



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 04:40 am BST

PDB ID : 1E5V / pdb_00001e5v
Title : OXIDIZED DMSO REDUCTASE EXPOSED TO HEPES BUFFER
Authors : Bailey, S.; Bennett, B.; Adams, B.; Smith, A.T.; Bray, R.C.
Deposited on : 2000-08-03
Resolution : 2.40 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	:	1.8.4, CSD as541be (2020)
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)	:	2.50

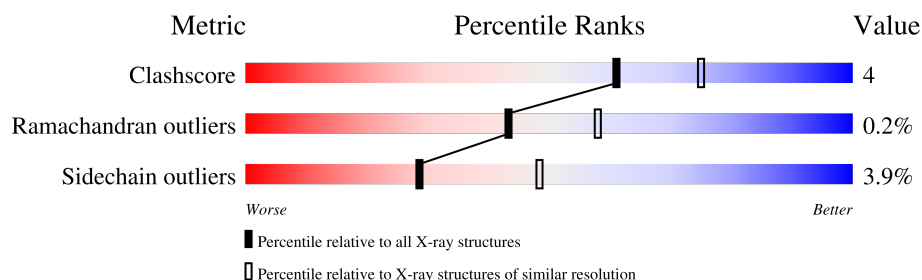
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	 72% 18% • 7%
1	C	823	 71% 19% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12440 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	766	Total	C	N	O	S	0	0	0
			5884	3741	996	1120	27			
1	C	766	Total	C	N	O	S	0	0	0
			5884	3741	996	1120	27			

There are 28 discrepancies between the modelled and reference sequences:

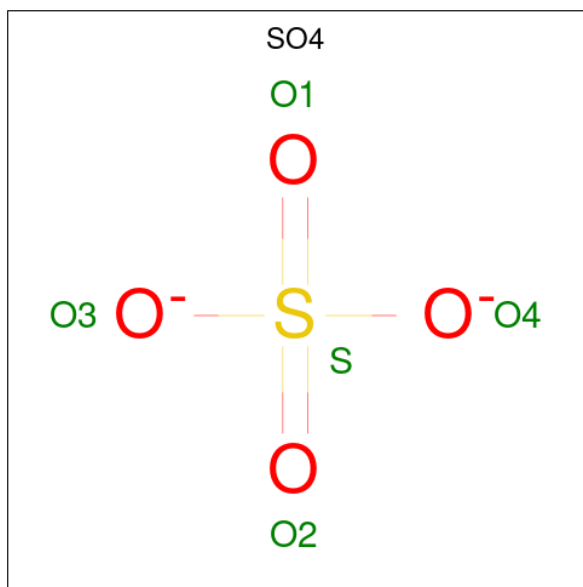
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	THR	conflict	UNP Q52675
A	43	ALA	GLU	conflict	UNP Q52675
A	107	GLU	GLN	conflict	UNP Q52675
A	234	GLU	ASP	conflict	UNP Q52675
A	236	ILE	VAL	conflict	UNP Q52675
A	280	ASP	MET	conflict	UNP Q52675
A	294	GLU	SER	conflict	UNP Q52675
A	295	GLY	ASP	conflict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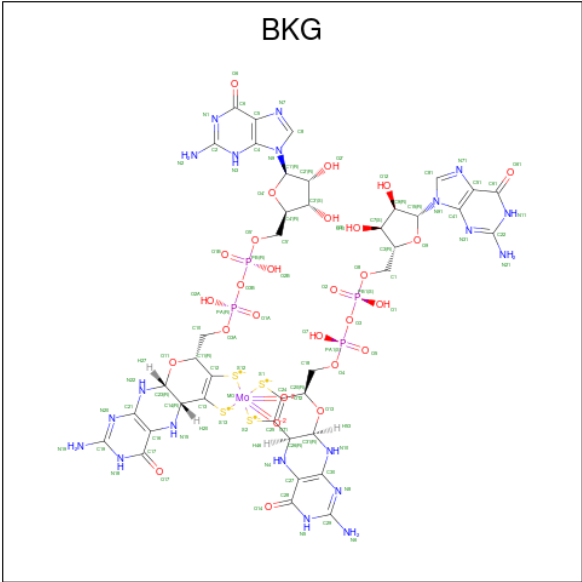
Chain	Residue	Modelled	Actual	Comment	Reference
C	526	ALA	LYS	conflict	UNP Q52675
C	552	ALA	GLY	conflict	UNP Q52675
C	555	GLN	GLU	conflict	UNP Q52675

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is bis-molybdopterin guanine dinucleotide dioxo molybdenum (CCD ID: BKG) (formula: C₄₀H₄₈MoN₂₀O₂₈P₄S₄).



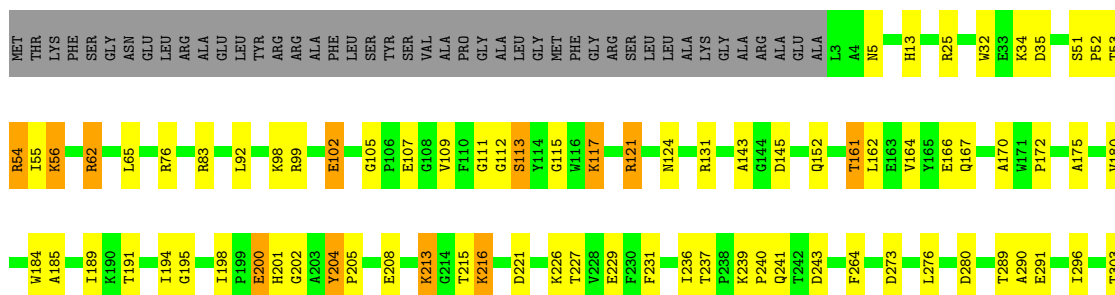
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Mo	N	O	P	S	0	0
			97	40	1	20	28	4	4		
3	C	1	Total	C	Mo	N	O	P	S	0	0
			97	40	1	20	28	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	261	Total	O	0	0
			261	261		
4	C	207	Total	O	0	0
			207	207		

Note EDS was not executed.

- Chain A: 72% 18% 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	70.35Å 117.18Å 233.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	80.4 (20.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12440	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: SO4, BKG

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	0/6041	1.83	126/8221 (1.5%)
1	C	0.81	1/6041 (0.0%)	1.83	121/8221 (1.5%)
All	All	0.82	1/12082 (0.0%)	1.83	247/16442 (1.5%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	121	ARG	CD-NE	-5.29	1.38	1.46

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	ARG	CD-NE-CZ	24.52	158.72	124.40
1	C	99	ARG	CD-NE-CZ	11.75	140.85	124.40
1	C	62	ARG	NE-CZ-NH2	10.81	128.93	119.20
1	A	693	ARG	CD-NE-CZ	10.09	138.53	124.40
1	A	653	ASN	OD1-CG-ND2	-9.70	112.90	122.60
1	C	492	ASN	OD1-CG-ND2	-9.48	113.12	122.60
1	C	458	HIS	CA-CB-CG	9.41	123.21	113.80
1	A	334	HIS	CA-CB-CG	-9.31	104.49	113.80
1	A	168	GLN	OE1-CD-NE2	8.86	131.46	122.60
1	C	442	ARG	NE-CZ-NH2	-8.74	111.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	HIS	CA-CB-CG	8.66	122.46	113.80
1	C	145	ASP	CA-CB-CG	8.40	121.00	112.60
1	C	781	GLU	CA-CB-CG	8.35	130.80	114.10
1	A	701	LYS	N-CA-CB	8.28	123.73	110.65
1	A	458	HIS	CA-CB-CG	8.18	121.98	113.80
1	C	703	THR	CB-CA-C	-8.12	92.65	109.94
1	A	5	ASN	CA-CB-CG	-8.11	104.49	112.60
1	C	467	ARG	CA-C-O	-8.02	111.04	120.10
1	C	492	ASN	CB-CG-ND2	7.92	128.28	116.40
1	A	62	ARG	CD-NE-CZ	7.81	135.33	124.40
1	A	275	PHE	CA-CB-CG	7.80	121.60	113.80
1	C	243	ASP	CA-CB-CG	-7.74	104.86	112.60
1	C	326	ARG	NE-CZ-NH2	-7.74	112.24	119.20
1	A	187	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	434	ASN	CA-CB-CG	7.65	120.25	112.60
1	A	564	ALA	CA-C-O	-7.49	112.96	120.82
1	A	669	CYS	CA-C-O	-7.48	112.54	120.40
1	C	707	MET	CA-C-O	7.48	129.71	121.56
1	C	395	SER	N-CA-C	-7.45	104.33	113.50
1	C	606	ASN	OD1-CG-ND2	7.45	130.05	122.60
1	C	567	ILE	O-C-N	-7.39	116.54	122.97
1	C	25	ARG	CD-NE-CZ	7.37	134.72	124.40
1	A	685	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	769	VAL	N-CA-CB	-7.33	98.63	111.39
1	A	401	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	C	418	THR	N-CA-CB	7.21	121.87	111.05
1	A	399	VAL	N-CA-C	7.18	118.81	110.62
1	A	605	LYS	CA-C-O	7.17	128.20	120.10
1	C	324	MET	CA-C-O	-7.13	109.78	119.05
1	A	438	HIS	CA-CB-CG	7.12	120.92	113.80
1	C	585	ARG	CD-NE-CZ	7.12	134.37	124.40
1	C	264	PHE	CA-CB-CG	-7.08	106.72	113.80
1	A	653	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	23	ASN	N-CA-CB	-7.01	101.32	111.70
1	C	351	GLY	CA-C-N	-7.01	115.93	121.82
1	C	351	GLY	C-N-CA	-7.01	115.93	121.82
1	A	398	PRO	CA-C-O	-6.94	113.75	121.32
1	A	703	THR	CB-CA-C	-6.87	95.31	109.94
1	C	627	ARG	NE-CZ-NH2	-6.85	113.03	119.20
1	A	688	ARG	CD-NE-CZ	6.81	133.94	124.40
1	A	700	VAL	N-CA-C	6.75	118.87	109.55
1	A	695	GLN	OE1-CD-NE2	6.71	129.31	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	HIS	CA-CB-CG	-6.69	107.11	113.80
1	C	688	ARG	CD-NE-CZ	6.69	133.77	124.40
1	A	232	GLY	O-C-N	-6.68	116.49	122.57
1	A	263	ASP	CA-C-O	-6.68	113.34	120.42
1	A	638	HIS	CA-C-O	-6.67	113.09	120.69
1	A	467	ARG	NE-CZ-NH2	6.66	125.19	119.20
1	A	70	ASN	CA-CB-CG	-6.64	105.96	112.60
1	C	626	GLU	CB-CG-CD	6.58	123.78	112.60
1	A	492	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	C	693	ARG	CD-NE-CZ	6.53	133.55	124.40
1	A	152	GLN	OE1-CD-NE2	-6.53	116.08	122.60
1	C	458	HIS	N-CA-CB	6.51	121.61	110.68
1	C	83	ARG	CD-NE-CZ	6.48	133.47	124.40
1	A	399	VAL	CB-CA-C	-6.47	103.56	112.04
1	C	568	VAL	CB-CA-C	-6.47	101.68	110.42
1	A	444	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	A	208	GLU	CB-CG-CD	6.45	123.56	112.60
1	A	439	HIS	CA-CB-CG	-6.43	107.37	113.80
1	C	606	ASN	CA-CB-CG	-6.40	106.20	112.60
1	C	579	VAL	O-C-N	-6.39	116.83	123.03
1	A	434	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	757	VAL	N-CA-C	6.37	117.47	108.17
1	C	573	THR	CA-C-O	-6.36	115.17	119.68
1	A	76	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	C	113	SER	N-CA-CB	-6.31	102.12	111.71
1	A	401	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	A	54	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	C	280	ASP	CA-CB-CG	-6.26	106.34	112.60
1	A	3	LEU	CA-C-O	6.25	131.43	120.80
1	C	102	GLU	CB-CG-CD	6.24	123.20	112.60
1	C	202	GLY	O-C-N	-6.23	115.64	122.68
1	C	334	HIS	CA-CB-CG	-6.22	107.58	113.80
1	C	76	ARG	CA-C-O	-6.22	114.35	121.19
1	A	471	ILE	CA-C-O	-6.20	113.88	120.39
1	C	605	LYS	CA-C-O	6.18	127.08	119.97
1	A	683	ASP	CA-CB-CG	-6.18	106.42	112.60
1	C	309	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	309	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	C	306	GLU	CB-CG-CD	6.14	123.04	112.60
1	A	530	GLU	CB-CG-CD	-6.10	102.22	112.60
1	A	720	ASP	CA-CB-CG	6.08	118.68	112.60
1	C	105	GLY	CA-C-N	6.06	125.94	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105	GLY	C-N-CA	6.06	125.94	119.28
1	A	33	GLU	CB-CG-CD	6.04	122.86	112.60
1	A	689	VAL	CA-C-O	-6.04	114.01	120.59
1	A	580	ARG	CB-CA-C	6.01	119.93	109.65
1	A	308	ALA	CA-C-N	5.98	128.30	120.28
1	A	308	ALA	C-N-CA	5.98	128.30	120.28
1	C	191	THR	N-CA-C	5.97	120.41	113.18
1	A	431	VAL	CA-C-O	-5.96	114.20	120.76
1	A	374	ALA	O-C-N	-5.96	115.13	123.11
1	C	716	GLY	N-CA-C	5.90	123.58	115.27
1	A	5	ASN	CA-C-O	-5.89	113.99	120.24
1	C	13	HIS	CA-CB-CG	5.88	119.68	113.80
1	C	643	HIS	CB-CA-C	5.88	117.90	109.26
1	C	396	VAL	CA-C-O	-5.85	114.12	120.67
1	C	394	ALA	N-CA-CB	5.84	119.16	110.40
1	A	562	PHE	CA-C-O	5.83	126.95	120.82
1	C	221	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	81	PHE	CA-C-N	5.82	130.84	123.10
1	A	81	PHE	C-N-CA	5.82	130.84	123.10
1	A	315	ARG	CD-NE-CZ	5.80	132.53	124.40
1	C	540	SER	CA-C-O	-5.80	113.29	119.97
1	C	204	TYR	O-C-N	-5.80	115.32	120.48
1	A	509	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	C	567	ILE	N-CA-C	5.75	115.82	107.88
1	C	568	VAL	CA-C-O	-5.73	114.48	120.27
1	A	311	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	29	PHE	CA-C-O	-5.71	114.40	120.40
1	C	717	GLY	O-C-N	-5.71	117.75	122.77
1	A	578	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	243	ASP	CA-CB-CG	-5.68	106.92	112.60
1	C	606	ASN	N-CA-CB	-5.66	101.50	110.28
1	A	62	ARG	NE-CZ-NH1	5.65	127.15	121.50
1	C	54	ARG	CA-C-O	-5.64	114.49	120.92
1	A	62	ARG	CA-C-O	-5.63	114.88	120.90
1	C	216	LYS	CA-C-O	5.63	126.73	120.43
1	C	273	ASP	CA-CB-CG	-5.62	106.98	112.60
1	C	56	LYS	N-CA-C	5.61	118.25	111.40
1	A	604	SER	CA-C-N	5.61	128.35	120.28
1	A	604	SER	C-N-CA	5.61	128.35	120.28
1	C	327	MET	CG-SD-CE	5.59	113.20	100.90
1	C	716	GLY	CA-C-N	5.59	126.36	120.43
1	C	716	GLY	C-N-CA	5.59	126.36	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	PHE	CA-C-O	-5.59	114.92	120.90
1	A	320	ALA	CA-C-N	5.58	128.42	121.83
1	A	320	ALA	C-N-CA	5.58	128.42	121.83
1	A	216	LYS	CA-C-O	5.58	127.05	120.69
1	C	167	GLN	CA-CB-CG	5.58	125.25	114.10
1	A	721	PRO	O-C-N	-5.57	116.30	123.03
1	C	76	ARG	CA-C-N	-5.56	113.79	122.51
1	C	76	ARG	C-N-CA	-5.56	113.79	122.51
1	C	559	PHE	CA-CB-CG	-5.55	108.25	113.80
1	C	769	VAL	CA-CB-CG1	5.55	119.84	110.40
1	C	316	THR	N-CA-C	5.55	117.94	108.90
1	A	61	ARG	NE-CZ-NH2	-5.55	114.21	119.20
1	C	460	PHE	N-CA-C	-5.54	106.41	114.12
1	A	326	ARG	CA-C-O	5.54	129.74	120.65
1	C	326	ARG	CD-NE-CZ	5.54	132.15	124.40
1	A	42	LEU	N-CA-CB	5.52	118.72	110.22
1	C	276	LEU	CA-C-N	5.52	124.71	118.97
1	C	276	LEU	C-N-CA	5.52	124.71	118.97
1	A	276	LEU	CA-C-N	5.51	124.97	119.24
1	A	276	LEU	C-N-CA	5.51	124.97	119.24
1	A	506	TYR	CB-CA-C	-5.51	110.20	116.54
1	C	204	TYR	CA-C-O	5.51	124.13	118.73
1	A	113	SER	N-CA-CB	-5.51	103.33	111.71
1	A	748	LEU	O-C-N	-5.51	116.30	122.03
1	C	109	VAL	CB-CA-C	-5.51	102.92	110.96
1	C	631	PRO	CA-C-O	-5.49	115.35	121.23
1	A	312	GLU	OE1-CD-OE2	-5.48	109.75	122.90
1	A	425	VAL	CA-C-O	-5.47	114.60	121.11
1	A	703	THR	CA-CB-OG1	5.45	117.77	109.60
1	C	614	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	195	GLY	O-C-N	-5.43	118.52	123.57
1	C	339	THR	O-C-N	-5.43	116.22	122.09
1	A	769	VAL	CB-CA-C	5.43	118.71	110.62
1	A	641	ALA	N-CA-CB	-5.42	101.93	110.49
1	A	612	TYR	CA-C-O	-5.41	114.43	120.54
1	C	640	ALA	CA-C-O	-5.37	115.37	121.66
1	A	142	GLY	O-C-N	-5.37	116.77	123.21
1	C	92	LEU	CB-CA-C	5.36	119.97	110.85
1	A	81	PHE	O-C-N	-5.36	116.98	123.03
1	A	161	THR	CA-C-O	-5.35	115.52	121.51
1	C	769	VAL	N-CA-CB	-5.34	99.20	111.81
1	A	194	ILE	CB-CG1-CD1	-5.34	102.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	658	ARG	N-CA-C	5.34	117.79	111.33
1	C	687	VAL	CA-C-O	-5.33	116.08	121.67
1	A	766	GLY	CA-C-N	5.31	125.25	119.78
1	A	766	GLY	C-N-CA	5.31	125.25	119.78
1	C	559	PHE	N-CA-C	5.31	117.49	111.11
1	C	688	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	C	505	LEU	CD1-CG-CD2	-5.30	99.13	110.80
1	C	164	VAL	N-CA-C	5.30	116.02	110.62
1	C	399	VAL	N-CA-C	5.30	120.36	109.34
1	A	585	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	653	ASN	N-CA-CB	5.29	117.98	110.16
1	C	229	GLU	CA-CB-CG	-5.28	103.54	114.10
1	A	672	HIS	CA-CB-CG	-5.28	108.52	113.80
1	C	442	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	769	VAL	O-C-N	-5.26	117.50	123.18
1	A	635	TYR	CB-CA-C	5.25	116.95	108.91
1	C	5	ASN	OD1-CG-ND2	5.25	127.85	122.60
1	C	651	GLN	N-CA-CB	5.25	117.68	109.97
1	A	13	HIS	CA-CB-CG	5.24	119.04	113.80
1	A	346	GLN	CG-CD-NE2	5.23	124.25	116.40
1	A	639	ILE	N-CA-CB	5.23	116.96	111.00
1	C	470	ASP	N-CA-C	-5.22	105.19	112.45
1	C	536	GLY	O-C-N	-5.22	117.13	122.19
1	A	638	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	653	ASN	N-CA-C	-5.19	105.70	111.36
1	C	649	HIS	CB-CA-C	-5.19	110.17	117.23
1	C	434	ASN	CA-C-N	5.19	124.85	119.56
1	C	434	ASN	C-N-CA	5.19	124.85	119.56
1	A	658	ARG	CA-C-N	5.18	127.74	120.28
1	A	658	ARG	C-N-CA	5.18	127.74	120.28
1	A	109	VAL	CB-CA-C	-5.18	104.26	110.99
1	C	200	GLU	CA-C-O	5.17	125.47	119.32
1	A	205	PRO	CA-C-N	5.17	125.68	119.94
1	A	205	PRO	C-N-CA	5.17	125.68	119.94
1	A	486	THR	O-C-N	-5.17	116.76	122.86
1	A	733	TYR	CA-C-O	-5.16	113.86	120.31
1	C	521	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	777	PRO	O-C-N	-5.15	116.57	122.85
1	C	658	ARG	CA-C-N	5.14	127.69	120.28
1	C	658	ARG	C-N-CA	5.14	127.69	120.28
1	C	331	GLU	O-C-N	-5.14	116.20	122.22
1	A	105	GLY	CA-C-N	5.13	124.75	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLY	C-N-CA	5.13	124.75	119.56
1	C	442	ARG	CA-C-O	-5.13	115.41	120.90
1	A	130	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	C	424	ASP	CA-C-O	-5.13	116.34	122.13
1	A	722	SER	N-CA-CB	5.12	117.74	110.16
1	A	425	VAL	N-CA-CB	-5.12	103.25	110.26
1	A	158	VAL	CA-C-O	-5.11	115.32	120.69
1	A	67	LYS	N-CA-C	5.11	120.15	112.94
1	A	459	ASP	CA-C-O	-5.10	115.97	121.38
1	C	121	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
1	A	196	TRP	N-CA-C	-5.09	105.64	111.14
1	A	606	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	C	111	GLY	O-C-N	-5.08	116.09	122.70
1	C	394	ALA	CB-CA-C	-5.08	102.88	110.50
1	C	92	LEU	N-CA-CB	-5.07	102.66	110.16
1	C	579	VAL	CA-C-O	5.07	125.28	120.31
1	A	57	TYR	CB-CA-C	-5.06	101.53	109.22
1	C	717	GLY	CA-C-O	5.06	125.74	120.98
1	C	775	VAL	O-C-N	-5.06	117.56	122.97
1	C	601	GLU	CA-C-O	5.05	126.30	120.84
1	C	345	GLY	O-C-N	-5.05	117.46	122.41
1	A	87	ASP	CA-C-O	-5.03	115.22	120.55
1	C	467	ARG	O-C-N	5.03	128.11	122.22
1	A	333	ALA	N-CA-C	5.02	116.44	111.07
1	A	23	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	C	180	VAL	CA-C-O	-5.02	115.20	120.27
1	C	372	ALA	O-C-N	-5.01	117.35	123.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	231	PHE	Mainchain

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	5884	0	5690	39	0
1	C	5884	0	5690	58	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	97	0	0	0	0
3	C	97	0	0	2	0
4	A	261	0	0	2	0
4	C	207	0	0	1	0
All	All	12440	0	11380	97	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 (97) 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:671:MET:HE1	1:C:761:VAL:HG11	1.53	0.90
1:A:97:VAL:HG22	1:A:427:MET:HE1	1.54	0.89
1:C:54:ARG:NH1	1:C:505:LEU:HD12	2.09	0.68
1:A:223:VAL:HG22	1:A:706:VAL:HG12	1.75	0.67
1:C:732:LYS:HD2	1:C:769:VAL:HG13	1.77	0.65
1:C:627:ARG:HD2	4:C:2152:HOH:O	1.98	0.64
1:C:131:ARG:HB2	1:C:378:ASP:HA	1.79	0.63
1:C:410:GLY:O	1:C:421:LYS:HG2	1.97	0.63
1:C:703:THR:HG22	1:C:705:ALA:H	1.63	0.63
1:C:152:GLN:HB2	1:C:162:LEU:HD11	1.85	0.59
1:A:520:GLU:OE1	1:A:525:GLY:HA3	2.02	0.58
1:C:161:THR:HB	1:C:166:GLU:OE2	2.04	0.58
1:A:653:ASN:ND2	1:A:718:TRP:H	2.01	0.58
1:C:412:GLU:HA	1:C:420:SER:O	2.04	0.57
1:C:56:LYS:HG2	1:C:506:TYR:CD2	2.40	0.57
1:C:398:PRO:HG2	1:C:401:ARG:HG3	1.87	0.56
1:C:653:ASN:ND2	1:C:718:TRP:H	2.04	0.55
1:A:639:ILE:HG12	1:A:711:ILE:HD11	1.88	0.55
1:A:59:MET:HE2	1:A:780:ALA:HB2	1.87	0.55
1:A:294:GLU:HG3	1:A:299:VAL:O	2.09	0.53
1:C:625:LEU:HD23	1:C:626:GLU:HG2	1.91	0.53
1:C:170:ALA:HB1	1:C:172:PRO:HD2	1.92	0.51
1:A:618:HIS:HB2	1:A:619:PRO:HD2	1.92	0.51
1:C:32:TRP:CE2	1:C:34:LYS:HB2	2.45	0.51
1:A:701:LYS:HG2	4:A:2220:HOH:O	2.10	0.51
1:A:112:GLY:O	1:A:113:SER:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:GLU:OE2	1:C:305:LYS:NZ	2.43	0.50
1:A:397:ILE:O	1:A:397:ILE:HG13	2.12	0.49
1:C:703:THR:CG2	1:C:705:ALA:H	2.24	0.49
1:C:595:THR:HB	1:C:596:PRO:CD	2.44	0.48
1:C:185:ALA:O	1:C:321:GLY:HA3	2.14	0.48
1:C:98:LYS:HE3	1:C:102:GLU:OE2	2.14	0.48
1:A:521:ARG:HH11	1:A:521:ARG:HG3	1.78	0.48
1:C:189:ILE:HD12	1:C:227:THR:HA	1.96	0.48
1:A:407:GLU:OE1	1:A:444:ARG:NH2	2.29	0.47
1:C:239:LYS:O	1:C:240:PRO:C	2.57	0.47
1:C:194:ILE:C	1:C:194:ILE:HD12	2.39	0.47
1:A:161:THR:HB	1:A:166:GLU:OE2	2.15	0.47
1:C:241:GLN:HG2	1:C:327:MET:SD	2.55	0.47
1:C:530:GLU:HG3	1:C:532:LYS:HE3	1.96	0.47
1:C:407:GLU:OE1	1:C:444:ARG:NH2	2.42	0.46
1:C:595:THR:HB	1:C:596:PRO:HD2	1.98	0.46
1:C:743:ILE:O	1:C:743:ILE:HG13	2.15	0.46
1:A:332:GLN:OE1	1:A:619:PRO:HA	2.16	0.46
1:A:562:PHE:CD1	1:A:568:VAL:HG23	2.51	0.46
1:C:184:TRP:O	1:C:185:ALA:HB3	2.16	0.45
1:C:638:HIS:HA	1:C:758:LEU:HD23	1.99	0.45
1:A:189:ILE:HD12	1:A:230:PHE:HB2	1.97	0.45
1:A:252:HIS:CE1	1:A:289:THR:HG22	2.52	0.45
1:A:258:ASP:CG	1:A:262:LYS:HZ1	2.22	0.45
1:C:327:MET:HE1	3:C:902:BKG:O61	2.17	0.45
1:A:185:ALA:O	1:A:321:GLY:HA3	2.17	0.45
1:C:204:TYR:HB2	1:C:205:PRO:HD3	1.97	0.45
1:A:241:GLN:HG2	1:A:327:MET:SD	2.56	0.45
1:C:115:GLY:HA2	3:C:902:BKG:O2A	2.17	0.45
1:A:562:PHE:HD1	1:A:568:VAL:HG23	1.82	0.44
1:A:477:THR:HG1	1:A:479:TYR:HD2	1.61	0.44
1:A:503:GLU:O	1:A:504:PRO:C	2.59	0.44
1:A:663:VAL:HB	1:A:699:GLY:HA3	1.99	0.44
1:C:143:ALA:HB2	1:C:396:VAL:CG1	2.47	0.44
1:C:240:PRO:O	1:C:241:GLN:HB2	2.16	0.44
1:C:445:MET:HE3	1:C:449:TRP:CZ3	2.52	0.44
1:C:327:MET:O	1:C:745:THR:HG22	2.17	0.44
1:A:51:SER:HB2	1:A:52:PRO:HD2	2.00	0.44
1:A:144:GLY:HA2	1:A:152:GLN:OE1	2.17	0.43
1:A:550:LYS:O	1:A:551:ALA:C	2.60	0.43
1:C:55:ILE:HG22	1:C:474:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:HA	1:A:154:ILE:HG22	2.00	0.42
1:C:51:SER:HB2	1:C:52:PRO:HD2	2.01	0.42
1:C:430:TRP:O	1:C:457:VAL:HA	2.19	0.42
1:A:56:LYS:HG2	1:A:506:TYR:CD2	2.54	0.42
1:A:467:ARG:HD3	4:A:2150:HOH:O	2.18	0.42
1:C:35:ASP:CG	1:C:201:HIS:HD1	2.26	0.42
1:C:732:LYS:CD	1:C:769:VAL:HG13	2.47	0.42
1:C:237:THR:O	1:C:237:THR:OG1	2.36	0.42
1:A:435:PRO:HB2	1:A:445:MET:HE1	2.01	0.42
1:A:535:MET:HE1	1:A:559:PHE:HZ	1.85	0.42
1:C:634:LYS:HG2	1:C:635:TYR:CE2	2.54	0.42
1:C:152:GLN:HB2	1:C:162:LEU:CD1	2.49	0.42
1:A:412:GLU:HA	1:A:420:SER:O	2.20	0.42
1:C:424:ASP:OD1	1:C:451:LYS:NZ	2.50	0.41
1:A:150:ALA:HB1	1:A:331:GLU:HG3	2.02	0.41
1:C:98:LYS:HA	1:C:98:LYS:HD2	1.80	0.41
1:C:62:ARG:NH1	1:C:62:ARG:HG3	2.35	0.41
1:C:175:ALA:O	1:C:213:LYS:HD2	2.20	0.41
1:C:112:GLY:O	1:C:113:SER:C	2.63	0.41
1:C:622:MET:HE3	1:C:622:MET:HB2	1.97	0.41
1:C:117:LYS:HE2	1:C:124:ASN:OD1	2.21	0.41
1:A:250:MET:HE2	1:A:307:LEU:HB3	2.03	0.40
1:A:97:VAL:CG2	1:A:427:MET:HE1	2.39	0.40
1:A:211:LYS:HE3	1:A:230:PHE:O	2.21	0.40
1:C:289:THR:O	1:C:290:ALA:C	2.63	0.40
1:C:603:TYR:OH	1:C:608:GLU:OE2	2.36	0.40
1:C:340:LEU:O	1:C:344:LEU:HG	2.21	0.40
1:A:116:TRP:O	1:A:117:LYS:C	2.64	0.40
1:C:107:GLU:CD	1:C:107:GLU:H	2.30	0.40
1:C:204:TYR:O	1:C:208:GLU:HG3	2.22	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	762/823 (93%)	736 (97%)	25 (3%)	1 (0%)	48	64
1	C	762/823 (93%)	736 (97%)	24 (3%)	2 (0%)	36	50
All	All	1524/1646 (93%)	1472 (97%)	49 (3%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	117	LYS
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	610/648 (94%)	586 (96%)	24 (4%)	28	48
1	C	610/648 (94%)	586 (96%)	24 (4%)	28	48
All	All	1220/1296 (94%)	1172 (96%)	48 (4%)	28	48

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	33	GLU
1	A	53	THR
1	A	65	LEU
1	A	161	THR
1	A	189	ILE
1	A	200	GLU
1	A	216	LYS
1	A	306	GLU
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	419	ARG
1	A	420	SER
1	A	430	TRP
1	A	438	HIS
1	A	504	PRO
1	A	547	LYS
1	A	560	ASP
1	A	586	GLU
1	A	589	LEU
1	A	606	ASN
1	A	703	THR
1	A	757	VAL
1	A	769	VAL
1	A	778	LYS
1	C	53	THR
1	C	65	LEU
1	C	121	ARG
1	C	161	THR
1	C	198	ILE
1	C	200	GLU
1	C	213	LYS
1	C	215	THR
1	C	216	LYS
1	C	226	LYS
1	C	236	ILE
1	C	296	ILE
1	C	303	THR
1	C	307	LEU
1	C	337	LEU
1	C	376	ILE
1	C	430	TRP
1	C	451	LYS
1	C	547	LYS
1	C	568	VAL
1	C	590	LEU
1	C	625	LEU
1	C	703	THR
1	C	769	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
1	A	606	ASN
1	A	653	ASN
1	A	712	GLN
1	C	88	GLN
1	C	241	GLN
1	C	443	ASN
1	C	482	ASN
1	C	653	ASN

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](#)

4 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	SO4	A	901	-	4,4,4	0.36	0	6,6,6	0.48	0
2	SO4	C	901	-	4,4,4	0.53	0	6,6,6	0.56	0
3	BKG	A	902	1	92,110,110	2.27	26 (28%)	103,181,181	2.40	31 (30%)
3	BKG	C	902	1	92,110,110	2.27	28 (30%)	103,181,181	3.01	27 (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
3	BKG	A	902	1	-	7/44/160/160	0/14/14/14
3	BKG	C	902	1	-	5/44/160/160	0/14/14/14

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	BKG	C30-N10	7.82	1.44	1.35
3	A	902	BKG	C30-N10	7.41	1.43	1.35
3	A	902	BKG	C21-N22	7.24	1.43	1.35
3	C	902	BKG	C21-N22	6.73	1.42	1.35
3	C	902	BKG	PA1-O5	6.04	1.72	1.50
3	A	902	BKG	PA1-O5	5.96	1.72	1.50
3	A	902	BKG	PB1-O2	5.66	1.71	1.50
3	A	902	BKG	PA-O1A	5.46	1.70	1.50
3	A	902	BKG	PB-O1B	5.40	1.70	1.50
3	C	902	BKG	PB-O1B	5.23	1.69	1.50
3	C	902	BKG	PA-O1A	5.02	1.68	1.50
3	C	902	BKG	PB1-O2	5.02	1.68	1.50
3	A	902	BKG	PB-O5'	4.17	1.76	1.59
3	C	902	BKG	O11-C11	-4.11	1.38	1.43
3	A	902	BKG	O13-C20	-3.91	1.38	1.43
3	A	902	BKG	C29-N6	3.83	1.43	1.34
3	C	902	BKG	PB1-O8	3.79	1.74	1.59
3	C	902	BKG	PB-O2B	3.59	1.72	1.55
3	C	902	BKG	C29-N6	3.54	1.42	1.34
3	C	902	BKG	PA1-O4	3.49	1.73	1.59
3	C	902	BKG	C26-N4	3.39	1.50	1.46
3	A	902	BKG	PB1-O1	3.37	1.71	1.55
3	C	902	BKG	PA-O3A	3.37	1.72	1.59
3	A	902	BKG	PA-O3A	3.32	1.72	1.59
3	C	902	BKG	C19-N19	3.20	1.41	1.34
3	A	902	BKG	PA1-O4	3.20	1.72	1.59
3	A	902	BKG	PA1-O7	3.06	1.69	1.55
3	C	902	BKG	PA-O2A	3.02	1.69	1.55
3	A	902	BKG	C19-N19	2.96	1.41	1.34
3	C	902	BKG	PB1-O1	2.96	1.69	1.55
3	A	902	BKG	C10-C11	2.95	1.56	1.52
3	A	902	BKG	PB1-O8	2.83	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	BKG	C2-N2	2.81	1.40	1.34
3	C	902	BKG	PA1-O7	2.80	1.68	1.55
3	C	902	BKG	C23-N22	2.70	1.49	1.45
3	A	902	BKG	C22-N21	2.68	1.40	1.34
3	C	902	BKG	O4'-C4'	-2.61	1.39	1.45
3	C	902	BKG	PB-O5'	2.56	1.69	1.59
3	A	902	BKG	PA-O2A	2.54	1.67	1.55
3	C	902	BKG	C22-N21	2.52	1.40	1.34
3	C	902	BKG	C5-N7	-2.48	1.34	1.39
3	C	902	BKG	C6-C5	-2.43	1.38	1.45
3	A	902	BKG	C51-N71	-2.40	1.34	1.39
3	A	902	BKG	PB-O2B	2.37	1.66	1.55
3	A	902	BKG	O9-C3	-2.34	1.39	1.45
3	C	902	BKG	C51-N71	-2.32	1.34	1.39
3	C	902	BKG	O3A-C10	-2.31	1.35	1.44
3	A	902	BKG	C4-N9	-2.28	1.34	1.37
3	A	902	BKG	C6-C5	-2.24	1.38	1.45
3	A	902	BKG	O11-C23	-2.23	1.40	1.43
3	A	902	BKG	C31-C26	2.22	1.55	1.53
3	C	902	BKG	C10-C11	2.16	1.54	1.52
3	C	902	BKG	O2'-C2'	-2.04	1.38	1.43
3	C	902	BKG	C2-N2	2.04	1.39	1.34

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	BKG	C25-C24-S1	-21.58	107.90	120.15
3	A	902	BKG	C25-C24-S1	-11.55	113.59	120.15
3	A	902	BKG	C24-C25-S2	-9.45	114.79	120.15
3	C	902	BKG	C24-C25-S2	-8.86	115.12	120.15
3	C	902	BKG	C5-C4-N9	8.70	110.31	106.23
3	A	902	BKG	C5-C4-N9	7.40	109.70	106.23
3	C	902	BKG	C8-N9-C4	-4.85	102.67	106.71
3	A	902	BKG	C51-C41-N31	-4.49	121.17	128.46
3	A	902	BKG	C19-N20-C21	4.36	121.30	113.43
3	C	902	BKG	C29-N8-C30	4.24	121.08	113.43
3	C	902	BKG	C13-C12-S12	4.12	122.49	120.15
3	A	902	BKG	C22-N31-C41	4.08	119.57	112.30
3	A	902	BKG	O6-C6-N1	-4.03	113.38	120.23
3	A	902	BKG	PA-O3B-PB	4.00	146.57	132.83
3	C	902	BKG	O11-C23-C14	-3.93	106.34	108.96
3	A	902	BKG	C29-N8-C30	3.79	120.27	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	BKG	C13-C12-S12	-3.52	118.15	120.15
3	C	902	BKG	C19-N20-C21	3.50	119.75	113.43
3	C	902	BKG	C22-N31-C41	3.50	118.53	112.30
3	C	902	BKG	C51-C41-N31	-3.49	122.79	128.46
3	A	902	BKG	O17-C17-C16	-3.36	119.54	127.24
3	C	902	BKG	C51-C41-N91	3.23	111.49	105.63
3	C	902	BKG	O61-C61-N11	-3.20	113.97	120.12
3	C	902	BKG	O6-C6-N1	-3.20	114.78	120.23
3	C	902	BKG	PA-O3B-PB	3.08	143.40	132.83
3	A	902	BKG	C51-C41-N91	3.01	111.08	105.63
3	C	902	BKG	C28-C27-N4	2.84	124.37	116.76
3	C	902	BKG	O4'-C1'-C2'	-2.83	100.47	106.64
3	A	902	BKG	C19-N18-C17	-2.79	120.01	125.10
3	A	902	BKG	O13-C31-C26	2.73	110.78	108.96
3	C	902	BKG	C17-C16-N15	2.71	124.02	116.76
3	C	902	BKG	O14-C28-N5	-2.69	114.96	120.12
3	C	902	BKG	C3-O9-C15	-2.67	103.57	109.47
3	A	902	BKG	PA1-O3-PB1	2.64	141.90	132.83
3	A	902	BKG	O4'-C1'-N9	-2.50	102.64	108.36
3	A	902	BKG	O9-C15-C9	-2.46	101.28	106.64
3	C	902	BKG	N6-C29-N5	2.41	121.84	116.71
3	A	902	BKG	C16-C17-N18	2.38	119.41	112.31
3	A	902	BKG	O13-C31-N10	-2.38	106.12	108.57
3	C	902	BKG	C27-C28-N5	2.36	119.34	112.31
3	C	902	BKG	C19-N18-C17	-2.36	120.80	125.10
3	A	902	BKG	N19-C19-N18	2.32	121.66	116.71
3	A	902	BKG	N3-C2-N1	-2.32	119.00	123.32
3	C	902	BKG	O17-C17-N18	-2.31	115.68	120.12
3	C	902	BKG	N2-C2-N3	2.25	121.50	116.71
3	A	902	BKG	N6-C29-N5	2.24	121.48	116.71
3	A	902	BKG	C17-C16-N15	2.24	122.76	116.76
3	C	902	BKG	C29-N5-C28	-2.22	121.05	125.10
3	A	902	BKG	C5'-C4'-C3'	-2.20	106.94	115.18
3	A	902	BKG	PA1-O4-C18	-2.15	109.08	121.68
3	A	902	BKG	O14-C28-C27	-2.14	122.34	127.24
3	C	902	BKG	PA1-O3-PB1	2.14	140.16	132.83
3	A	902	BKG	C41-C51-N71	-2.12	107.36	110.72
3	A	902	BKG	C28-C27-N4	2.12	122.46	116.76
3	A	902	BKG	N2-C2-N3	2.10	121.19	116.71
3	A	902	BKG	O4'-C1'-C2'	-2.10	102.06	106.64
3	C	902	BKG	C16-C17-N18	2.06	118.46	112.31
3	A	902	BKG	N5-C29-N8	-2.05	119.50	123.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

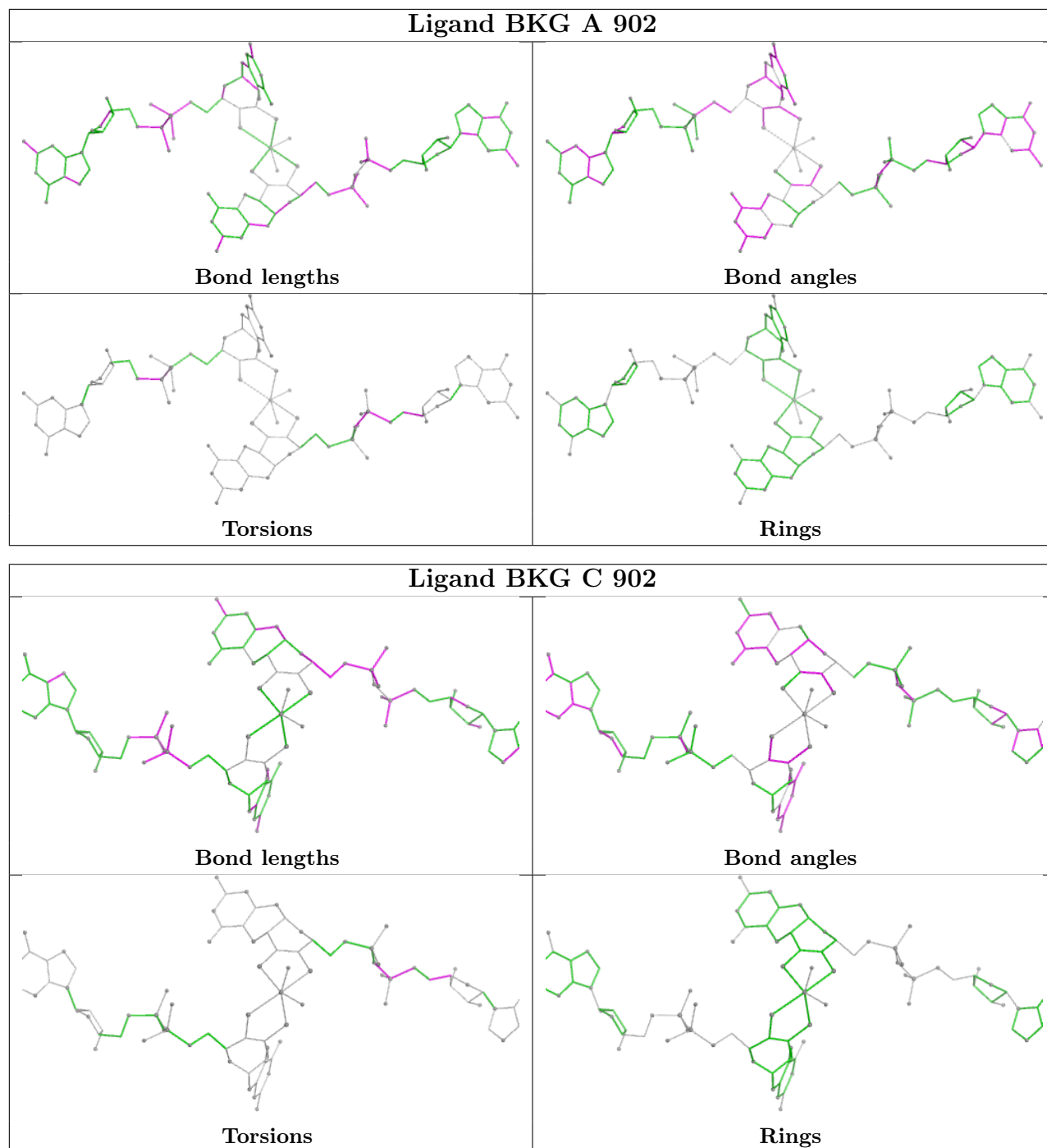
Mol	Chain	Res	Type	Atoms
3	A	902	BKG	PA-O3B-PB-O5'
3	A	902	BKG	C5'-O5'-PB-O2B
3	C	902	BKG	C5'-O5'-PB-O1B
3	C	902	BKG	C5'-O5'-PB-O2B
3	A	902	BKG	PA1-O3-PB1-O8
3	C	902	BKG	PA-O3B-PB-O5'
3	A	902	BKG	C5'-O5'-PB-O3B
3	A	902	BKG	C5'-O5'-PB-O1B
3	A	902	BKG	O4'-C4'-C5'-O5'
3	C	902	BKG	C5'-O5'-PB-O3B
3	A	902	BKG	C1-O8-PB1-O2
3	C	902	BKG	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	902	BKG	2	0

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



5.7 Other polymers [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.