



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:13 AM UTC

PDB ID : 1SRI / pdb_00001sri
Title : STRUCTURE-BASED DESIGN OF SYNTHETIC AZOBENZENE LIG-
ANDS FOR STREPTAVIDIN
Authors : Weber, P.C.; Salemme, F.R.
Deposited on : 1994-02-17
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

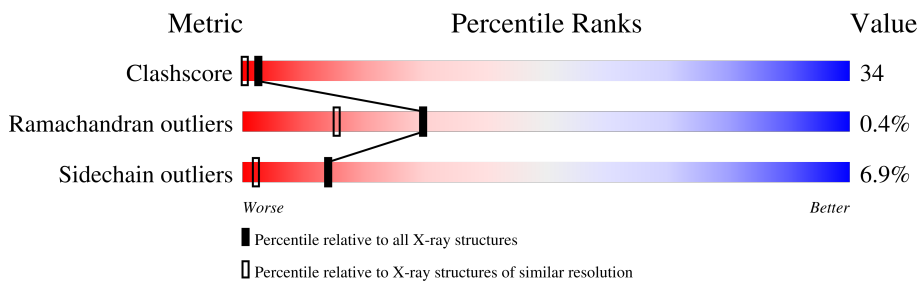
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)

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	121	 53% 36% 6% . .
1	B	121	 59% 33% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMB	A	300	-	-	X	-
2	DMB	B	300	-	-	X	-

2 Entry composition [i](#)

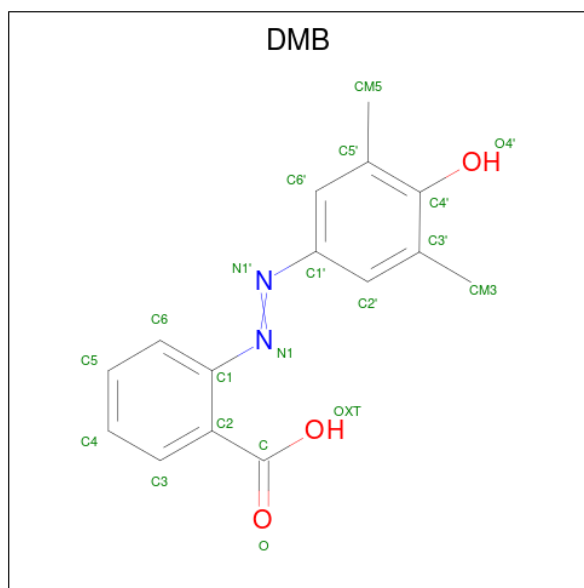
There are 3 unique types of molecules in this entry. The entry contains 1958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STREPTAVIDIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	0	1	0
			883	552	153	178			
1	B	121	Total	C	N	O	0	0	0
			901	562	156	183			

- Molecule 2 is 2-((3',5'-DIMETHYL-4'-HYDROXYPHENYL)AZO)BENZOIC ACID (CCD ID: DMB) (formula: C₁₅H₁₄N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	15	2	3		
2	B	1	Total	C	N	O	0	0
			20	15	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	65	Total	O	0	0
			65	65		

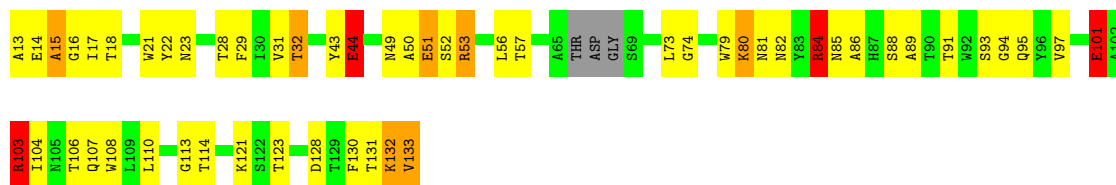
3 Residue-property plots [i](#)

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.

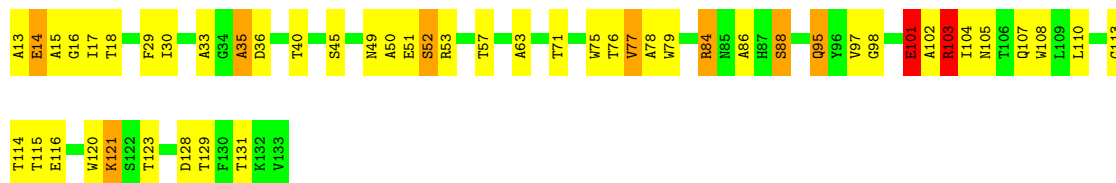
• Molecule 1: STREPTAVIDIN

Chain A:  53% 36% 6% . .



• Molecule 1: STREPTAVIDIN

Chain B:  59% 33% 7% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.60Å 106.00Å 47.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, PROLSQ	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1958	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: DMB

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	1.91	15/909 (1.7%)	2.07	33/1243 (2.7%)
1	B	1.84	11/923 (1.2%)	2.18	40/1264 (3.2%)
All	All	1.87	26/1832 (1.4%)	2.12	73/2507 (2.9%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	GLU	N-CA	7.40	1.55	1.46
1	B	98	GLY	N-CA	7.32	1.52	1.45
1	B	104	ILE	CA-C	6.99	1.61	1.52
1	B	105	ASN	N-CA	6.91	1.54	1.46
1	A	101	GLU	CA-CB	-6.86	1.46	1.53
1	B	71	THR	CA-CB	6.39	1.62	1.53
1	A	133	VAL	C-O	6.28	1.36	1.23
1	A	29	PHE	N-CA	5.92	1.53	1.46
1	B	78	ALA	C-O	5.84	1.31	1.24
1	A	57	THR	CA-C	5.83	1.59	1.52
1	A	81	ASN	CA-CB	-5.83	1.46	1.53
1	B	123	THR	CA-CB	5.62	1.62	1.53
1	A	84	ARG	N-CA	5.60	1.53	1.45
1	A	106	THR	CA-CB	5.51	1.63	1.53
1	A	74	GLY	CA-C	5.47	1.57	1.51
1	A	94	GLY	N-CA	5.46	1.52	1.45
1	B	29	PHE	N-CA	5.33	1.52	1.46
1	B	79	TRP	CA-CB	5.29	1.59	1.52
1	B	113	GLY	N-CA	5.28	1.53	1.45
1	A	113	GLY	N-CA	5.27	1.52	1.45
1	A	97	VAL	N-CA	5.26	1.53	1.46
1	A	56	LEU	N-CA	5.26	1.52	1.45
1	A	31	VAL	N-CA	5.23	1.52	1.46
1	A	123	THR	CA-CB	5.17	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	ARG	N-CA	5.14	1.52	1.45
1	B	18	THR	CA-CB	5.03	1.61	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	PHE	CA-CB-CG	13.97	127.77	113.80
1	A	53	ARG	CA-CB-CG	11.63	137.37	114.10
1	B	104	ILE	O-C-N	11.54	135.44	123.20
1	B	29	PHE	CA-CB-CG	11.18	124.98	113.80
1	A	80	LYS	CA-CB-CG	9.69	133.47	114.10
1	B	14	GLU	CA-CB-CG	9.23	132.56	114.10
1	A	133	VAL	CA-C-O	-8.70	106.00	120.80
1	B	104	ILE	CA-C-O	-8.17	111.89	120.39
1	B	84	ARG	CD-NE-CZ	-7.91	113.33	124.40
1	B	35	ALA	CA-C-N	7.83	136.84	121.58
1	B	35	ALA	C-N-CA	7.83	136.84	121.58
1	B	101	GLU	CB-CA-C	-7.75	101.01	112.09
1	B	128	ASP	CA-CB-CG	7.75	120.35	112.60
1	B	84	ARG	NE-CZ-NH1	-7.69	113.81	121.50
1	B	105	ASN	O-C-N	7.50	131.74	123.27
1	B	63	ALA	O-C-N	7.45	126.63	121.19
1	A	101	GLU	CA-CB-CG	7.22	128.54	114.10
1	A	57	THR	O-C-N	7.10	131.35	123.33
1	B	97	VAL	CA-C-N	-7.05	115.29	122.27
1	B	97	VAL	C-N-CA	-7.05	115.29	122.27
1	B	84	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	A	84	ARG	CD-NE-CZ	-6.86	114.80	124.40
1	A	91	THR	CA-C-O	-6.70	113.12	120.36
1	A	107	GLN	CA-CB-CG	-6.58	100.94	114.10
1	A	101	GLU	N-CA-CB	6.57	120.85	111.19
1	B	95	GLN	OE1-CD-NE2	-6.49	116.11	122.60
1	B	107	GLN	CA-CB-CG	-6.48	101.14	114.10
1	B	105	ASN	CA-C-O	-6.46	113.38	120.43
1	A	32	THR	CA-C-O	-6.42	113.43	120.36
1	A	17	ILE	N-CA-C	6.35	116.50	110.53
1	B	77	VAL	CA-C-O	-6.34	113.87	120.27
1	B	84	ARG	O-C-N	6.33	130.19	123.42
1	A	89	ALA	O-C-N	6.12	130.37	123.27
1	A	84	ARG	N-CA-CB	-6.11	101.46	111.66
1	B	75	TRP	O-C-N	6.08	129.93	123.42
1	B	30	ILE	CA-C-O	-6.05	113.72	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ALA	CA-C-O	-6.03	113.28	120.10
1	A	123	THR	N-CA-C	6.03	118.24	108.41
1	A	53	ARG	CD-NE-CZ	5.92	132.68	124.40
1	B	57	THR	CA-CB-OG1	-5.89	100.76	109.60
1	B	104	ILE	CA-C-N	-5.75	114.79	122.72
1	B	104	ILE	C-N-CA	-5.75	114.79	122.72
1	B	40	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	82	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	B	84	ARG	CA-CB-CG	5.72	125.53	114.10
1	B	116	GLU	CB-CG-CD	5.66	122.21	112.60
1	A	43	TYR	CA-C-N	-5.62	115.08	123.00
1	A	43	TYR	C-N-CA	-5.62	115.08	123.00
1	A	57	THR	CA-CB-CG2	5.49	119.83	110.50
1	B	88	SER	O-C-N	5.49	129.02	123.26
1	A	128	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	49	ASN	O-C-N	5.45	128.95	122.46
1	A	132	LYS	CG-CD-CE	5.45	123.83	111.30
1	A	57	THR	CA-C-O	-5.45	114.89	120.99
1	B	113	GLY	N-CA-C	-5.45	101.56	111.15
1	B	36	ASP	OD1-CG-OD2	-5.43	109.86	122.90
1	B	98	GLY	O-C-N	5.43	128.03	122.88
1	B	29	PHE	O-C-N	5.31	130.13	123.12
1	A	89	ALA	CA-C-O	-5.30	114.92	121.06
1	A	85	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	104	ILE	O-C-N	5.24	128.75	123.20
1	A	93	SER	CA-C-N	-5.20	114.17	120.51
1	A	93	SER	C-N-CA	-5.20	114.17	120.51
1	B	123	THR	N-CA-C	5.20	116.87	108.34
1	A	103	ARG	N-CA-CB	-5.16	103.04	111.66
1	A	49	ASN	CA-CB-CG	-5.14	107.46	112.60
1	B	115	THR	N-CA-C	-5.14	103.90	110.53
1	B	107	GLN	N-CA-C	-5.13	101.51	109.72
1	A	15	ALA	O-C-N	5.11	127.53	122.12
1	A	107	GLN	N-CA-C	-5.09	101.46	109.50
1	B	102	ALA	O-C-N	5.09	129.07	122.81
1	B	14	GLU	N-CA-CB	-5.05	101.96	110.49
1	B	78	ALA	N-CA-C	-5.03	101.12	109.46

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	883	0	825	54	1
1	B	901	0	839	69	0
2	A	20	0	13	22	0
2	B	20	0	13	24	0
3	A	69	0	0	1	0
3	B	65	0	0	4	0
All	All	1958	0	1690	120	1

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 34.

All (120) 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:50:ALA:HB2	2:B:300:DMB:CM3	1.51	1.39
1:B:103:ARG:NH1	1:B:131:THR:HG22	1.44	1.28
1:A:50:ALA:CB	2:B:300:DMB:HM32	1.64	1.25
2:A:300:DMB:CM3	1:B:50:ALA:HB2	1.74	1.18
2:A:300:DMB:HM33	1:B:50:ALA:HB2	1.26	1.14
1:B:103:ARG:HH12	1:B:131:THR:CG2	1.63	1.10
1:A:28:THR:HB	1:A:44:GLU:CG	1.83	1.09
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.20	1.06
2:A:300:DMB:H6'	1:B:110:LEU:HD21	1.37	1.06
1:A:13:ALA:O	1:A:16:GLY:N	1.90	1.04
1:B:51:GLU:HG2	1:B:84:ARG:HD2	1.37	1.03
1:B:14:GLU:HA	1:B:33:ALA:HB3	1.36	1.03
1:B:13:ALA:O	1:B:17:ILE:N	1.93	1.02
1:A:28:THR:HB	1:A:44:GLU:HG3	1.41	1.00
1:B:14:GLU:HA	1:B:33:ALA:CB	1.96	0.94
2:A:300:DMB:H6'	1:B:110:LEU:CD2	1.98	0.93
1:A:95:GLN:HE22	1:B:114:THR:H	1.14	0.92
1:B:14:GLU:HG3	1:B:33:ALA:O	1.68	0.91
1:B:120:TRP:CE2	1:B:121:LYS:HD2	2.06	0.90
1:A:28:THR:HB	1:A:44:GLU:HG2	1.54	0.90
1:A:114:THR:H	1:B:95:GLN:HE22	1.19	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:HH11	1:B:103:ARG:CG	1.86	0.87
2:A:300:DMB:HM32	1:B:50:ALA:HB2	1.60	0.83
1:A:22:TYR:HE2	1:A:133:VAL:HG21	1.45	0.80
1:B:51:GLU:HB3	1:B:84:ARG:NH1	1.98	0.79
1:B:51:GLU:HG2	1:B:84:ARG:CD	2.13	0.77
1:A:101:GLU:HB2	1:A:103:ARG:NH2	1.99	0.77
1:A:22:TYR:CE2	1:A:133:VAL:HG21	2.21	0.76
1:A:108:TRP:NE1	2:B:300:DMB:H4	2.02	0.74
1:A:79:TRP:CE3	2:B:300:DMB:HM33	2.23	0.73
2:A:300:DMB:OXT	1:B:45:SER:OG	2.03	0.73
1:A:108:TRP:CE2	2:B:300:DMB:H5	2.24	0.72
1:A:108:TRP:CZ2	2:B:300:DMB:H5	2.25	0.72
2:A:300:DMB:O4'	1:B:86:ALA:CB	2.40	0.70
1:A:50:ALA:CB	2:B:300:DMB:CM3	2.42	0.70
1:B:103:ARG:HH12	1:B:131:THR:HG22	0.69	0.69
1:B:13:ALA:O	1:B:14:GLU:C	2.34	0.69
1:B:103:ARG:NH1	1:B:131:THR:CG2	2.37	0.69
1:A:103:ARG:NH1	1:A:131:THR:HG23	2.08	0.69
2:A:300:DMB:C6'	1:B:110:LEU:HD21	2.20	0.68
1:B:13:ALA:O	1:B:16:GLY:N	2.27	0.67
1:A:51:GLU:CG	1:A:84:ARG:HH21	2.06	0.67
1:B:103:ARG:NH2	1:B:129:THR:HG21	2.09	0.67
1:B:51:GLU:O	1:B:52:SER:HB3	1.94	0.67
1:A:108:TRP:CH2	2:B:300:DMB:H5	2.31	0.66
2:A:300:DMB:H5	1:B:108:TRP:CD2	2.31	0.66
1:A:108:TRP:CE2	2:B:300:DMB:H4	2.30	0.66
2:A:300:DMB:H4	1:B:108:TRP:NE1	2.11	0.65
1:A:88:SER:OG	2:B:300:DMB:HM53	1.96	0.65
1:B:53:ARG:HD3	3:B:703:HOH:O	1.96	0.65
1:B:103:ARG:NH2	1:B:129:THR:CG2	2.60	0.64
1:A:13:ALA:O	1:A:16:GLY:CA	2.44	0.64
1:A:110:LEU:HD21	2:B:300:DMB:H6'	1.79	0.64
1:B:51:GLU:CB	1:B:84:ARG:NH1	2.61	0.64
1:A:28:THR:CB	1:A:44:GLU:HG3	2.23	0.63
2:A:300:DMB:HM32	1:B:49:ASN:C	2.24	0.62
1:A:51:GLU:OE2	1:A:84:ARG:NH2	2.31	0.62
1:B:51:GLU:CG	1:B:84:ARG:NH1	2.63	0.62
1:B:103:ARG:NH1	1:B:103:ARG:HG2	2.00	0.61
1:A:51:GLU:HG2	1:A:84:ARG:HH21	1.65	0.60
1:A:79:TRP:CE3	2:B:300:DMB:CM3	2.85	0.60
1:A:108:TRP:CE2	2:B:300:DMB:C5	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:NH1	1:B:103:ARG:CG	2.53	0.59
1:A:86:ALA:CB	2:B:300:DMB:O4'	2.52	0.57
1:A:108:TRP:CE2	2:B:300:DMB:C4	2.88	0.56
1:B:14:GLU:OE1	1:B:35:ALA:HA	2.05	0.56
1:B:51:GLU:HG2	1:B:84:ARG:NH1	2.21	0.56
1:B:51:GLU:O	1:B:52:SER:CB	2.54	0.56
1:A:50:ALA:HB2	2:B:300:DMB:HM32	0.68	0.56
1:B:14:GLU:CA	1:B:33:ALA:HB3	2.22	0.56
1:B:51:GLU:HB3	1:B:84:ARG:HH12	1.71	0.55
1:A:101:GLU:HB2	1:A:103:ARG:HH22	1.71	0.55
1:B:14:GLU:HB2	3:B:660:HOH:O	2.05	0.55
1:B:120:TRP:CZ2	1:B:121:LYS:HD2	2.42	0.55
2:A:300:DMB:HM32	1:B:50:ALA:CB	2.36	0.54
1:A:108:TRP:CD2	2:B:300:DMB:H5	2.44	0.53
1:A:18:THR:HG23	1:A:32:THR:HA	1.90	0.52
1:A:28:THR:O	1:A:44:GLU:HG2	2.08	0.52
1:A:51:GLU:O	1:A:52[A]:SER:HB3	2.09	0.52
1:A:108:TRP:CZ3	2:B:300:DMB:H5	2.45	0.52
1:A:114:THR:H	1:B:95:GLN:NE2	1.98	0.51
2:A:300:DMB:HM52	1:B:110:LEU:HD11	1.92	0.51
1:A:13:ALA:O	1:A:14:GLU:C	2.54	0.51
2:A:300:DMB:H4	1:B:108:TRP:CD1	2.46	0.50
1:B:51:GLU:OE2	1:B:84:ARG:CZ	2.59	0.50
1:A:108:TRP:CZ2	2:B:300:DMB:C5	2.92	0.50
1:A:13:ALA:C	1:A:16:GLY:H	2.17	0.50
2:A:300:DMB:HM52	1:B:88:SER:OG	2.12	0.49
1:B:14:GLU:CD	1:B:35:ALA:HA	2.37	0.49
2:A:300:DMB:H4	1:B:108:TRP:CE2	2.47	0.49
1:B:101:GLU:CG	1:B:101:GLU:O	2.59	0.49
2:A:300:DMB:H5	1:B:108:TRP:CE3	2.48	0.48
1:A:110:LEU:CD2	2:B:300:DMB:H6'	2.43	0.48
1:A:51:GLU:CD	1:A:84:ARG:HH21	2.20	0.48
1:B:103:ARG:NH1	1:B:103:ARG:CB	2.76	0.48
1:A:13:ALA:C	1:A:15:ALA:N	2.70	0.47
1:A:21:TRP:CZ2	1:A:132:LYS:HD3	2.49	0.47
2:A:300:DMB:H5	1:B:108:TRP:CE2	2.50	0.47
1:A:86:ALA:HB3	2:B:300:DMB:O4'	2.15	0.47
1:A:84:ARG:HG2	3:A:650:HOH:O	2.15	0.46
1:B:103:ARG:HH11	1:B:103:ARG:CB	2.29	0.45
2:A:300:DMB:C4	1:B:108:TRP:CE2	3.00	0.45
1:A:108:TRP:CE3	2:B:300:DMB:H5	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:TRP:CZ3	2:B:300:DMB:HM33	2.52	0.44
2:A:300:DMB:C5	1:B:108:TRP:CE2	3.01	0.44
1:B:76:THR:HG22	1:B:77:VAL:N	2.33	0.44
1:B:13:ALA:HB2	3:B:697:HOH:O	2.17	0.43
1:A:51:GLU:CG	1:A:84:ARG:NH2	2.78	0.43
2:A:300:DMB:HO4'	1:B:86:ALA:CB	2.31	0.43
1:A:51:GLU:HB3	1:A:84:ARG:NH2	2.33	0.43
2:A:300:DMB:CM3	1:B:50:ALA:CB	2.68	0.43
1:B:13:ALA:CB	3:B:697:HOH:O	2.67	0.43
1:B:103:ARG:NH2	1:B:129:THR:HG22	2.33	0.43
1:A:88:SER:OG	2:B:300:DMB:CM5	2.66	0.42
1:B:14:GLU:HA	1:B:33:ALA:HB1	1.89	0.42
1:B:120:TRP:NE1	1:B:121:LYS:HD2	2.32	0.42
1:B:103:ARG:NH1	1:B:103:ARG:HB3	2.35	0.41
1:A:101:GLU:CD	1:A:103:ARG:HH21	2.28	0.41
1:B:14:GLU:O	1:B:15:ALA:C	2.63	0.41
1:A:23:ASN:HB3	1:A:130:PHE:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:OH	1:A:22:TYR:OH[3_655]	1.87	0.33

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	115/121 (95%)	111 (96%)	4 (4%)	0	100	100
1	B	119/121 (98%)	114 (96%)	4 (3%)	1 (1%)	16	4
All	All	234/242 (97%)	225 (96%)	8 (3%)	1 (0%)	30	15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	SER

5.3.2 Protein sidechains [i](#)

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	87/88 (99%)	78 (90%)	9 (10%)	7	1
1	B	88/88 (100%)	85 (97%)	3 (3%)	32	10
All	All	175/176 (99%)	163 (93%)	12 (7%)	14	2

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	51	GLU
1	A	53	ARG
1	A	73	LEU
1	A	80	LYS
1	A	84	ARG
1	A	101	GLU
1	A	103	ARG
1	A	121	LYS
1	B	101	GLU
1	B	103	ARG
1	B	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	B	49	ASN
1	B	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	DMB	A	300	-	21,21,21	2.22	4 (19%)	29,29,29	1.42	3 (10%)
2	DMB	B	300	-	21,21,21	2.22	5 (23%)	29,29,29	1.39	7 (24%)

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	DMB	A	300	-	-	3/9/9/9	0/2/2/2
2	DMB	B	300	-	-	2/9/9/9	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	DMB	O-C	7.38	1.43	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	DMB	O-C	7.24	1.43	1.22
2	B	300	DMB	C1-N1	3.77	1.50	1.42
2	A	300	DMB	OXT-C	-3.55	1.20	1.30
2	A	300	DMB	C1-N1	3.25	1.49	1.42
2	B	300	DMB	OXT-C	-2.97	1.21	1.30
2	A	300	DMB	O4'-C4'	2.94	1.43	1.36
2	B	300	DMB	O4'-C4'	2.85	1.43	1.36
2	B	300	DMB	C2-C	2.04	1.54	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	DMB	OXT-C-C2	3.78	126.03	115.28
2	A	300	DMB	O-C-C2	-3.38	113.91	121.97
2	B	300	DMB	C2'-C3'-C4'	3.07	120.47	118.08
2	B	300	DMB	O-C-C2	-2.71	115.50	121.97
2	B	300	DMB	C1'-C2'-C3'	-2.63	119.08	121.54
2	B	300	DMB	OXT-C-C2	2.47	122.30	115.28
2	A	300	DMB	C2'-C3'-C4'	2.33	119.90	118.08
2	B	300	DMB	C2-C1-N1	2.07	121.60	117.50
2	B	300	DMB	C5'-C4'-C3'	-2.07	120.27	121.70
2	B	300	DMB	C1-N1-N1'	-2.04	110.03	114.51

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	DMB	C1-N1-N1'-C1'
2	A	300	DMB	C6'-C1'-N1'-N1
2	A	300	DMB	C2'-C1'-N1'-N1
2	B	300	DMB	C6'-C1'-N1'-N1
2	B	300	DMB	C2'-C1'-N1'-N1

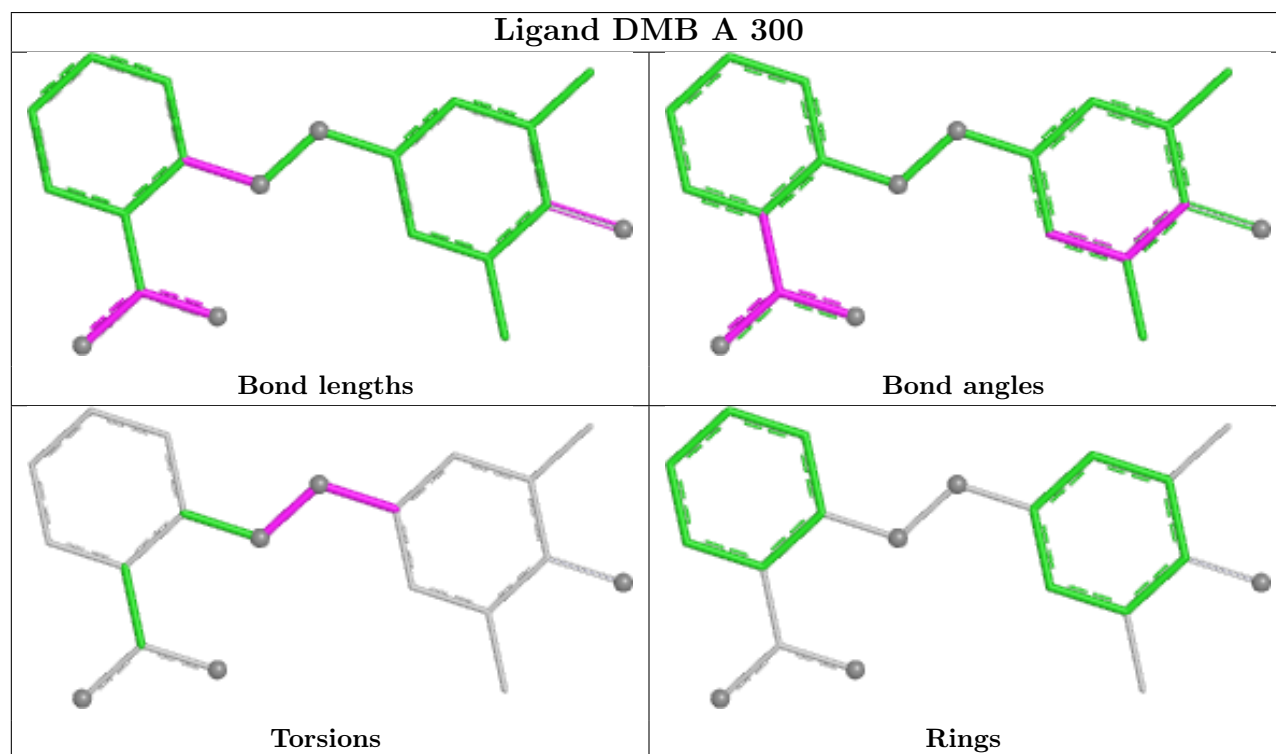
There are no ring outliers.

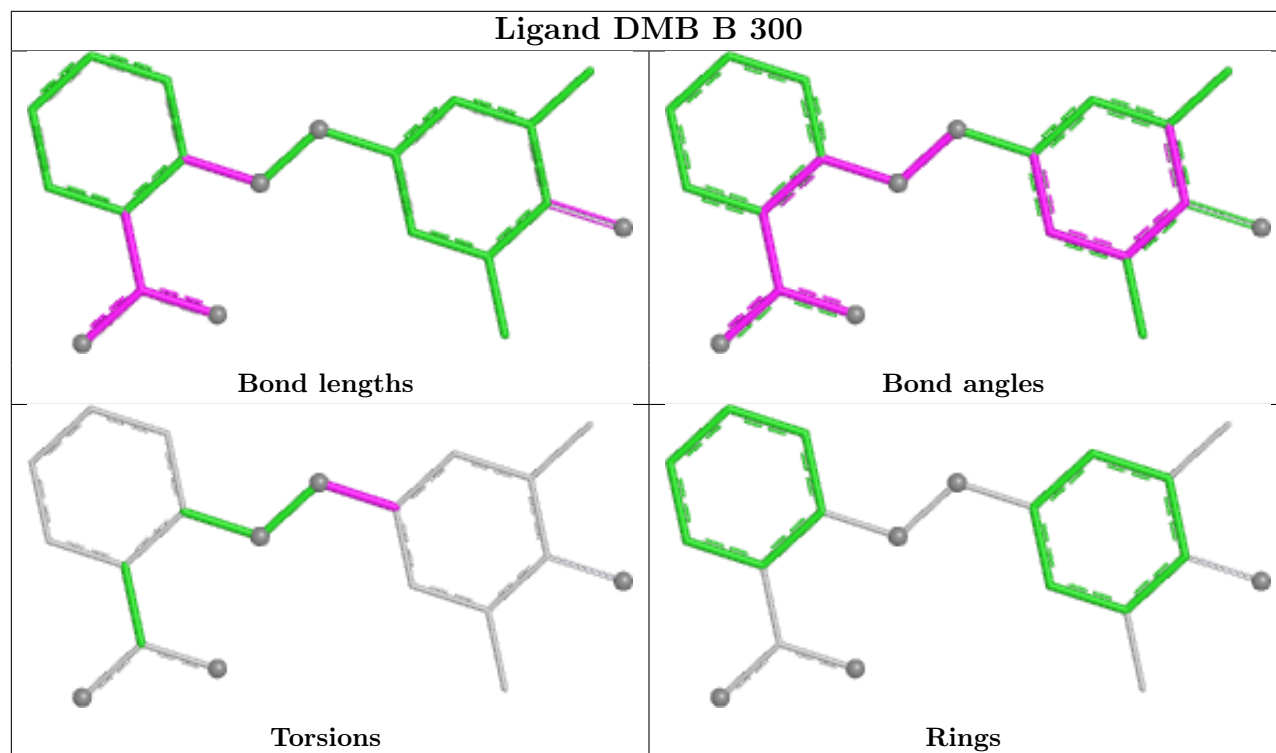
2 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	DMB	22	0
2	B	300	DMB	24	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.