



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:39 AM UTC

PDB ID : 1E60 / pdb_00001e60
Title : OXIDIZED DMSO REDUCTASE EXPOSED TO HEPES - Structure II BUFFER
Authors : Bailey, S.; Bennett, B.; Adams, B.; Smith, A.T.; Bray, R.C.
Deposited on : 2000-08-06
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

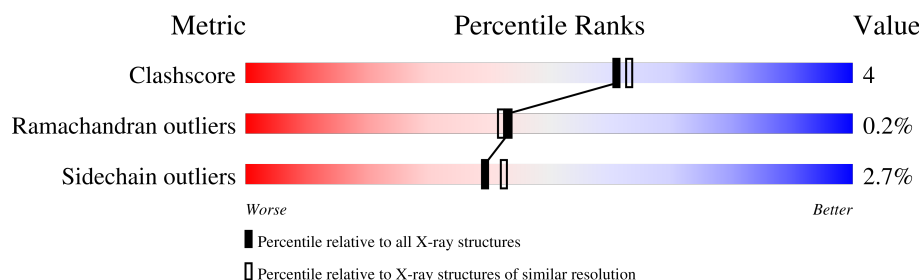
1 Overall quality at a glance

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	 81% 11% • 5%
1	C	823	 79% 12% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13400 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	778	Total	C	N	O	S	0	0	0
			5964	3791	1009	1137	27			
1	C	770	Total	C	N	O	S	0	0	0
			5904	3752	999	1126	27			

There are 26 discrepancies between the modelled and reference sequences:

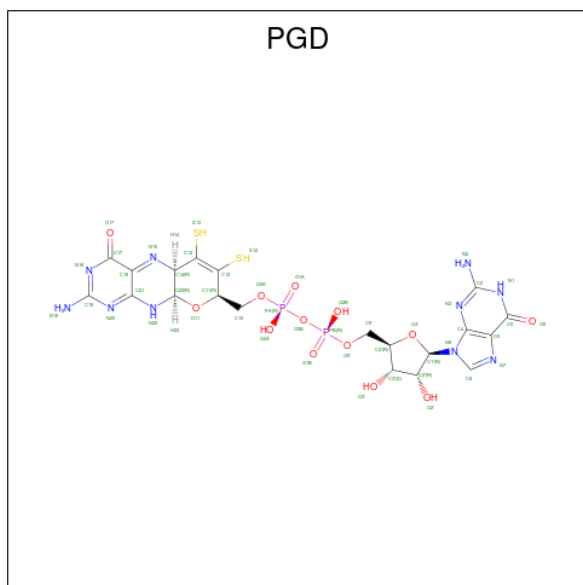
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	THR	conflict	UNP Q52675
A	43	ALA	GLU	conflict	UNP Q52675
A	107	GLU	GLN	conflict	UNP Q52675
A	234	GLU	ASP	conflict	UNP Q52675
A	236	ILE	VAL	conflict	UNP Q52675
A	280	ASP	MET	conflict	UNP Q52675
A	294	GLU	SER	conflict	UNP Q52675
A	295	GLY	ASP	conflict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

Continued on next page...

Continued from previous page...

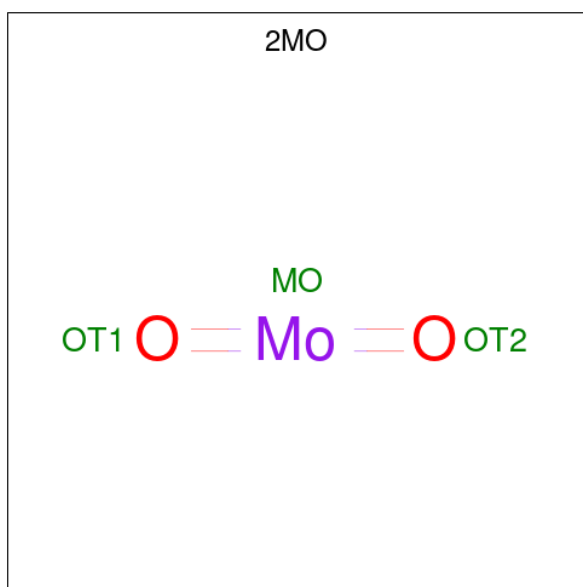
Chain	Residue	Modelled	Actual	Comment	Reference
C	552	ALA	GLY	conflict	UNP Q52675

- 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: $C_{20}H_{24}N_{10}O_{13}P_2S_2$).



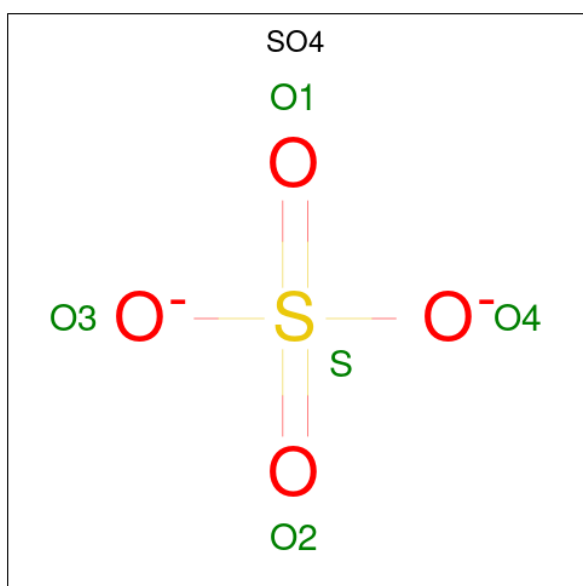
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 3 is MOLYBDENUM (IV)OXIDE (CCD ID: 2MO) (formula: MoO_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Mo	O	0	0
			3	1	2		
3	C	1	Total	Mo	O	0	0
			3	1	2		

- 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	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	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	686	Total	O	0	0
			686	686		
5	C	632	Total	O	0	0
			632	632		

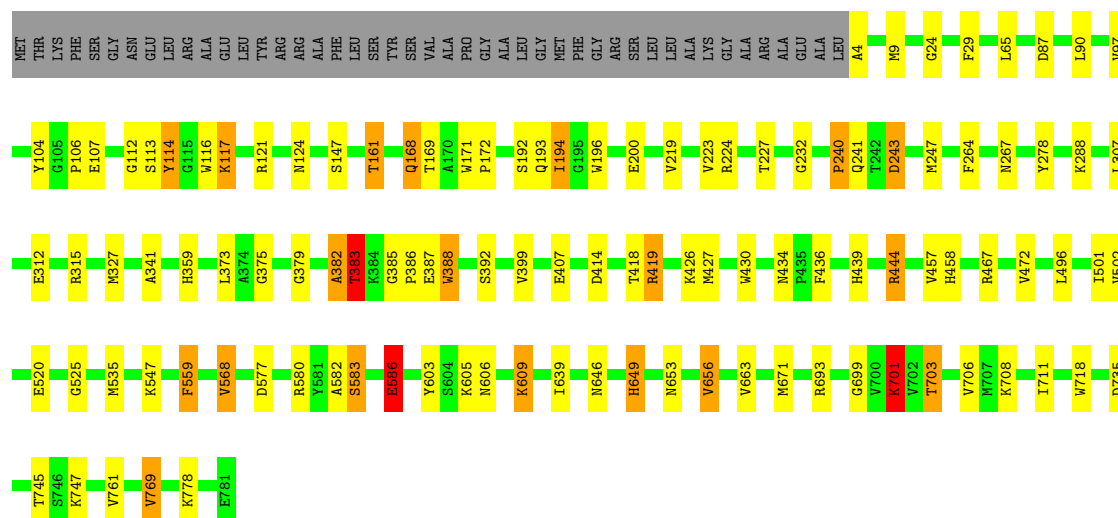
3 Residue-property plots

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.

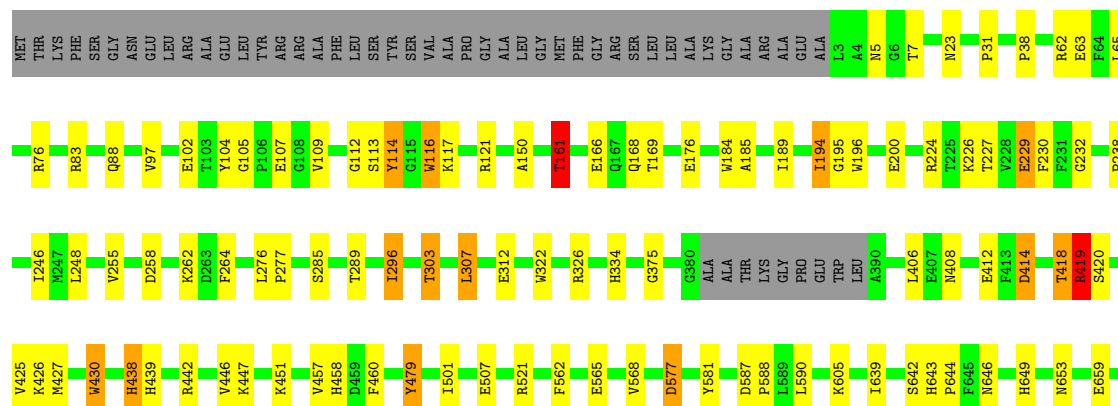
- Molecule 1: Dimethyl sulfoxide/trimethylamine N-oxide reductase

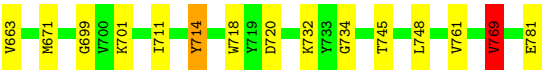
Chain A: 



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

Chain C: 





4 Data and refinement statistics

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	68.55Å 115.92Å 229.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.1 (20.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13400	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: PGD, SO4, 2MO

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	0.76	0/6125	1.59	67/8338 (0.8%)
1	C	0.75	0/6061	1.56	60/8248 (0.7%)
All	All	0.76	0/12186	1.58	127/16586 (0.8%)

There are no bond length outliers.

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	VAL	CB-CA-C	-10.79	94.58	110.33
1	A	577	ASP	CA-CB-CG	10.61	123.21	112.60
1	C	102	GLU	CB-CG-CD	9.87	129.38	112.60
1	A	703	THR	CB-CA-C	-9.47	92.82	110.16
1	A	383	THR	N-CA-CB	8.92	127.10	111.13
1	A	769	VAL	N-CA-CB	-8.71	97.16	111.44
1	C	62	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	A	224	ARG	CD-NE-CZ	8.47	136.26	124.40
1	A	568	VAL	N-CA-CB	8.46	123.86	111.52
1	A	419	ARG	CA-CB-CG	8.42	130.94	114.10
1	A	583	SER	CB-CA-C	7.85	125.74	110.67
1	A	194	ILE	CA-CB-CG2	7.84	123.83	110.50
1	C	577	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	312	GLU	CG-CD-OE2	7.58	135.84	118.40
1	C	334	HIS	CA-CB-CG	-7.46	106.34	113.80
1	A	359	HIS	CA-CB-CG	-7.27	106.53	113.80
1	C	224	ARG	CD-NE-CZ	7.21	134.49	124.40
1	A	388	TRP	CA-CB-CG	7.18	127.23	113.60
1	A	458	HIS	CA-CB-CG	7.10	120.90	113.80
1	C	63	GLU	CB-CG-CD	7.10	124.67	112.60
1	A	264	PHE	CA-CB-CG	-6.90	106.90	113.80
1	C	458	HIS	N-CA-CB	6.89	122.25	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	VAL	CB-CA-C	-6.78	101.64	112.16
1	C	646	ASN	CA-CB-CG	-6.76	105.84	112.60
1	A	90	LEU	CA-C-O	6.70	127.65	120.55
1	A	703	THR	CA-C-O	-6.64	113.58	120.89
1	C	312	GLU	CG-CD-OE2	6.63	133.66	118.40
1	C	114	TYR	CA-CB-CG	-6.48	102.24	113.90
1	A	196	TRP	N-CA-C	-6.37	104.26	111.14
1	C	248	LEU	CA-C-N	6.34	127.13	120.03
1	C	248	LEU	C-N-CA	6.34	127.13	120.03
1	C	414	ASP	CA-CB-CG	-6.33	106.27	112.60
1	A	693	ARG	CG-CD-NE	6.29	125.83	112.00
1	C	460	PHE	N-CA-CB	6.23	119.81	110.65
1	A	568	VAL	CA-C-O	-6.20	113.79	120.36
1	C	521	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	385	GLY	N-CA-C	-6.14	99.82	112.34
1	A	649	HIS	CB-CA-C	-6.08	108.96	117.23
1	A	373	LEU	CA-C-O	-6.05	113.60	120.32
1	A	419	ARG	N-CA-CB	6.01	120.36	110.69
1	C	23	ASN	CA-CB-CG	-6.01	106.59	112.60
1	A	701	LYS	CA-CB-CG	5.98	126.06	114.10
1	A	232	GLY	N-CA-C	-5.98	103.00	113.76
1	A	399	VAL	N-CA-C	5.97	117.43	110.62
1	A	193	GLN	CA-C-N	-5.97	114.47	122.77
1	A	193	GLN	C-N-CA	-5.97	114.47	122.77
1	A	29	PHE	CA-CB-CG	5.95	119.75	113.80
1	C	326	ARG	N-CA-C	-5.92	103.45	111.55
1	C	303	THR	N-CA-C	-5.83	105.01	111.36
1	A	444	ARG	CD-NE-CZ	5.82	132.55	124.40
1	C	408	ASN	N-CA-C	5.82	119.09	109.79
1	C	88	GLN	CB-CG-CD	5.78	122.42	112.60
1	A	458	HIS	N-CA-CB	5.70	120.75	110.83
1	A	114	TYR	CA-CB-CG	-5.69	103.66	113.90
1	A	701	LYS	CG-CD-CE	5.67	124.34	111.30
1	A	434	ASN	CA-C-O	5.65	127.49	121.28
1	C	296	ILE	CB-CA-C	-5.64	104.65	112.04
1	A	243	ASP	CA-CB-CG	-5.64	106.96	112.60
1	C	5	ASN	CA-CB-CG	-5.64	106.96	112.60
1	C	161	THR	N-CA-CB	5.61	120.35	111.43
1	A	693	ARG	CA-CB-CG	-5.60	102.89	114.10
1	C	229	GLU	CA-CB-CG	-5.59	102.92	114.10
1	A	646	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	C	419	ARG	CB-CA-C	-5.58	101.15	110.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	HIS	CA-CB-CG	-5.57	108.23	113.80
1	A	434	ASN	O-C-N	-5.57	116.72	121.23
1	C	116	TRP	CA-CB-CG	-5.54	103.08	113.60
1	A	312	GLU	OE1-CD-OE2	-5.53	109.62	122.90
1	C	442	ARG	CA-C-O	-5.53	115.01	120.82
1	A	436	PHE	CA-C-N	5.52	131.91	121.97
1	A	436	PHE	C-N-CA	5.52	131.91	121.97
1	C	322	TRP	N-CA-C	5.52	120.69	113.30
1	A	341	ALA	CA-C-O	-5.45	114.77	120.55
1	A	240	PRO	CB-CA-C	5.45	118.48	111.56
1	C	255	VAL	CA-C-N	5.44	127.57	120.28
1	C	255	VAL	C-N-CA	5.44	127.57	120.28
1	A	609	LYS	CB-CG-CD	5.44	123.81	111.30
1	A	227	THR	CA-C-O	5.42	126.28	120.70
1	A	267	ASN	N-CA-C	5.41	119.93	113.23
1	C	479	TYR	CA-CB-CG	-5.38	104.21	113.90
1	A	580	ARG	CA-C-O	-5.38	115.14	121.16
1	C	748	LEU	CA-C-O	5.37	126.43	120.90
1	C	62	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	C	769	VAL	N-CA-CB	-5.34	100.85	111.91
1	C	408	ASN	N-CA-CB	-5.34	102.37	110.75
1	C	105	GLY	CA-C-N	5.33	125.14	119.28
1	C	105	GLY	C-N-CA	5.33	125.14	119.28
1	C	194	ILE	CA-CB-CG2	5.32	119.55	110.50
1	C	232	GLY	N-CA-C	-5.32	104.18	113.76
1	A	559	PHE	CA-CB-CG	-5.32	108.48	113.80
1	C	643	HIS	CB-CA-C	5.32	117.77	109.42
1	A	472	VAL	CA-C-O	-5.31	114.85	120.53
1	A	192	SER	CA-C-O	5.30	126.06	119.12
1	A	419	ARG	CB-CA-C	-5.30	99.84	109.38
1	C	460	PHE	N-CA-C	-5.29	106.84	113.72
1	C	714	TYR	CA-C-O	-5.29	115.94	121.55
1	A	603	TYR	CA-C-O	-5.28	114.66	120.36
1	C	312	GLU	OE1-CD-OE2	-5.27	110.25	122.90
1	C	264	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	467	ARG	O-C-N	5.23	128.70	122.27
1	C	194	ILE	CA-C-O	5.22	127.21	121.67
1	A	161	THR	N-CA-CB	5.21	120.06	111.62
1	C	7	THR	CA-C-O	-5.21	115.01	121.11
1	A	161	THR	CB-CA-C	-5.21	99.06	110.67
1	C	446	VAL	N-CA-CB	-5.20	104.74	110.51
1	A	224	ARG	NE-CZ-NH1	5.20	126.70	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	THR	OG1-CB-CG2	5.18	119.66	109.30
1	C	439	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	586	GLU	CB-CA-C	5.15	120.15	110.63
1	C	425	VAL	N-CA-C	5.15	115.68	108.89
1	C	438	HIS	CA-CB-CG	5.14	118.94	113.80
1	A	87	ASP	CA-CB-CG	-5.13	107.47	112.60
1	C	161	THR	CB-CA-C	-5.11	100.17	110.30
1	A	219	VAL	CA-C-O	-5.11	115.03	120.39
1	C	720	ASP	CA-C-N	5.11	125.02	119.76
1	C	720	ASP	C-N-CA	5.11	125.02	119.76
1	C	196	TRP	N-CA-C	-5.09	105.38	111.03
1	A	168	GLN	OE1-CD-NE2	5.09	127.69	122.60
1	C	581	TYR	CA-C-N	5.08	127.04	120.44
1	C	581	TYR	C-N-CA	5.08	127.04	120.44
1	A	382	ALA	N-CA-C	5.08	121.61	110.80
1	A	457	VAL	CB-CA-C	-5.04	102.73	110.50
1	C	418	THR	CA-C-O	5.04	126.14	120.70
1	C	408	ASN	O-C-N	-5.04	116.48	121.17
1	A	559	PHE	N-CA-C	5.03	117.15	111.11
1	C	289	THR	N-CA-C	5.01	116.58	110.41
1	C	76	ARG	CG-CD-NE	5.01	123.03	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5964	0	5763	51	0
1	C	5904	0	5706	49	0
2	A	94	0	42	4	0
2	C	94	0	42	2	0
3	A	3	0	0	1	0
3	C	3	0	0	1	0
4	A	10	0	0	1	0
4	C	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	686	0	0	4	0
5	C	632	0	0	5	0
All	All	13400	0	11553	100	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 (100) 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:114:TYR:OH	3:A:803:2MO:OT1	1.84	0.95
1:C:114:TYR:OH	3:C:803:2MO:OT1	1.94	0.84
1:A:407:GLU:OE1	1:A:444:ARG:NH2	2.09	0.83
1:C:562:PHE:HD1	1:C:568:VAL:HG23	1.49	0.77
1:C:562:PHE:CD1	1:C:568:VAL:HG23	2.22	0.74
1:A:97:VAL:HG22	1:A:427:MET:HE1	1.75	0.69
1:C:97:VAL:HG22	1:C:427:MET:HE1	1.73	0.69
1:C:194:ILE:C	1:C:194:ILE:HD12	2.20	0.67
1:C:414:ASP:OD1	1:C:419:ARG:HG2	1.93	0.67
1:C:671:MET:HE1	1:C:761:VAL:HG11	1.77	0.67
1:A:535:MET:HE1	1:A:559:PHE:HZ	1.57	0.66
1:C:176:GLU:HG3	5:C:2074:HOH:O	1.94	0.66
1:C:189:ILE:HD12	1:C:227:THR:HA	1.76	0.65
1:A:701:LYS:HD3	5:A:2616:HOH:O	1.97	0.63
1:C:568:VAL:HG22	5:C:2452:HOH:O	1.99	0.61
1:A:407:GLU:HG2	5:A:2382:HOH:O	2.02	0.60
1:A:106:PRO:HB2	1:A:388:TRP:CZ3	2.37	0.60
1:A:107:GLU:HG3	1:A:388:TRP:CE2	2.38	0.58
1:A:671:MET:HE1	1:A:761:VAL:HG11	1.84	0.58
1:C:121:ARG:HB3	1:C:375:GLY:HA3	1.85	0.58
1:A:535:MET:HE1	1:A:559:PHE:CZ	2.39	0.58
1:A:414:ASP:OD2	1:A:747:LYS:HE3	2.04	0.57
1:A:383:THR:HG23	5:A:2153:HOH:O	2.05	0.57
1:C:479:TYR:HB3	1:C:501:ILE:HD12	1.87	0.57
1:A:582:ALA:O	1:A:586:GLU:HB3	2.05	0.56
1:C:107:GLU:CD	1:C:107:GLU:H	2.16	0.53
1:A:653:ASN:ND2	1:A:718:TRP:H	2.08	0.52
1:C:732:LYS:HD2	1:C:769:VAL:HG13	1.92	0.51
1:C:406:LEU:O	1:C:451:LYS:HD2	2.10	0.51
1:C:168:GLN:O	1:C:169:THR:C	2.53	0.51
1:A:414:ASP:OD1	1:A:419:ARG:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:ASN:ND2	1:C:718:TRP:H	2.09	0.51
1:A:663:VAL:HB	1:A:699:GLY:HA3	1.93	0.50
1:C:642:SER:HB2	2:C:802:PGD:O1B	2.11	0.50
1:C:663:VAL:HB	1:C:699:GLY:HA3	1.93	0.50
1:A:194:ILE:HD12	1:A:194:ILE:C	2.37	0.50
1:A:520:GLU:OE1	1:A:525:GLY:HA3	2.12	0.49
1:C:781:GLU:OE1	5:C:2624:HOH:O	2.20	0.49
1:C:161:THR:HB	1:C:166:GLU:OE2	2.13	0.49
1:C:303:THR:HG22	1:C:307:LEU:HD22	1.95	0.48
1:A:9:MET:HE3	1:A:496:LEU:HD11	1.95	0.48
1:A:107:GLU:HG3	1:A:388:TRP:NE1	2.28	0.48
1:A:121:ARG:HB3	1:A:375:GLY:HA3	1.95	0.48
1:A:535:MET:CE	1:A:559:PHE:CZ	2.97	0.48
1:C:104:TYR:CD2	1:C:426:LYS:HG3	2.49	0.48
1:A:639:ILE:HG12	1:A:711:ILE:HD11	1.94	0.47
1:A:107:GLU:HG2	1:A:392:SER:HB3	1.96	0.47
1:A:117:LYS:HE2	1:A:124:ASN:OD1	2.14	0.47
1:C:116:TRP:O	1:C:117:LYS:C	2.57	0.47
1:A:315:ARG:HA	4:A:902:SO4:O2	2.15	0.47
1:C:109:VAL:HG13	1:C:427:MET:HE2	1.96	0.47
1:A:147:SER:HA	2:A:801:PGD:S13	2.55	0.47
1:A:379:GLY:O	1:A:382:ALA:HB3	2.15	0.47
1:C:150:ALA:HB2	1:C:745:THR:HG21	1.96	0.46
1:C:412:GLU:HA	1:C:420:SER:O	2.15	0.46
1:C:663:VAL:CG2	1:C:701:LYS:HE3	2.45	0.46
1:A:4:ALA:HB3	1:A:24:GLY:HA2	1.96	0.46
1:A:112:GLY:O	1:A:113:SER:C	2.58	0.45
1:C:31:PRO:HB3	1:C:38:PRO:HB3	1.99	0.45
1:C:184:TRP:O	1:C:185:ALA:HB3	2.17	0.45
1:C:430:TRP:O	1:C:457:VAL:HA	2.17	0.45
1:C:104:TYR:CE2	1:C:426:LYS:HG3	2.53	0.44
1:A:708:LYS:HG2	5:A:2248:HOH:O	2.17	0.44
1:C:238:PRO:HB3	1:C:246:ILE:CD1	2.48	0.44
1:A:327:MET:O	1:A:745:THR:HG22	2.18	0.44
1:A:104:TYR:CD2	1:A:426:LYS:HG3	2.53	0.44
1:C:447:LYS:HD3	5:C:2359:HOH:O	2.17	0.43
1:A:104:TYR:CE2	1:A:426:LYS:HG3	2.53	0.43
1:C:194:ILE:HD12	1:C:195:GLY:N	2.33	0.43
1:C:189:ILE:HD11	1:C:230:PHE:CB	2.49	0.42
1:C:258:ASP:OD1	1:C:262:LYS:NZ	2.42	0.42
1:A:243:ASP:O	1:A:247:MET:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TYR:CZ	1:A:288:LYS:HE2	2.54	0.42
1:C:605:LYS:HG3	5:C:2267:HOH:O	2.19	0.42
1:A:606:ASN:HD22	1:A:606:ASN:HA	1.67	0.42
1:A:116:TRP:O	1:A:117:LYS:C	2.62	0.42
1:A:535:MET:HE3	1:A:535:MET:HA	2.02	0.42
1:C:276:LEU:HB3	1:C:277:PRO:HD3	2.02	0.41
1:C:83:ARG:NH2	1:C:507:GLU:OE2	2.53	0.41
1:A:171:TRP:N	1:A:172:PRO:HD2	2.35	0.41
1:C:238:PRO:HB3	1:C:246:ILE:HD11	2.03	0.41
1:C:649:HIS:CG	2:C:801:PGD:H102	2.55	0.41
1:A:501:ILE:HG22	1:A:502:VAL:HG13	2.02	0.41
1:A:735:ASP:OD1	1:A:735:ASP:C	2.64	0.41
1:A:147:SER:OG	2:A:802:PGD:S12	2.77	0.41
1:A:223:VAL:HG22	1:A:706:VAL:HG12	2.02	0.41
1:A:241:GLN:HG2	1:A:327:MET:SD	2.61	0.41
1:A:116:TRP:HB2	2:A:801:PGD:O2B	2.21	0.41
1:A:605:LYS:HB3	1:A:609:LYS:NZ	2.36	0.41
1:C:121:ARG:HB3	1:C:375:GLY:CA	2.50	0.41
1:C:116:TRP:CZ3	1:C:194:ILE:HD13	2.55	0.41
1:C:587:ASP:CG	1:C:590:LEU:HB2	2.46	0.41
1:C:112:GLY:O	1:C:113:SER:C	2.64	0.41
1:A:649:HIS:CG	2:A:801:PGD:H102	2.55	0.40
1:C:639:ILE:HG12	1:C:711:ILE:HD11	2.02	0.40
1:A:107:GLU:H	1:A:107:GLU:CD	2.30	0.40
1:A:240:PRO:O	1:A:241:GLN:HB2	2.21	0.40
1:A:168:GLN:O	1:A:169:THR:C	2.64	0.40
1:C:644:PRO:HA	1:C:714:TYR:CG	2.55	0.40
1:C:587:ASP:HA	1:C:588:PRO:HD2	1.97	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	776/823 (94%)	746 (96%)	28 (4%)	2 (0%)	36	35
1	C	766/823 (93%)	745 (97%)	20 (3%)	1 (0%)	48	46
All	All	1542/1646 (94%)	1491 (97%)	48 (3%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	PRO
1	A	117	LYS
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	616/648 (95%)	599 (97%)	17 (3%)	38	41
1	C	611/648 (94%)	595 (97%)	16 (3%)	40	44
All	All	1227/1296 (95%)	1194 (97%)	33 (3%)	39	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	161	THR
1	A	200	GLU
1	A	307	LEU
1	A	383	THR
1	A	387	GLU
1	A	418	THR
1	A	430	TRP
1	A	547	LYS
1	A	568	VAL
1	A	583	SER
1	A	586	GLU
1	A	656	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	701	LYS
1	A	703	THR
1	A	769	VAL
1	A	778	LYS
1	C	65	LEU
1	C	161	THR
1	C	200	GLU
1	C	226	LYS
1	C	229	GLU
1	C	285	SER
1	C	296	ILE
1	C	307	LEU
1	C	418	THR
1	C	419	ARG
1	C	430	TRP
1	C	438	HIS
1	C	565	GLU
1	C	577	ASP
1	C	659	GLU
1	C	769	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	241	GLN
1	A	606	ASN
1	A	653	ASN
1	C	241	GLN
1	C	653	ASN

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](#)

10 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	$\# Z > 2$
2	PGD	C	802	-	46,52,52	3.63	17 (36%)	56,81,81	1.64	10 (17%)
4	SO4	C	901	-	4,4,4	0.61	0	6,6,6	0.65	0
2	PGD	A	801	3	46,52,52	3.53	15 (32%)	56,81,81	1.77	13 (23%)
3	2MO	C	803	2,1	0,2,2	-	-	-	-	-
4	SO4	C	902	-	4,4,4	0.71	0	6,6,6	0.41	0
2	PGD	A	802	-	46,52,52	3.67	15 (32%)	56,81,81	1.77	15 (26%)
3	2MO	A	803	2,1	0,2,2	-	-	-	-	-
4	SO4	A	901	-	4,4,4	0.37	0	6,6,6	0.30	0
2	PGD	C	801	3	46,52,52	3.58	13 (28%)	56,81,81	1.87	16 (28%)
4	SO4	A	902	-	4,4,4	0.65	0	6,6,6	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGD	C	802	-	-	3/22/82/82	0/6/6/6
2	PGD	A	802	-	-	3/22/82/82	0/6/6/6
2	PGD	A	801	3	-	5/22/82/82	0/6/6/6
2	PGD	C	801	3	-	7/22/82/82	0/6/6/6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	PGD	C16-N15	18.94	1.46	1.28
2	C	801	PGD	C16-N15	18.85	1.46	1.28
2	C	802	PGD	C16-N15	18.38	1.45	1.28
2	A	801	PGD	C16-N15	17.01	1.44	1.28
2	A	802	PGD	C21-N22	8.05	1.43	1.35
2	A	801	PGD	C21-N22	7.72	1.43	1.35
2	C	802	PGD	C21-N22	6.81	1.42	1.35
2	A	801	PGD	PA-O1A	6.49	1.73	1.50
2	C	801	PGD	PB-O1B	6.29	1.72	1.50
2	C	801	PGD	PA-O1A	6.24	1.72	1.50
2	A	801	PGD	PB-O3B	6.21	1.66	1.59
2	C	801	PGD	C21-N22	5.89	1.41	1.35
2	C	802	PGD	PB-O1B	5.74	1.70	1.50
2	C	802	PGD	PA-O1A	5.43	1.69	1.50
2	A	802	PGD	PB-O1B	5.12	1.68	1.50
2	A	801	PGD	PB-O1B	5.08	1.68	1.50
2	A	802	PGD	PA-O3B	4.90	1.64	1.59
2	A	802	PGD	PA-O1A	4.74	1.67	1.50
2	C	801	PGD	PB-O5'	4.07	1.75	1.59
2	C	802	PGD	PA-O3A	4.02	1.75	1.59
2	A	801	PGD	PB-O5'	3.88	1.74	1.59
2	C	802	PGD	PB-O5'	3.73	1.74	1.59
2	A	802	PGD	PA-O2A	3.67	1.72	1.55
2	A	802	PGD	PB-O5'	3.62	1.73	1.59
2	A	801	PGD	PA-O3B	3.56	1.63	1.59
2	A	802	PGD	PB-O2B	3.52	1.71	1.55
2	C	802	PGD	PB-O3B	3.50	1.63	1.59
2	A	801	PGD	PA-O3A	3.49	1.73	1.59
2	C	801	PGD	PA-O3B	3.46	1.63	1.59
2	C	802	PGD	C10-C11	3.45	1.56	1.51
2	C	801	PGD	C2-N2	3.42	1.42	1.34
2	A	802	PGD	C2-N2	3.22	1.41	1.34
2	A	802	PGD	PA-O3A	3.17	1.71	1.59
2	C	802	PGD	PA-O3B	3.17	1.62	1.59
2	C	802	PGD	PB-O2B	3.16	1.70	1.55
2	C	802	PGD	PA-O2A	3.16	1.70	1.55
2	C	802	PGD	O11-C11	-3.13	1.37	1.43
2	C	802	PGD	C2-N2	3.12	1.41	1.34
2	C	801	PGD	C17-C16	-3.06	1.39	1.47
2	A	801	PGD	PB-O2B	3.02	1.69	1.55
2	A	801	PGD	C17-C16	-2.99	1.39	1.47
2	A	801	PGD	C2-N2	2.95	1.41	1.34
2	C	801	PGD	C19-N19	2.85	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	802	PGD	C19-N19	2.84	1.42	1.34
2	C	802	PGD	C17-C16	-2.78	1.39	1.47
2	C	801	PGD	PA-O3A	2.77	1.70	1.59
2	C	801	PGD	PA-O2A	2.76	1.68	1.55
2	A	802	PGD	C21-N20	2.76	1.37	1.32
2	A	801	PGD	C19-N19	2.61	1.41	1.34
2	A	801	PGD	PA-O2A	2.57	1.67	1.55
2	A	802	PGD	C17-C16	-2.50	1.40	1.47
2	A	802	PGD	C10-C11	2.40	1.55	1.51
2	A	801	PGD	C10-C11	2.37	1.55	1.51
2	A	801	PGD	C2-N3	2.35	1.38	1.33
2	C	802	PGD	C5-N7	-2.35	1.34	1.39
2	C	801	PGD	PB-O3B	2.34	1.62	1.59
2	A	802	PGD	C19-N19	2.31	1.40	1.34
2	C	801	PGD	PB-O2B	2.25	1.65	1.55
2	A	802	PGD	O11-C23	-2.16	1.40	1.43
2	C	802	PGD	C21-N20	2.06	1.36	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	PGD	C17-C16-N15	6.47	125.06	118.06
2	C	802	PGD	C17-C16-N15	5.77	124.31	118.06
2	C	801	PGD	C17-C16-N15	5.43	123.94	118.06
2	A	802	PGD	C5-C4-N3	-4.59	121.09	128.39
2	C	802	PGD	N20-C19-N18	-4.56	119.22	126.44
2	C	801	PGD	N20-C19-N18	-4.41	119.46	126.44
2	A	801	PGD	N20-C19-N18	-4.37	119.52	126.44
2	A	802	PGD	C2-N3-C4	3.97	119.13	112.30
2	C	801	PGD	C5-C4-N3	-3.90	122.18	128.39
2	A	802	PGD	C17-C16-N15	3.68	122.04	118.06
2	C	801	PGD	C2-N1-C6	-3.57	118.64	125.11
2	A	802	PGD	O11-C23-C14	3.28	113.38	108.73
2	C	801	PGD	O3B-PB-O1B	-3.27	100.86	110.70
2	A	802	PGD	C5-C4-N9	3.22	111.42	105.66
2	A	801	PGD	N19-C19-N18	3.20	122.04	117.09
2	A	802	PGD	N20-C19-N18	-3.10	121.53	126.44
2	A	802	PGD	O11-C23-N22	-3.03	105.86	108.61
2	C	802	PGD	O3A-C10-C11	-2.89	101.44	108.58
2	C	801	PGD	C4'-O4'-C1'	-2.88	103.11	109.47
2	C	802	PGD	C4'-O4'-C1'	-2.87	103.13	109.47
2	C	801	PGD	N19-C19-N18	2.83	121.46	117.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	PGD	C5-C4-N9	2.82	110.70	105.66
2	C	802	PGD	PA-O3A-C10	-2.77	105.46	121.35
2	A	801	PGD	C5-C4-N3	-2.76	124.00	128.39
2	A	801	PGD	O11-C23-N22	-2.72	106.14	108.61
2	A	802	PGD	C2-N1-C6	-2.63	120.33	125.11
2	C	801	PGD	C2-N3-C4	2.58	116.75	112.30
2	C	801	PGD	PB-O5'-C5'	-2.58	106.57	121.35
2	A	801	PGD	C4'-O4'-C1'	-2.54	103.85	109.47
2	C	802	PGD	N19-C19-N18	2.54	121.02	117.09
2	A	801	PGD	O4'-C1'-N9	-2.49	102.72	108.36
2	C	802	PGD	C5-C4-N3	-2.39	124.59	128.39
2	A	802	PGD	O3A-C10-C11	-2.37	102.72	108.58
2	C	802	PGD	C5'-C4'-C3'	-2.34	106.78	115.21
2	A	801	PGD	O3A-C10-C11	-2.33	102.83	108.58
2	C	801	PGD	C5-C4-N9	2.33	109.82	105.66
2	A	802	PGD	O4'-C1'-C2'	-2.31	101.66	106.62
2	C	801	PGD	O4'-C4'-C3'	2.26	109.64	105.15
2	A	802	PGD	N19-C19-N18	2.25	120.57	117.09
2	C	801	PGD	O11-C23-N22	-2.25	106.56	108.61
2	A	802	PGD	O6-C6-N1	-2.23	115.92	120.11
2	C	801	PGD	O4'-C1'-N9	-2.21	103.36	108.36
2	C	801	PGD	C5-C6-N1	2.20	118.87	113.25
2	A	802	PGD	PA-O3A-C10	-2.19	108.79	121.35
2	A	802	PGD	C4-C5-N7	-2.19	107.20	110.67
2	A	801	PGD	O6-C6-N1	-2.18	116.01	120.11
2	A	801	PGD	O3B-PB-O1B	-2.17	104.19	110.70
2	A	801	PGD	O17-C17-N18	-2.10	116.74	120.27
2	C	801	PGD	O11-C23-C14	2.10	111.70	108.73
2	C	802	PGD	C2-N3-C4	2.08	115.89	112.30
2	C	801	PGD	O3A-C10-C11	-2.08	103.44	108.58
2	A	801	PGD	C5-C4-N9	2.07	109.36	105.66
2	A	801	PGD	O17-C17-C16	2.06	127.35	122.35
2	A	802	PGD	O3B-PB-O1B	-2.01	104.67	110.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PGD	PA-O3B-PB-O5'
2	A	801	PGD	C5'-O5'-PB-O1B
2	A	801	PGD	C5'-O5'-PB-O2B
2	A	801	PGD	C5'-O5'-PB-O3B

Continued on next page...

Continued from previous page...

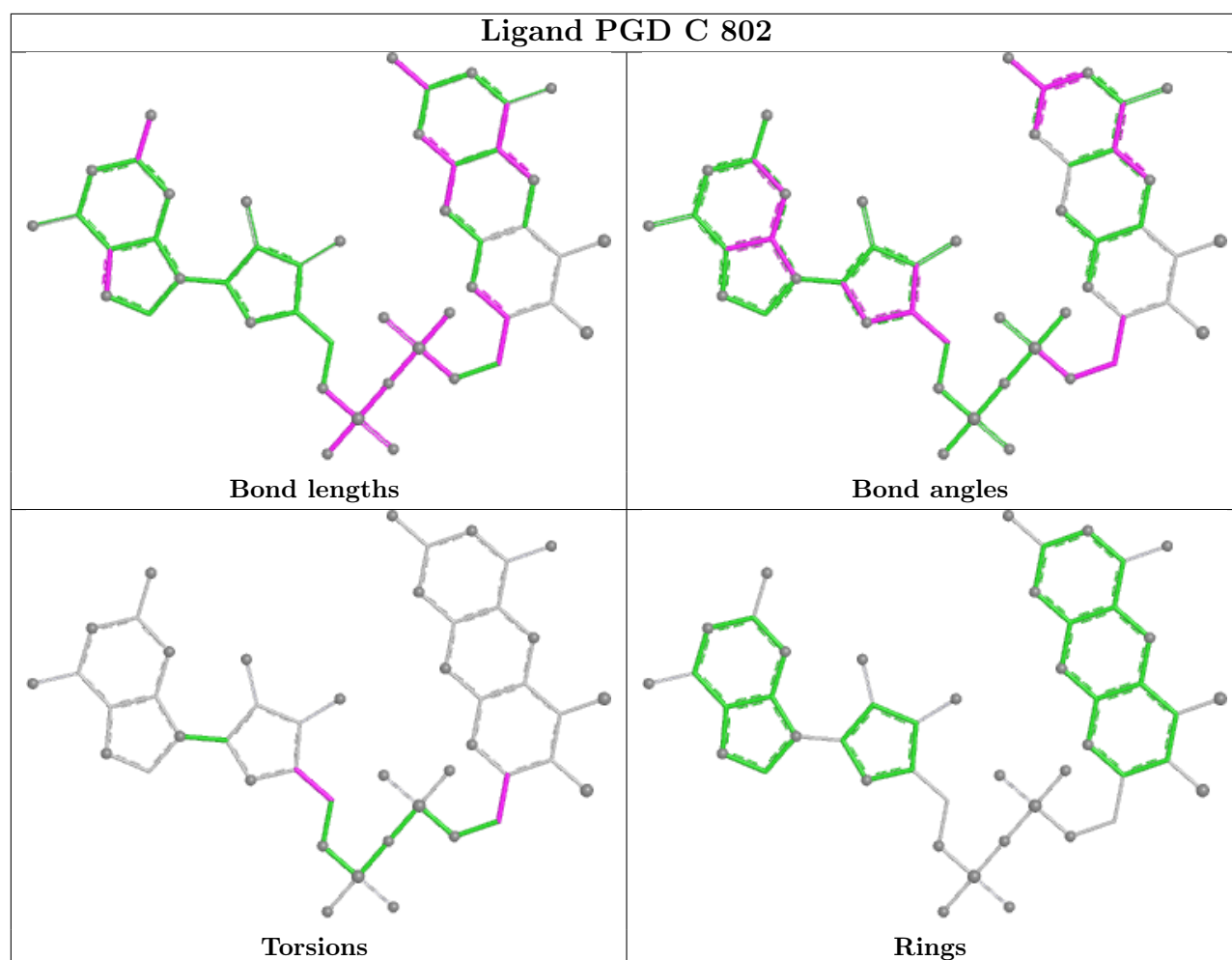
Mol	Chain	Res	Type	Atoms
2	A	802	PGD	O3A-C10-C11-C12
2	C	801	PGD	PA-O3B-PB-O5'
2	C	801	PGD	C5'-O5'-PB-O1B
2	C	801	PGD	C5'-O5'-PB-O2B
2	C	801	PGD	C5'-O5'-PB-O3B
2	A	801	PGD	O3A-C10-C11-C12
2	C	801	PGD	O3A-C10-C11-C12
2	C	802	PGD	O3A-C10-C11-C12
2	A	802	PGD	C5'-O5'-PB-O1B
2	A	802	PGD	O3A-C10-C11-O11
2	C	801	PGD	O3A-C10-C11-O11
2	C	802	PGD	O3A-C10-C11-O11
2	C	801	PGD	O4'-C4'-C5'-O5'
2	C	802	PGD	O4'-C4'-C5'-O5'

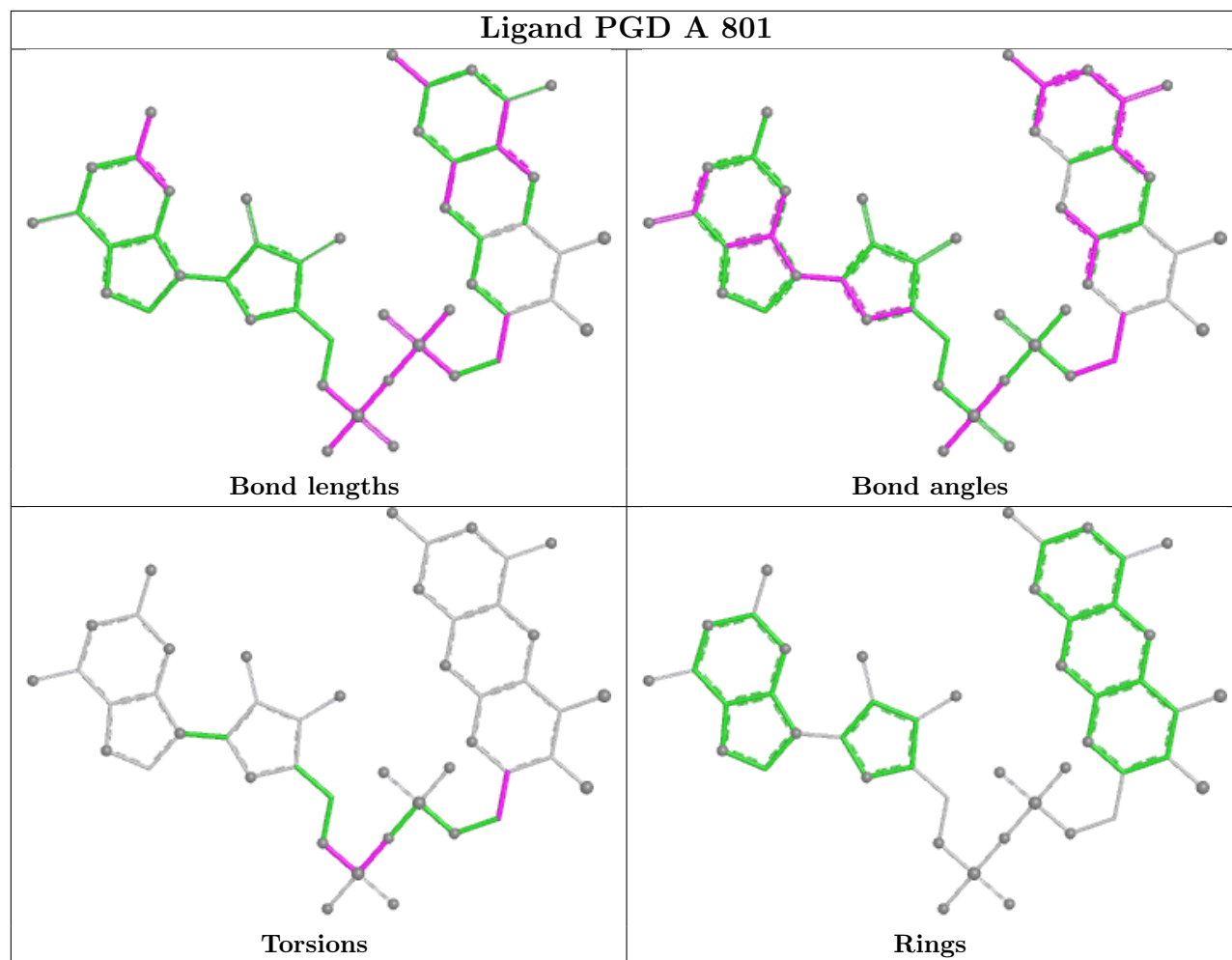
There are no ring outliers.

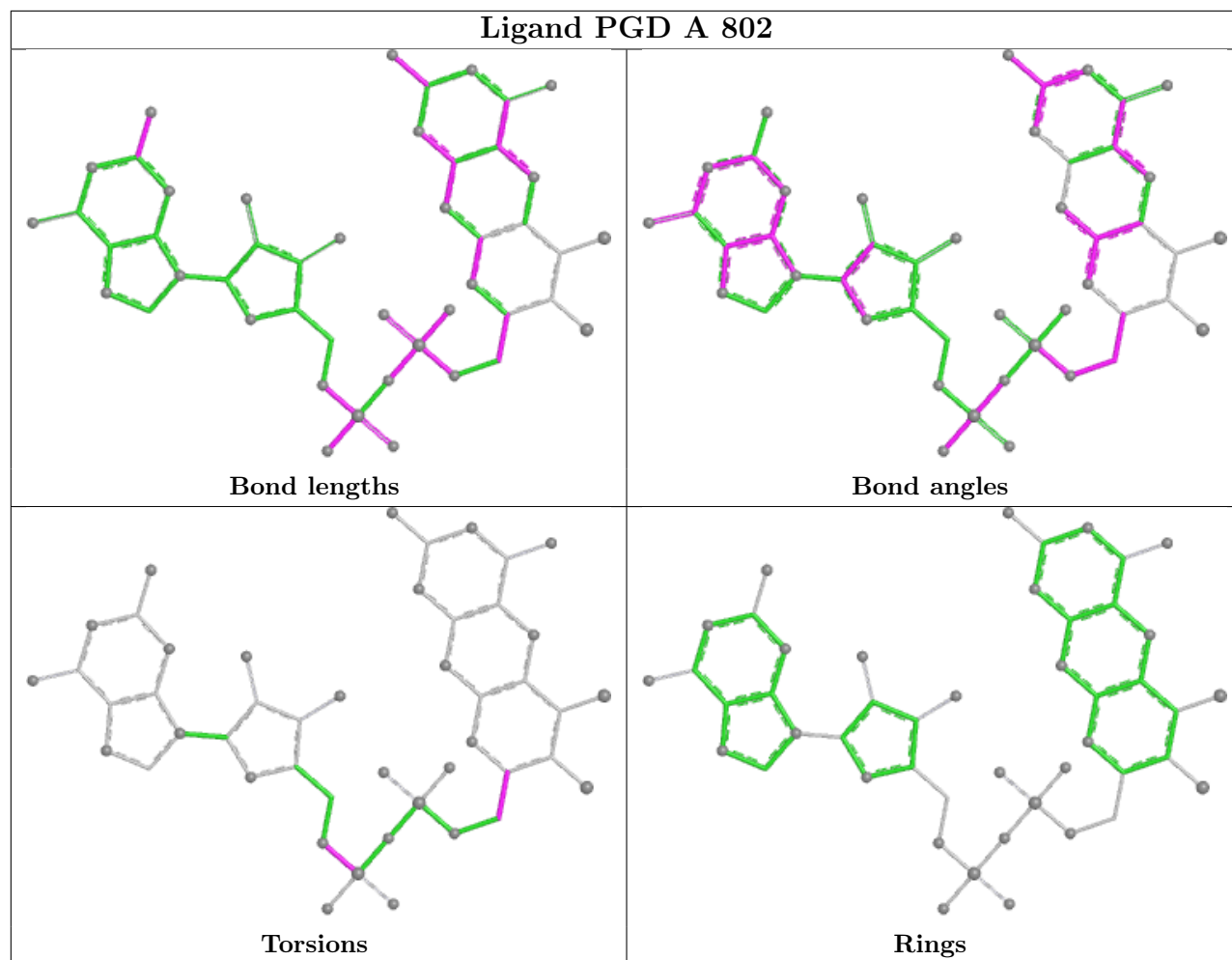
7 monomers are involved in 9 short contacts:

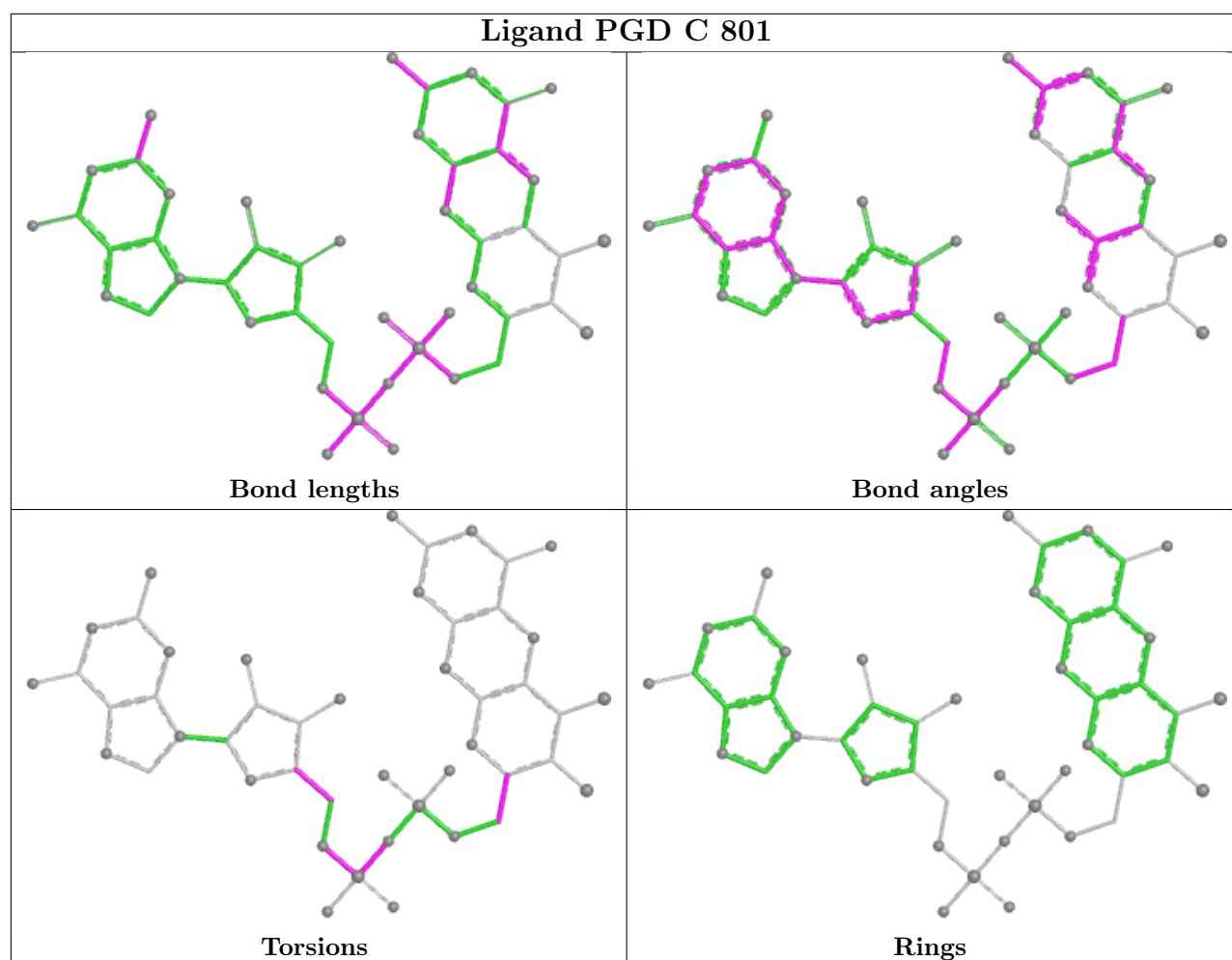
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	PGD	1	0
2	A	801	PGD	3	0
3	C	803	2MO	1	0
2	A	802	PGD	1	0
3	A	803	2MO	1	0
2	C	801	PGD	1	0
4	A	902	SO4	1	0

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.