N-CA-C	-6.02	105.06	112.77
1	C	399	VAL	CB-CA-C	-5.98	104.23	111.88
1	C	438	HIS	N-CA-C	5.92	119.76	112.54
1	C	139	TYR	CA-C-N	5.91	129.82	121.66
1	C	139	TYR	C-N-CA	5.91	129.82	121.66
1	C	408	ASN	N-CA-C	5.90	119.23	109.79
1	A	648	LEU	CA-C-O	-5.85	114.83	121.39
1	C	439	HIS	CA-CB-CG	-5.85	107.95	113.80
1	C	221	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	275	PHE	CA-CB-CG	5.84	119.64	113.80
1	C	568	VAL	CA-CB-CG2	5.83	120.32	110.40
1	C	475	ALA	CA-C-O	-5.80	114.87	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	693	ARG	CG-CD-NE	5.78	124.71	112.00
1	C	147	SER	N-CA-C	5.77	117.37	111.14
1	C	414	ASP	CA-CB-CG	-5.76	106.84	112.60
1	A	444	ARG	CA-C-O	5.72	126.62	120.55
1	A	161	THR	N-CA-CB	5.70	120.86	111.62
1	C	757	VAL	CB-CA-C	-5.70	101.27	110.28
1	A	775	VAL	CA-C-O	-5.67	114.70	121.28
1	A	280	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	312	GLU	OE1-CD-OE2	-5.62	109.41	122.90
1	A	62	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	130	ARG	NE-CZ-NH2	5.62	124.25	119.20
1	A	399	VAL	N-CA-C	5.60	117.01	110.62
1	C	738	VAL	CA-C-O	5.60	126.36	119.58
1	C	311	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	161	THR	CA-CB-OG1	5.57	117.96	109.60
1	A	439	HIS	CA-CB-CG	-5.53	108.27	113.80
1	C	264	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	583	SER	O-C-N	-5.48	115.90	122.15
1	C	438	HIS	CA-CB-CG	5.48	119.28	113.80
1	A	419	ARG	N-CA-CB	5.48	119.17	110.57
1	A	634	LYS	N-CA-C	5.46	117.04	111.14
1	A	585	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	A	334	HIS	CA-CB-CG	-5.38	108.42	113.80
1	C	224	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	130	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	C	683	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	720	ASP	CA-C-N	5.33	125.25	119.76
1	A	720	ASP	C-N-CA	5.33	125.25	119.76
1	C	229	GLU	N-CA-C	5.32	117.08	111.28
1	C	614	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	649	HIS	CB-CA-C	-5.31	110.01	117.23
1	C	778	LYS	N-CA-C	5.27	117.03	111.28
1	A	8	VAL	CA-C-O	-5.25	115.02	120.64
1	A	479	TYR	CA-CB-CG	-5.25	104.44	113.90
1	C	769	VAL	N-CA-CB	-5.25	101.05	111.91
1	A	706	VAL	N-CA-CB	5.23	117.78	110.56
1	C	229	GLU	CA-CB-CG	-5.23	103.64	114.10
1	C	610	MET	CA-C-O	-5.22	113.97	119.97
1	A	547	LYS	CA-C-O	5.22	126.08	120.55
1	C	446	VAL	N-CA-CB	-5.21	103.95	110.47
1	C	224	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	C	234	GLU	N-CA-C	-5.20	102.16	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	399	VAL	N-CA-C	5.16	115.78	110.36
1	C	703	THR	OG1-CB-CG2	5.15	119.60	109.30
1	A	123	HIS	CA-C-N	5.13	129.64	122.41
1	A	123	HIS	C-N-CA	5.13	129.64	122.41
1	C	83	ARG	CD-NE-CZ	5.11	131.56	124.40
1	C	62	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	438	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	530	GLU	N-CA-CB	-5.10	104.55	112.30
1	C	412	GLU	CA-C-O	-5.10	115.24	121.36
1	A	583	SER	CB-CA-C	5.10	119.51	110.85
1	A	427	MET	CA-C-N	-5.08	115.32	122.94
1	A	427	MET	C-N-CA	-5.08	115.32	122.94
1	A	341	ALA	CA-C-O	-5.08	115.17	120.55
1	A	715	GLU	CA-C-O	-5.07	115.99	121.87
1	A	738	VAL	O-C-N	-5.07	115.41	122.05
1	A	228	VAL	N-CA-CB	5.06	116.47	110.55
1	C	446	VAL	CA-CB-CG2	-5.00	101.90	110.40

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	5867	0	5668	28	0
1	C	5877	0	5677	33	0
2	A	94	0	40	1	0
2	C	94	0	40	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	652	0	0	7	0
5	C	582	0	0	4	0
All	All	13178	0	11425	61	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 (61) 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:189:ILE:HD12	1:C:227:THR:HA	1.54	0.89
1:A:407:GLU:OE1	1:A:444:ARG:NH2	2.07	0.88
1:A:671:MET:HE1	1:A:761:VAL:HG11	1.64	0.78
1:A:147:SER:HA	2:A:1782:PGD:S13	2.28	0.73
1:A:149:GLY:HA2	5:A:2159:HOH:O	1.89	0.72
1:C:530:GLU:HG3	1:C:532:LYS:HZ3	1.59	0.65
1:C:147:SER:HA	2:C:1782:PGD:S13	2.37	0.65
1:C:414:ASP:OD1	1:C:419:ARG:HG2	1.98	0.64
1:C:144:GLY:HA3	5:C:2129:HOH:O	1.98	0.63
1:A:407:GLU:HG2	5:A:2354:HOH:O	2.00	0.60
1:C:97:VAL:HG22	1:C:427:MET:HE1	1.81	0.59
1:C:146:TYR:HH	1:C:439:HIS:HD1	1.50	0.59
1:A:414:ASP:OD1	1:A:419:ARG:HG2	2.01	0.59
1:C:143:ALA:O	1:C:399:VAL:HG22	2.03	0.59
1:A:451:LYS:HG2	5:A:2372:HOH:O	2.05	0.56
1:C:109:VAL:HG13	1:C:427:MET:HE2	1.88	0.56
1:A:772:THR:OG1	5:A:2640:HOH:O	2.18	0.56
1:C:530:GLU:HG3	1:C:532:LYS:NZ	2.22	0.55
1:C:703:THR:HG22	1:C:705:ALA:H	1.71	0.55
1:C:653:ASN:ND2	1:C:718:TRP:H	2.05	0.55
1:C:147:SER:HB3	2:C:1783:PGD:S12	2.49	0.53
1:A:663:VAL:HB	1:A:699:GLY:HA3	1.93	0.51
1:A:107:GLU:H	1:A:107:GLU:CD	2.20	0.50
1:A:224:ARG:HD2	5:A:2223:HOH:O	2.11	0.49
1:C:148:THR:HB	1:C:151:ALA:HB3	1.95	0.48
1:A:406:LEU:O	1:A:451:LYS:HD2	2.14	0.48
1:C:412:GLU:OE1	1:C:419:ARG:NH1	2.47	0.47
1:A:69:VAL:HG22	5:A:2019:HOH:O	2.15	0.47
1:A:114:TYR:OH	1:A:145:ASP:HB2	2.15	0.47
1:C:104:TYR:CE1	1:C:426:LYS:HG3	2.49	0.47
1:C:303:THR:O	1:C:307:LEU:HD22	2.15	0.47
1:A:112:GLY:O	1:A:113:SER:C	2.58	0.46
1:A:635:TYR:CZ	1:A:691:ASN:HA	2.51	0.46
1:A:303:THR:HG22	1:A:307:LEU:HD23	1.98	0.45
1:C:3:LEU:N	5:C:2001:HOH:O	2.48	0.45
1:C:303:THR:HG22	1:C:307:LEU:HD22	1.99	0.45
1:A:290:ALA:HB3	1:A:305:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:HIS:CE1	1:C:289:THR:HG22	2.52	0.45
1:C:418:THR:HG23	5:C:2300:HOH:O	2.16	0.45
1:A:671:MET:CE	1:A:761:VAL:HG11	2.41	0.44
1:C:104:TYR:CD1	1:C:426:LYS:HG3	2.53	0.44
1:C:168:GLN:O	1:C:169:THR:C	2.61	0.44
1:A:161:THR:HG22	5:A:2169:HOH:O	2.18	0.43
1:C:663:VAL:HB	1:C:699:GLY:HA3	2.00	0.43
1:C:116:TRP:O	1:C:117:LYS:C	2.61	0.43
1:C:241:GLN:HG2	1:C:327:MET:SD	2.59	0.43
1:C:238:PRO:HB3	1:C:246:ILE:HD11	2.01	0.43
1:C:314:LYS:NZ	5:C:2257:HOH:O	2.26	0.43
1:A:104:TYR:CE1	1:A:426:LYS:HG3	2.54	0.42
1:A:371:PRO:HD2	1:A:570:PHE:CZ	2.55	0.42
1:A:167:GLN:O	1:A:580:ARG:HD2	2.20	0.42
1:C:703:THR:CG2	1:C:705:ALA:H	2.32	0.42
1:A:114:TYR:CE1	1:A:145:ASP:HA	2.55	0.42
1:A:362:GLY:O	1:A:363:GLY:C	2.62	0.42
1:A:168:GLN:O	1:A:169:THR:C	2.64	0.41
1:C:113:SER:O	1:C:114:TYR:C	2.64	0.41
1:A:520:GLU:OE1	1:A:525:GLY:HA3	2.21	0.41
1:C:312:GLU:O	1:C:312:GLU:HG3	2.21	0.40
1:C:332:GLN:OE1	1:C:619:PRO:HA	2.22	0.40
1:C:643:HIS:CD2	1:C:643:HIS:N	2.87	0.40
1:A:440:GLN:CD	1:A:440:GLN:N	2.80	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	761/823 (92%)	735 (97%)	24 (3%)	2 (0%)	36 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	762/823 (93%)	740 (97%)	21 (3%)	1 (0%)	48	46
All	All	1523/1646 (92%)	1475 (97%)	45 (3%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LYS
1	A	734	GLY
1	C	734	GLY

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	607/648 (94%)	597 (98%)	10 (2%)	55	62
1	C	608/648 (94%)	593 (98%)	15 (2%)	42	45
All	All	1215/1296 (94%)	1190 (98%)	25 (2%)	47	52

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	98	LYS
1	A	161	THR
1	A	200	GLU
1	A	307	LEU
1	A	418	THR
1	A	430	TRP
1	A	568	VAL
1	A	769	VAL
1	A	778	LYS
1	C	65	LEU
1	C	161	THR
1	C	200	GLU

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Mol	Chain	Res	Type
1	C	226	LYS
1	C	229	GLU
1	C	307	LEU
1	C	399	VAL
1	C	418	THR
1	C	419	ARG
1	C	430	TRP
1	C	568	VAL
1	C	583	SER
1	C	703	THR
1	C	765	THR
1	C	769	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	434	ASN
1	A	606	ASN
1	C	152	GLN
1	C	241	GLN
1	C	606	ASN
1	C	664	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PGD	C	1782	3	46,52,52	3.71	15 (32%)	56,81,81	1.64	11 (19%)
4	SO4	A	1785	-	4,4,4	0.45	0	6,6,6	0.22	0
2	PGD	A	1782	3	46,52,52	3.56	15 (32%)	56,81,81	1.86	10 (17%)
4	SO4	C	1785	-	4,4,4	0.58	0	6,6,6	0.29	0
2	PGD	A	1783	3	46,52,52	3.52	19 (41%)	56,81,81	1.61	14 (25%)
2	PGD	C	1783	3	46,52,52	4.00	16 (34%)	56,81,81	1.74	15 (26%)

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	PGD	A	1783	3	-	1/22/82/82	0/6/6/6
2	PGD	C	1783	3	-	2/22/82/82	0/6/6/6
2	PGD	A	1782	3	-	5/22/82/82	0/6/6/6
2	PGD	C	1782	3	-	6/22/82/82	0/6/6/6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1783	PGD	C16-N15	20.67	1.47	1.28
2	C	1782	PGD	C16-N15	19.86	1.47	1.28
2	A	1782	PGD	C16-N15	17.65	1.45	1.28
2	A	1783	PGD	C16-N15	17.11	1.44	1.28
2	C	1783	PGD	C21-N22	8.52	1.44	1.35
2	A	1782	PGD	C21-N22	6.82	1.42	1.35
2	A	1782	PGD	PA-O1A	6.71	1.74	1.50
2	C	1782	PGD	C21-N22	6.35	1.42	1.35
2	C	1782	PGD	PA-O1A	6.27	1.72	1.50
2	A	1783	PGD	C21-N22	6.12	1.41	1.35
2	C	1783	PGD	PB-O3B	5.82	1.65	1.59
2	C	1783	PGD	PB-O1B	5.79	1.70	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1783	PGD	PB-O1B	5.62	1.70	1.50
2	C	1782	PGD	PB-O1B	5.59	1.70	1.50
2	C	1783	PGD	PA-O1A	5.31	1.69	1.50
2	A	1783	PGD	PA-O1A	5.16	1.68	1.50
2	A	1782	PGD	PB-O1B	5.16	1.68	1.50
2	A	1783	PGD	PA-O3B	4.49	1.64	1.59
2	A	1782	PGD	PA-O3B	4.47	1.64	1.59
2	A	1782	PGD	PB-O3B	4.28	1.64	1.59
2	A	1782	PGD	PB-O5'	4.14	1.75	1.59
2	C	1783	PGD	PA-O3A	4.03	1.75	1.59
2	A	1783	PGD	C10-C11	4.02	1.57	1.51
2	C	1782	PGD	PB-O5'	3.93	1.74	1.59
2	A	1782	PGD	PA-O3A	3.90	1.74	1.59
2	A	1783	PGD	PB-O5'	3.84	1.74	1.59
2	A	1783	PGD	PA-O3A	3.79	1.74	1.59
2	C	1783	PGD	PA-O3B	3.69	1.63	1.59
2	A	1783	PGD	C2-N2	3.65	1.42	1.34
2	C	1783	PGD	C2-N2	3.44	1.42	1.34
2	C	1782	PGD	C17-C16	-3.42	1.38	1.47
2	A	1783	PGD	PB-O3B	3.39	1.63	1.59
2	C	1782	PGD	C2-N2	3.32	1.41	1.34
2	C	1782	PGD	PA-O3A	3.24	1.72	1.59
2	C	1783	PGD	PB-O2B	3.20	1.70	1.55
2	A	1782	PGD	C19-N19	3.13	1.43	1.34
2	C	1783	PGD	O11-C23	-3.12	1.39	1.43
2	A	1783	PGD	PA-O2A	3.11	1.69	1.55
2	A	1783	PGD	C19-N19	3.11	1.42	1.34
2	C	1783	PGD	PB-O5'	3.07	1.71	1.59
2	A	1782	PGD	C17-C16	-3.02	1.39	1.47
2	A	1782	PGD	PB-O2B	2.94	1.69	1.55
2	C	1783	PGD	C19-N19	2.94	1.42	1.34
2	C	1782	PGD	PA-O2A	2.93	1.68	1.55
2	A	1782	PGD	C10-C11	2.92	1.55	1.51
2	A	1783	PGD	C21-N20	2.91	1.38	1.32
2	C	1783	PGD	PA-O2A	2.91	1.68	1.55
2	C	1783	PGD	C17-C16	-2.84	1.39	1.47
2	A	1783	PGD	PB-O2B	2.83	1.68	1.55
2	A	1782	PGD	C2-N2	2.74	1.40	1.34
2	C	1783	PGD	C21-N20	2.66	1.37	1.32
2	C	1782	PGD	PA-O3B	2.66	1.62	1.59
2	C	1782	PGD	PB-O2B	2.65	1.67	1.55
2	C	1782	PGD	C10-C11	2.56	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1783	PGD	C17-C16	-2.43	1.40	1.47
2	C	1782	PGD	C19-N19	2.34	1.40	1.34
2	C	1782	PGD	C5-N7	-2.34	1.34	1.39
2	A	1782	PGD	PA-O2A	2.29	1.65	1.55
2	A	1782	PGD	C2-N3	2.20	1.38	1.33
2	C	1783	PGD	C10-C11	2.19	1.54	1.51
2	A	1783	PGD	O11-C11	-2.13	1.39	1.43
2	C	1782	PGD	C21-N20	2.11	1.36	1.32
2	A	1783	PGD	C14-N15	2.08	1.48	1.46
2	A	1783	PGD	C5-N7	-2.07	1.34	1.39
2	A	1783	PGD	O11-C23	-2.07	1.40	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1782	PGD	C17-C16-N15	8.26	127.00	118.06
2	C	1783	PGD	N20-C19-N18	-4.35	119.54	126.44
2	A	1783	PGD	O11-C23-N22	-4.28	104.72	108.61
2	C	1782	PGD	C17-C16-N15	4.27	122.68	118.06
2	C	1783	PGD	C17-C16-N15	4.19	122.59	118.06
2	C	1782	PGD	C5-C4-N3	-4.14	121.79	128.39
2	A	1783	PGD	N20-C19-N18	-3.90	120.27	126.44
2	A	1782	PGD	C5-C4-N3	-3.77	122.38	128.39
2	C	1783	PGD	C4'-O4'-C1'	-3.58	101.57	109.47
2	C	1783	PGD	C2-N3-C4	3.43	118.20	112.30
2	C	1783	PGD	N19-C19-N18	3.41	122.36	117.09
2	A	1782	PGD	O11-C23-C14	3.41	113.56	108.73
2	A	1782	PGD	C2-N3-C4	3.37	118.10	112.30
2	C	1783	PGD	C5-C4-N3	-3.37	123.03	128.39
2	C	1782	PGD	C5-C4-N9	3.34	111.64	105.66
2	A	1782	PGD	C2-N1-C6	-3.28	119.16	125.11
2	A	1782	PGD	N20-C19-N18	-3.09	121.54	126.44
2	C	1783	PGD	C5-C4-N9	3.07	111.16	105.66
2	C	1782	PGD	N20-C19-N18	-3.04	121.62	126.44
2	C	1783	PGD	O3B-PB-O1B	-2.97	101.77	110.70
2	A	1783	PGD	C5-C4-N3	-2.91	123.75	128.39
2	A	1783	PGD	C5-C4-N9	2.86	110.78	105.66
2	A	1783	PGD	O3A-C10-C11	-2.86	101.53	108.58
2	C	1782	PGD	O4'-C1'-C2'	-2.74	100.75	106.62
2	A	1783	PGD	C4'-O4'-C1'	-2.74	103.42	109.47
2	C	1782	PGD	O11-C23-N22	2.66	111.02	108.61
2	C	1783	PGD	PA-O3A-C10	-2.64	106.20	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1783	PGD	PA-O3A-C10	-2.58	106.56	121.35
2	C	1782	PGD	O3B-PB-O1B	-2.53	103.08	110.70
2	C	1783	PGD	C2-N1-C6	-2.47	120.63	125.11
2	C	1782	PGD	N19-C19-N20	2.45	120.47	116.57
2	C	1783	PGD	O4'-C1'-C2'	-2.44	101.40	106.62
2	C	1782	PGD	C2-N3-C4	2.42	116.47	112.30
2	A	1782	PGD	C5-C6-N1	2.40	119.36	113.25
2	A	1782	PGD	N19-C19-N18	2.35	120.72	117.09
2	A	1783	PGD	O3B-PB-O1B	-2.33	103.71	110.70
2	C	1783	PGD	N2-C2-N1	2.32	121.66	116.76
2	A	1783	PGD	C17-C16-C21	2.31	120.02	117.40
2	A	1783	PGD	O6-C6-N1	-2.23	115.92	120.11
2	C	1783	PGD	O3A-C10-C11	-2.21	103.11	108.58
2	C	1783	PGD	O6-C6-N1	-2.21	115.95	120.11
2	A	1782	PGD	C5-C4-N9	2.21	109.61	105.66
2	A	1783	PGD	C4-C5-N7	-2.20	107.19	110.67
2	A	1783	PGD	C17-C16-N15	2.16	120.39	118.06
2	C	1783	PGD	C5'-C4'-C3'	-2.11	107.60	115.21
2	C	1782	PGD	PB-O5'-C5'	-2.08	109.40	121.35
2	A	1783	PGD	O5'-C5'-C4'	-2.08	101.89	108.99
2	A	1782	PGD	O17-C17-N18	-2.07	116.80	120.27
2	A	1783	PGD	N19-C19-N18	2.04	120.25	117.09
2	C	1782	PGD	C2-N1-C6	-2.04	121.41	125.11

There are no chirality outliers.

All (14) torsion outliers are listed below:

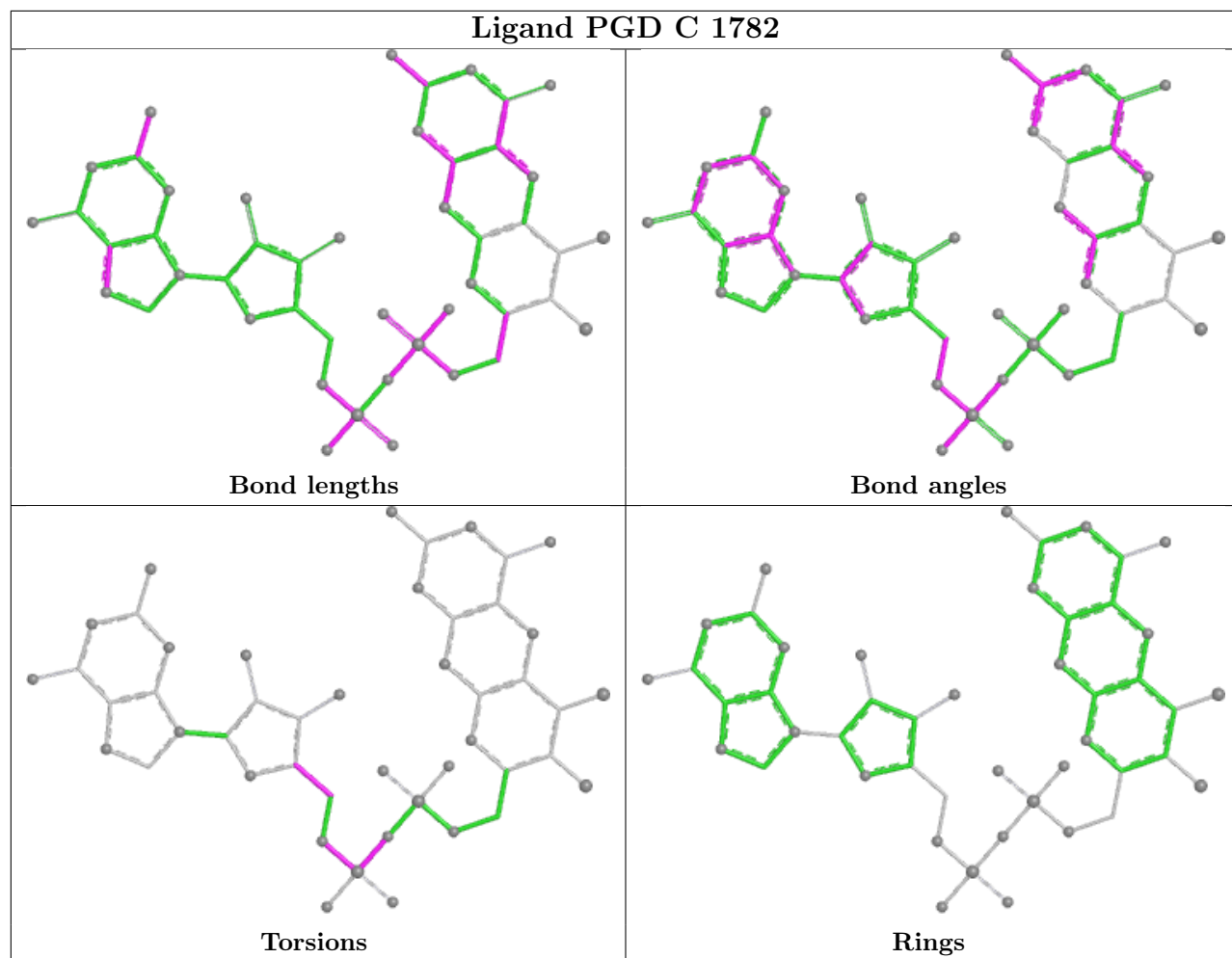
Mol	Chain	Res	Type	Atoms
2	A	1782	PGD	C5'-O5'-PB-O1B
2	A	1782	PGD	C5'-O5'-PB-O2B
2	A	1782	PGD	C5'-O5'-PB-O3B
2	C	1782	PGD	C5'-O5'-PB-O1B
2	C	1782	PGD	C5'-O5'-PB-O2B
2	C	1782	PGD	C5'-O5'-PB-O3B
2	A	1782	PGD	PA-O3B-PB-O5'
2	C	1782	PGD	PA-O3B-PB-O5'
2	C	1782	PGD	O4'-C4'-C5'-O5'
2	A	1782	PGD	O4'-C4'-C5'-O5'
2	C	1782	PGD	PA-O3B-PB-O1B
2	C	1783	PGD	O4'-C4'-C5'-O5'
2	A	1783	PGD	O3A-C10-C11-C12
2	C	1783	PGD	O3A-C10-C11-C12

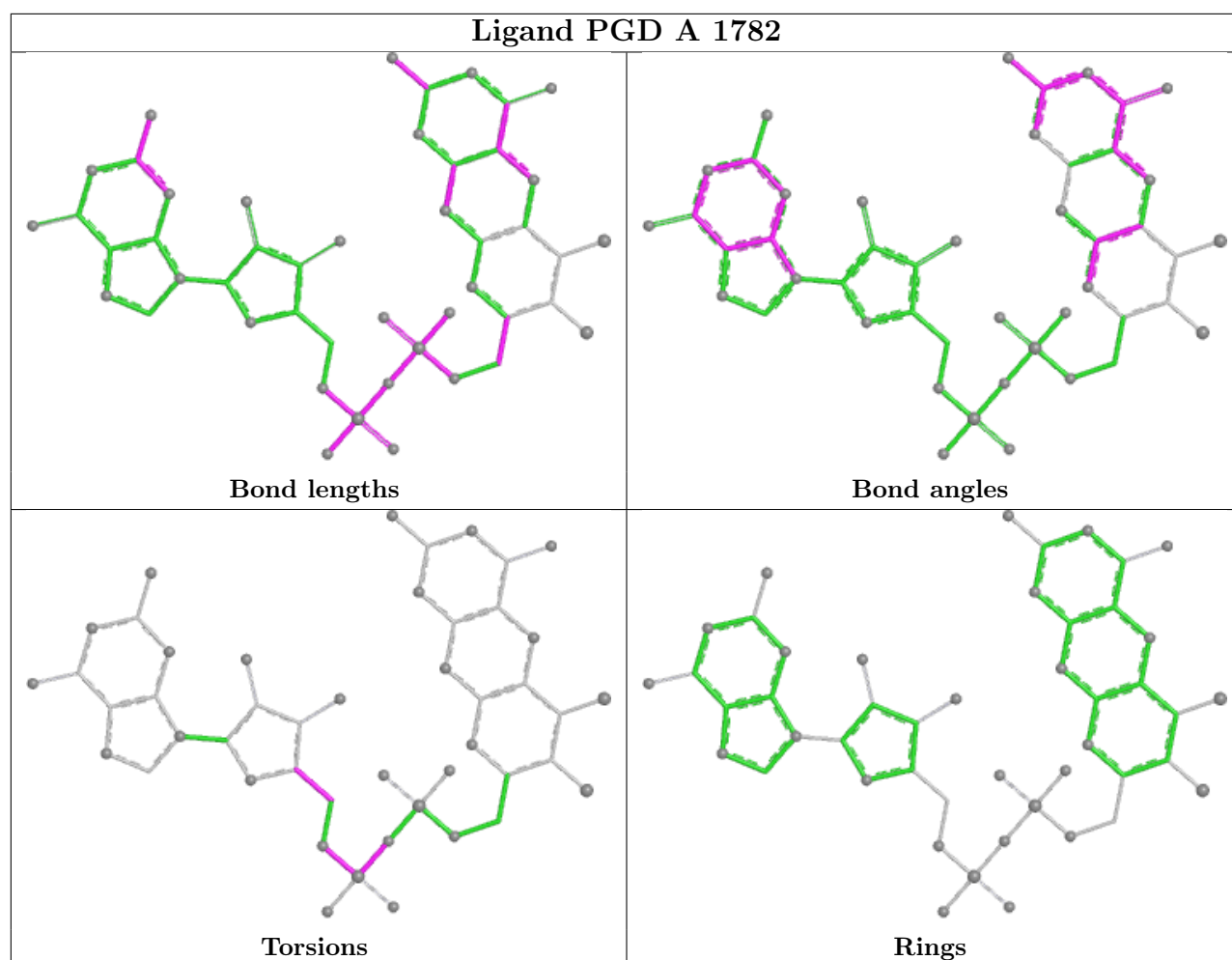
There are no ring outliers.

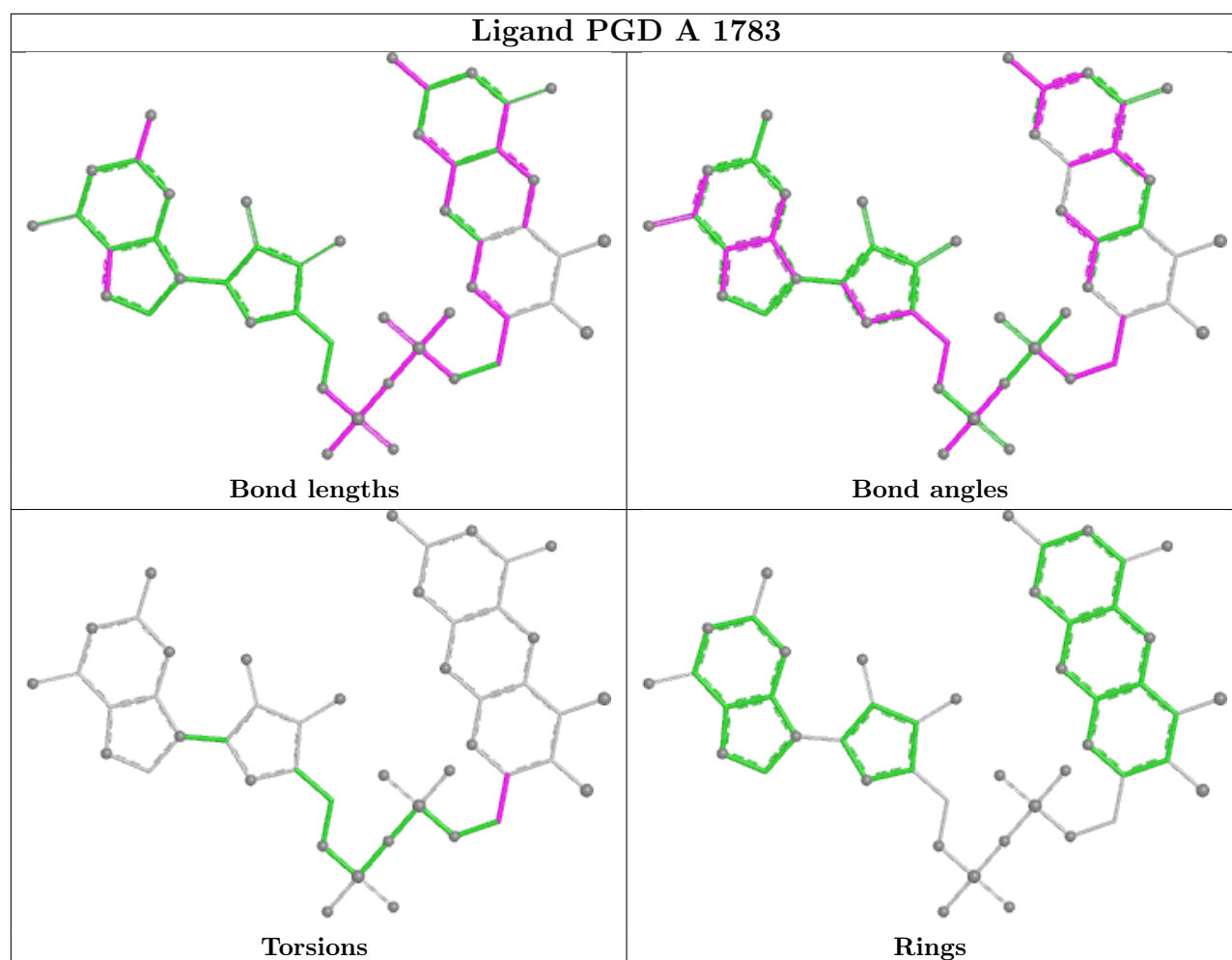
3 monomers are involved in 3 short contacts:

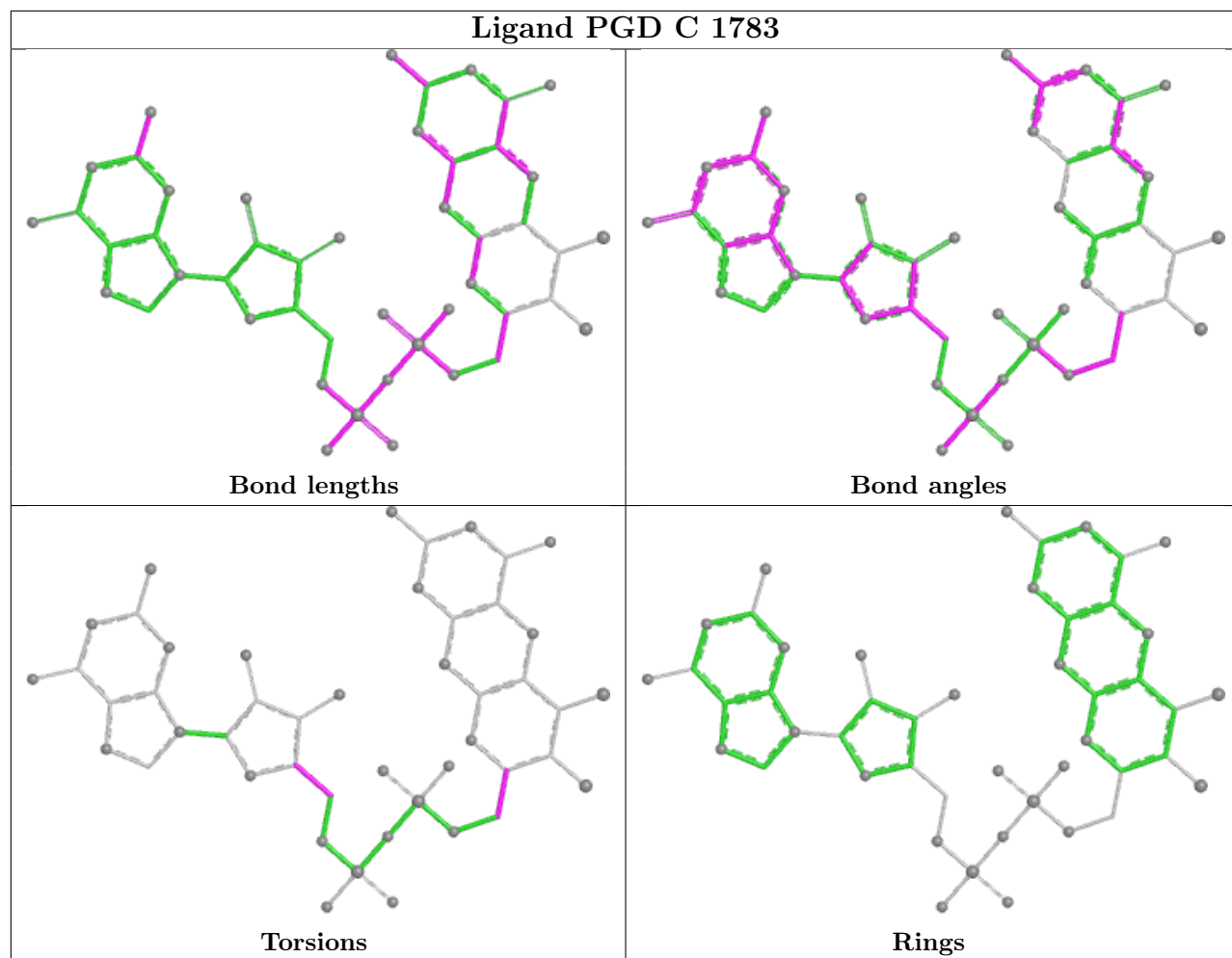
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1782	PGD	1	0
2	A	1782	PGD	1	0
2	C	1783	PGD	1	0

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.









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.