



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 01:49 PM EDT

PDB ID : 3VW2 / pdb_00003vw2
Title : Crystal Structure of The Berberine-bound Form of RamR (Transcriptional Regulator of TetR Family) from Salmonella Typhimurium
Authors : Sakurai, K.; Nikaido, E.; Nakashima, R.; Yamasaki, S.; Yamaguchi, A.; Nishino, K.
Deposited on : 2012-07-30
Resolution : 2.34 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

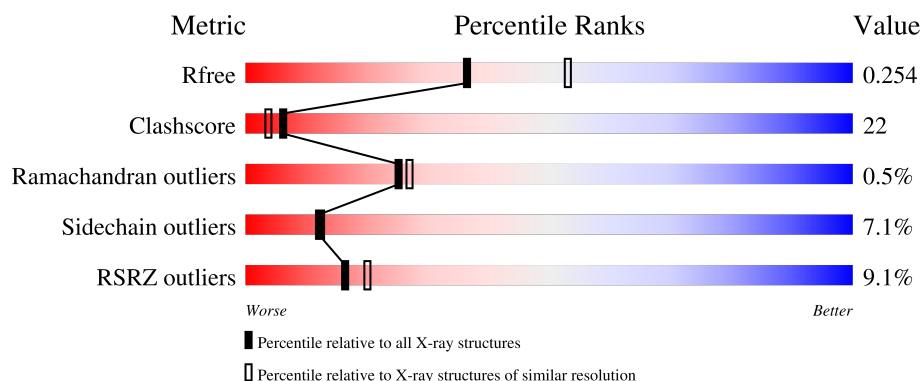
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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))
R_{free}	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	194	<div> <div>6%</div> <div>65%</div> <div>26%</div> <div>• 5%</div> </div>
1	B	194	<div> <div>16%</div> <div>56%</div> <div>35%</div> <div>• 5%</div> </div>
1	C	194	<div> <div>6%</div> <div>53%</div> <div>31%</div> <div>11%</div> <div>• 5%</div> </div>
1	D	194	<div> <div>7%</div> <div>56%</div> <div>35%</div> <div>• 6%</div> </div>

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	BER	A	301	-	X	-	-
2	BER	B	301	-	X	X	-
2	BER	D	301	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6032 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.

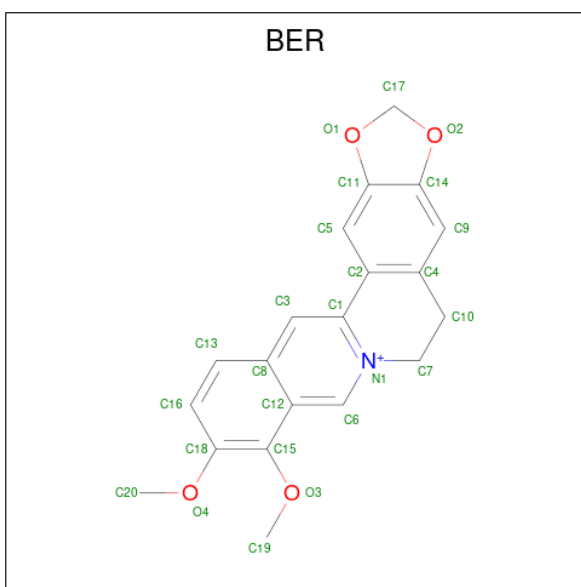
- Molecule 1 is a protein called Putative regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1462	922	258	271	11			
1	B	184	Total	C	N	O	S	0	0	0
			1462	922	258	271	11			
1	C	185	Total	C	N	O	S	0	0	0
			1468	926	259	272	11			
1	D	183	Total	C	N	O	S	0	0	0
			1453	917	257	268	11			

There are 8 discrepancies between the modelled and reference sequences:

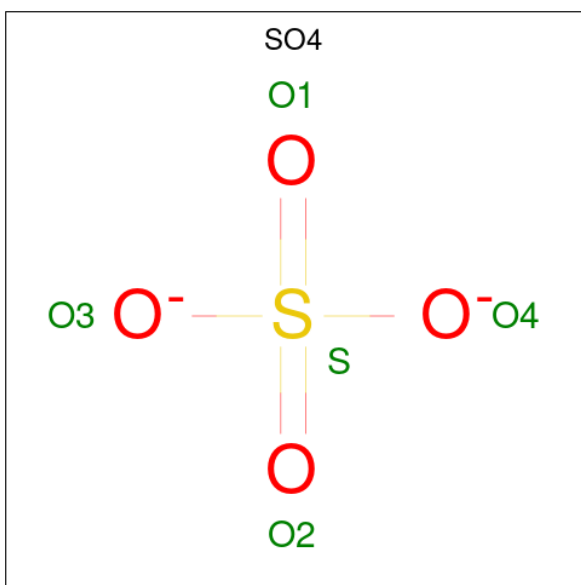
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP D0ZP76
A	1	VAL	-	expression tag	UNP D0ZP76
B	0	MET	-	expression tag	UNP D0ZP76
B	1	VAL	-	expression tag	UNP D0ZP76
C	0	MET	-	expression tag	UNP D0ZP76
C	1	VAL	-	expression tag	UNP D0ZP76
D	0	MET	-	expression tag	UNP D0ZP76
D	1	VAL	-	expression tag	UNP D0ZP76

- Molecule 2 is BERBERINE (CCD ID: BER) (formula: C₂₀H₁₈NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	20	1	4		
2	B	1	Total	C	N	O	0	0
			25	20	1	4		
2	C	1	Total	C	N	O	0	0
			25	20	1	4		
2	D	1	Total	C	N	O	0	0
			25	20	1	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

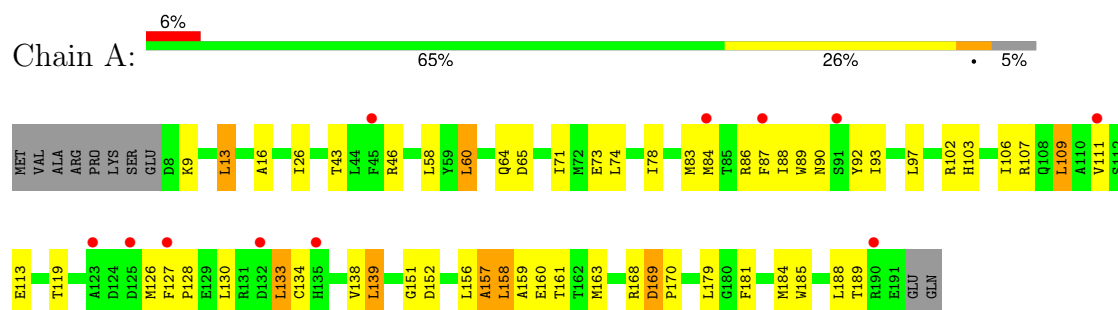
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	16	Total	O	0	0
			16	16		
4	C	16	Total	O	0	0
			16	16		
4	D	13	Total	O	0	0
			13	13		

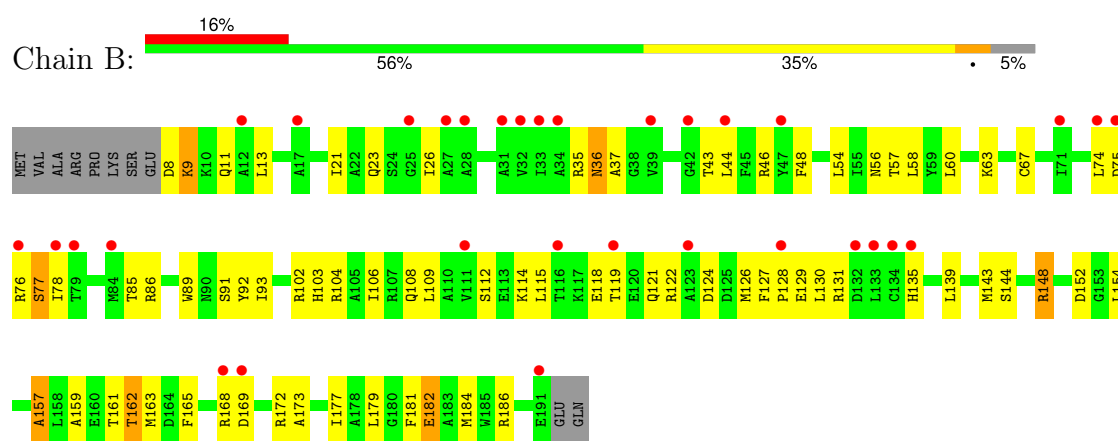
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

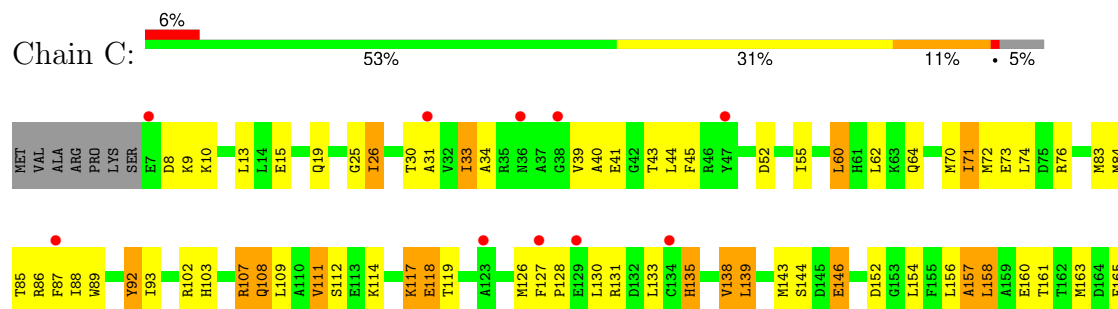
• Molecule 1: Putative regulatory protein

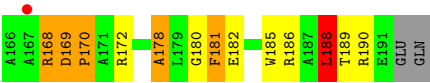


• Molecule 1: Putative regulatory protein

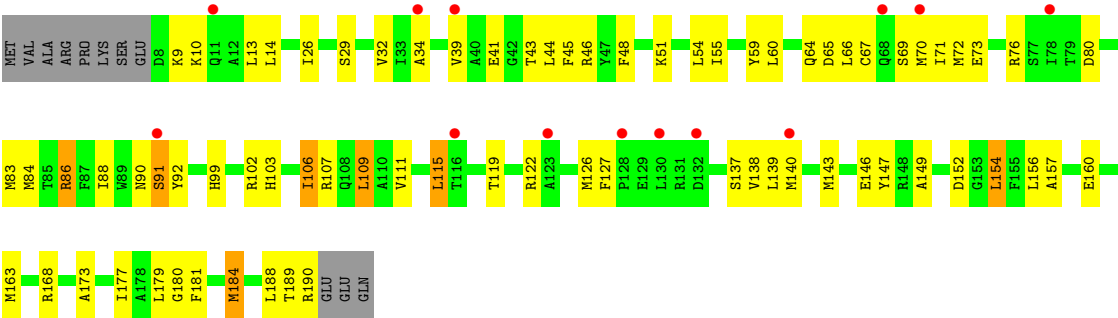


• Molecule 1: Putative regulatory protein





● Molecule 1: Putative regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.82Å 54.62Å 92.29Å 104.97° 97.74° 90.04°	Depositor
Resolution (Å)	41.29 – 2.34 41.29 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.6 (41.29-2.34) 94.8 (41.29-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.261 0.221 , 0.254	Depositor DCC
R_{free} test set	1693 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, BER

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	1.50	8/1488 (0.5%)	1.11	3/2006 (0.1%)
1	B	1.35	8/1488 (0.5%)	1.07	0/2006
1	C	1.52	15/1494 (1.0%)	1.19	4/2014 (0.2%)
1	D	1.31	4/1479 (0.3%)	1.15	1/1994 (0.1%)
All	All	1.42	35/5949 (0.6%)	1.13	8/8020 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	SER	N-CA	7.98	1.56	1.46
1	A	71	ILE	C-O	-7.67	1.15	1.24
1	C	178	ALA	CA-C	7.50	1.62	1.52
1	D	91	SER	N-CA	7.15	1.54	1.46
1	C	180	GLY	C-O	7.13	1.32	1.23
1	B	159	ALA	CA-CB	7.02	1.64	1.53
1	B	157	ALA	CA-CB	6.98	1.64	1.53
1	A	157	ALA	CA-CB	6.98	1.64	1.53
1	C	157	ALA	CA-CB	6.47	1.63	1.53
1	B	161	THR	CA-CB	6.42	1.63	1.53
1	A	158	LEU	C-O	-6.30	1.16	1.24
1	C	163	MET	CA-C	-6.12	1.44	1.52
1	B	154	LEU	N-CA	6.06	1.53	1.46
1	D	149	ALA	CA-CB	6.04	1.63	1.53
1	A	87	PHE	N-CA	6.01	1.53	1.46
1	D	154	LEU	N-CA	5.99	1.53	1.46
1	C	158	LEU	CA-C	5.97	1.60	1.52
1	C	111	VAL	CA-CB	5.64	1.61	1.54
1	C	71	ILE	C-O	-5.50	1.18	1.24
1	A	161	THR	N-CA	5.47	1.52	1.46
1	B	162	THR	CA-C	5.44	1.59	1.52
1	A	151	GLY	N-CA	5.39	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	ILE	CA-C	5.32	1.59	1.52
1	C	92	TYR	N-CA	5.30	1.52	1.46
1	C	138	VAL	CA-CB	5.29	1.60	1.54
1	A	16	ALA	CA-C	5.23	1.59	1.52
1	D	180	GLY	C-O	5.22	1.30	1.23
1	C	181	PHE	C-O	-5.21	1.18	1.24
1	C	161	THR	N-CA	5.20	1.52	1.46
1	A	90	ASN	CA-C	-5.17	1.46	1.52
1	C	185	TRP	CA-C	5.16	1.59	1.52
1	C	180	GLY	CA-C	-5.09	1.46	1.52
1	C	154	LEU	C-O	-5.09	1.18	1.24
1	C	189	THR	N-CA	5.05	1.51	1.45
1	B	182	GLU	CA-C	5.05	1.59	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	ASP	CA-C-N	7.76	128.17	119.32
1	C	169	ASP	C-N-CA	7.76	128.17	119.32
1	A	169	ASP	CA-C-N	5.83	125.69	119.28
1	A	169	ASP	C-N-CA	5.83	125.69	119.28
1	A	73	GLU	N-CA-C	-5.54	106.35	114.39
1	D	73	GLU	N-CA-C	-5.48	106.31	114.64
1	C	143	MET	N-CA-C	-5.34	107.13	113.97
1	C	188	LEU	N-CA-C	5.26	119.86	113.38

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	1462	0	1450	44	0
1	B	1462	0	1450	65	0
1	C	1468	0	1454	74	0
1	D	1453	0	1444	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	18	5	0
2	B	25	0	18	9	0
2	C	25	0	18	3	0
2	D	25	0	18	11	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	22	0	0	1	0
4	B	16	0	0	4	0
4	C	16	0	0	3	0
4	D	13	0	0	1	0
All	All	6032	0	5870	260	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 22.

All (260) 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)
2:D:301:BER:C19	2:D:301:BER:H61	1.61	1.27
1:B:75:ASP:HB3	1:B:78:ILE:HD11	1.17	1.16
2:D:301:BER:H193	2:D:301:BER:C6	1.72	1.15
2:B:301:BER:C19	2:B:301:BER:H61	1.75	1.14
2:B:301:BER:H61	2:B:301:BER:H193	1.28	1.08
2:A:301:BER:O4	2:A:301:BER:H192	1.53	1.07
2:B:301:BER:H193	2:B:301:BER:C6	1.86	1.02
1:D:60:LEU:HD21	1:D:119:THR:HG23	1.40	1.02
1:C:33:ILE:HG12	1:C:33:ILE:O	1.58	1.01
2:D:301:BER:H61	2:D:301:BER:H193	1.04	1.01
2:B:301:BER:O3	2:B:301:BER:H203	1.63	0.97
1:B:60:LEU:HD11	1:B:119:THR:HG23	1.44	0.95
1:B:118:GLU:HB3	4:B:405:HOH:O	1.64	0.95
1:D:60:LEU:CD2	1:D:119:THR:HG23	2.00	0.91
1:A:92:TYR:OH	1:A:103:HIS:CD2	2.24	0.91
2:D:301:BER:C19	2:D:301:BER:C6	2.30	0.90
2:B:301:BER:C19	2:B:301:BER:C6	2.43	0.90
1:D:86:ARG:HH12	1:D:90:ASN:HD21	1.17	0.89
1:D:86:ARG:NH1	1:D:90:ASN:HD21	1.72	0.88
1:C:165:PHE:CZ	1:D:111:VAL:HG21	2.09	0.86
1:A:92:TYR:OH	1:A:103:HIS:HD2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:MET:HE3	1:D:188:LEU:HD12	1.58	0.84
2:D:301:BER:H61	2:D:301:BER:H192	1.60	0.83
1:C:168:ARG:NH2	1:D:111:VAL:HG22	1.92	0.83
1:D:115:LEU:HD12	1:D:115:LEU:H	1.43	0.83
1:D:13:LEU:HD21	1:D:44:LEU:HA	1.61	0.82
1:D:106:ILE:HD12	2:D:301:BER:H201	1.60	0.82
1:D:86:ARG:HG3	1:D:86:ARG:HH11	1.45	0.82
2:B:301:BER:O3	2:B:301:BER:C20	2.30	0.80
1:C:70:MET:HE1	1:C:130:LEU:HD22	1.63	0.80
2:A:301:BER:O4	2:A:301:BER:C19	2.30	0.80
1:D:106:ILE:CD1	2:D:301:BER:H201	2.12	0.79
1:C:92:TYR:OH	1:C:103:HIS:CD2	2.35	0.79
1:D:184:MET:O	1:D:184:MET:HE2	1.83	0.79
2:B:301:BER:H61	2:B:301:BER:H192	1.63	0.79
1:D:70:MET:HG2	1:D:91:SER:HB3	1.65	0.78
1:B:43:THR:O	1:B:46:ARG:HG3	1.84	0.78
1:B:9:LYS:H	1:B:9:LYS:HD3	1.47	0.77
1:C:13:LEU:HD21	1:C:44:LEU:HA	1.66	0.77
1:D:29:SER:OG	1:D:32:VAL:HG23	1.85	0.77
1:B:60:LEU:CD1	1:B:119:THR:HG23	2.15	0.75
1:D:106:ILE:HD13	1:D:106:ILE:O	1.85	0.74
1:D:76:ARG:HB2	4:D:408:HOH:O	1.87	0.74
1:C:55:ILE:HG23	1:C:109:LEU:HD22	1.69	0.73
1:C:84:MET:O	1:C:88:ILE:HG12	1.88	0.73
1:A:134:CYS:O	1:A:138:VAL:HG23	1.87	0.73
1:A:60:LEU:HD13	1:A:119:THR:HG23	1.69	0.73
1:D:92:TYR:OH	1:D:103:HIS:HD2	1.73	0.72
1:C:172:ARG:HE	1:D:146:GLU:CD	1.99	0.70
1:C:128:PRO:HB3	1:C:131:ARG:NH2	2.06	0.70
1:D:99:HIS:HB3	1:D:102:ARG:HG3	1.73	0.70
1:D:138:VAL:HB	1:D:143:MET:HE1	1.74	0.70
1:C:152:ASP:OD1	2:C:301:BER:H61	1.93	0.68
1:D:71:ILE:HD11	1:D:127:PHE:CD2	2.29	0.68
1:A:88:ILE:HD13	1:A:130:LEU:HD13	1.76	0.67
1:D:92:TYR:HE2	1:D:163:MET:HE1	1.60	0.66
1:D:106:ILE:HD12	2:D:301:BER:C20	2.25	0.66
1:C:92:TYR:OH	1:C:103:HIS:HD2	1.77	0.66
1:C:117:LYS:NZ	1:C:117:LYS:HB2	2.11	0.66
1:D:13:LEU:HD23	1:D:48:PHE:CE2	2.31	0.65
1:B:124:ASP:HB3	1:B:131:ARG:HD3	1.77	0.65
1:C:60:LEU:HD13	1:C:119:THR:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ARG:NH2	1:D:111:VAL:O	2.31	0.64
1:D:109:LEU:O	1:D:115:LEU:HD11	1.98	0.64
1:A:64:GLN:HB2	1:A:126:MET:HE1	1.80	0.63
1:C:139:LEU:HD13	1:C:190:ARG:HA	1.79	0.63
1:A:74:LEU:HD22	1:A:127:PHE:HZ	1.64	0.63
1:C:168:ARG:HH22	1:D:111:VAL:HG22	1.62	0.63
1:A:111:VAL:HG22	1:A:111:VAL:O	1.99	0.62
1:B:148:ARG:HG3	1:B:148:ARG:HH11	1.65	0.62
1:B:103:HIS:CG	1:B:163:MET:HE1	2.35	0.61
1:D:111:VAL:HG22	1:D:111:VAL:O	1.99	0.61
1:C:107:ARG:NH2	1:C:160:GLU:OE1	2.33	0.61
1:D:13:LEU:HD23	1:D:48:PHE:HE2	1.65	0.61
1:C:25:GLY:HA2	1:C:108:GLN:HG2	1.83	0.60
1:D:60:LEU:HD21	1:D:119:THR:CG2	2.24	0.60
1:C:118:GLU:CD	1:C:118:GLU:H	2.08	0.60
1:D:64:GLN:HB2	1:D:126:MET:HE1	1.83	0.60
1:D:106:ILE:HD13	1:D:106:ILE:C	2.26	0.60
1:D:122:ARG:O	1:D:126:MET:HG3	2.03	0.59
1:B:104:ARG:O	1:B:108:GLN:HG3	2.02	0.59
1:D:92:TYR:CE2	1:D:163:MET:HE1	2.36	0.59
1:C:30:THR:HG22	4:C:410:HOH:O	2.02	0.59
1:C:64:GLN:NE2	1:C:126:MET:HE2	2.18	0.59
1:A:152:ASP:OD1	2:A:301:BER:H61	2.03	0.59
1:B:148:ARG:HH11	1:B:148:ARG:CG	2.15	0.58
1:D:70:MET:HG2	1:D:91:SER:CB	2.33	0.58
1:D:66:LEU:HG	1:D:70:MET:HE2	1.84	0.58
1:B:48:PHE:CE1	1:B:57:THR:HG21	2.38	0.58
1:A:86:ARG:HD2	1:A:181:PHE:CD2	2.38	0.58
1:B:75:ASP:HB3	1:B:78:ILE:CD1	2.11	0.58
1:C:111:VAL:HG12	1:C:111:VAL:O	2.03	0.58
1:C:107:ARG:NH1	1:C:157:ALA:HA	2.19	0.57
1:A:156:LEU:HD11	2:A:301:BER:H193	1.86	0.57
1:A:127:PHE:CG	1:A:130:LEU:HB3	2.40	0.56
1:B:23:GLN:HG3	4:B:410:HOH:O	2.04	0.56
2:D:301:BER:C6	2:D:301:BER:H192	2.28	0.56
1:C:144:SER:HB2	1:C:146:GLU:OE2	2.06	0.56
1:C:31:ALA:O	1:C:34:ALA:HB3	2.06	0.55
1:B:54:LEU:HA	1:B:57:THR:HG22	1.88	0.55
1:C:139:LEU:CD1	1:C:190:ARG:HA	2.36	0.55
1:C:30:THR:HG21	1:C:45:PHE:HZ	1.72	0.55
1:C:102:ARG:HG3	3:C:302:SO4:O3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MET:CE	1:C:130:LEU:HD22	2.36	0.54
1:C:30:THR:HG21	1:C:45:PHE:CZ	2.43	0.54
1:B:56:ASN:O	1:B:60:LEU:HD13	2.07	0.54
1:D:86:ARG:HD2	1:D:181:PHE:CD2	2.43	0.54
1:C:13:LEU:HD13	1:C:39:VAL:HG21	1.89	0.54
1:D:54:LEU:HD23	1:D:54:LEU:C	2.32	0.54
1:A:111:VAL:HG23	1:B:165:PHE:CZ	2.44	0.53
1:D:84:MET:O	1:D:88:ILE:HG12	2.08	0.53
1:C:33:ILE:HD13	1:C:44:LEU:HD11	1.91	0.53
1:A:157:ALA:HB1	1:B:157:ALA:HB1	1.90	0.53
1:D:86:ARG:NH1	1:D:86:ARG:HG3	2.19	0.53
1:B:89:TRP:CD1	1:B:181:PHE:HB2	2.44	0.53
1:B:13:LEU:HD21	1:B:44:LEU:HA	1.90	0.52
1:B:121:GLN:HE22	1:D:10:LYS:NZ	2.07	0.52
1:B:35:ARG:C	1:B:37:ALA:H	2.18	0.52
1:A:60:LEU:CD1	1:A:119:THR:HG23	2.38	0.51
1:C:107:ARG:HD3	1:C:156:LEU:HB3	1.92	0.51
1:C:92:TYR:HH	1:C:103:HIS:CD2	2.28	0.51
1:A:78:ILE:CG2	1:A:83:MET:HG2	2.41	0.51
1:A:84:MET:HG2	1:A:133:LEU:HD11	1.93	0.51
1:C:146:GLU:CD	1:C:146:GLU:H	2.18	0.51
1:A:9:LYS:O	1:A:13:LEU:HD22	2.11	0.51
1:C:70:MET:HE1	1:C:130:LEU:CD2	2.38	0.50
1:C:117:LYS:HB2	1:C:117:LYS:HZ2	1.75	0.50
1:B:121:GLN:HE22	1:D:10:LYS:HZ2	1.59	0.50
1:B:76:ARG:O	1:B:77:SER:HB3	2.12	0.50
1:A:103:HIS:CD2	1:A:163:MET:HE1	2.46	0.50
1:C:152:ASP:HA	2:C:301:BER:H72	1.94	0.50
1:B:148:ARG:CG	1:B:148:ARG:NH1	2.74	0.50
1:B:56:ASN:OD1	1:B:115:LEU:HA	2.12	0.50
1:C:52:ASP:OD1	1:C:114:LYS:HD2	2.13	0.49
1:C:138:VAL:HG12	1:C:139:LEU:O	2.13	0.49
1:A:103:HIS:CE1	1:A:160:GLU:OE1	2.66	0.49
1:D:64:GLN:HB2	1:D:126:MET:CE	2.42	0.49
1:A:84:MET:HG3	4:A:413:HOH:O	2.11	0.49
1:D:184:MET:CE	1:D:188:LEU:HB2	2.42	0.49
1:D:67:CYS:SG	1:D:127:PHE:HB2	2.53	0.49
1:B:182:GLU:HG3	1:B:186:ARG:NH1	2.28	0.49
1:C:30:THR:HG23	1:C:41:GLU:OE1	2.12	0.49
1:B:92:TYR:OH	1:B:103:HIS:HD2	1.95	0.49
1:A:78:ILE:HG23	1:A:83:MET:HG2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:C	1:A:170:PRO:HD3	2.38	0.48
1:B:168:ARG:HG3	1:B:169:ASP:N	2.27	0.48
1:B:26:ILE:HG21	1:B:112:SER:HB2	1.95	0.48
1:A:169:ASP:N	1:A:170:PRO:HD3	2.28	0.48
1:B:75:ASP:HA	4:B:413:HOH:O	2.13	0.48
1:D:9:LYS:HD3	1:D:39:VAL:CG1	2.44	0.48
1:C:182:GLU:HB3	1:C:186:ARG:NH1	2.28	0.48
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.79	0.47
1:B:85:THR:HG22	1:B:181:PHE:HE1	1.79	0.47
1:D:45:PHE:HA	1:D:48:PHE:O	2.14	0.47
1:A:92:TYR:HH	1:A:103:HIS:CD2	2.29	0.47
1:B:26:ILE:HD12	1:B:114:LYS:NZ	2.29	0.47
1:D:71:ILE:HG12	1:D:127:PHE:CE2	2.49	0.47
1:D:137:SER:N	1:D:190:ARG:HH21	2.13	0.47
1:B:152:ASP:HA	2:B:301:BER:H72	1.96	0.46
1:D:139:LEU:HD21	1:D:189:THR:O	2.15	0.46
2:A:301:BER:H31	2:A:301:BER:H51	1.69	0.46
1:C:182:GLU:HB3	1:C:186:ARG:HH12	1.81	0.46
1:A:126:MET:C	1:A:128:PRO:HD3	2.41	0.46
1:B:8:ASP:OD2	1:B:9:LYS:NZ	2.49	0.46
1:D:43:THR:O	1:D:46:ARG:HB3	2.16	0.46
1:A:84:MET:HE2	1:A:84:MET:HB2	1.71	0.46
1:A:89:TRP:CD1	1:A:181:PHE:HB2	2.51	0.46
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.80	0.45
1:B:173:ALA:O	1:B:177:ILE:HG13	2.16	0.45
1:C:83:MET:HG2	1:C:87:PHE:CE2	2.51	0.45
1:C:139:LEU:HD22	1:C:188:LEU:C	2.42	0.45
1:A:103:HIS:O	1:A:106:ILE:HG22	2.17	0.45
1:C:10:LYS:O	1:C:13:LEU:N	2.49	0.45
1:A:89:TRP:O	1:A:93:ILE:HG12	2.16	0.45
1:A:111:VAL:CG2	1:B:165:PHE:CZ	3.00	0.45
1:A:139:LEU:HD13	1:A:189:THR:O	2.16	0.45
1:D:146:GLU:HG2	1:D:147:TYR:CE2	2.52	0.45
1:B:21:ILE:HD13	1:B:109:LEU:HD11	1.98	0.45
1:D:9:LYS:HD3	1:D:39:VAL:HG11	1.99	0.45
1:C:40:ALA:HB3	1:C:43:THR:OG1	2.17	0.45
1:C:44:LEU:C	1:C:44:LEU:HD23	2.41	0.45
1:C:76:ARG:NH2	4:C:413:HOH:O	2.50	0.45
1:B:102:ARG:HG3	3:B:302:SO4:O4	2.17	0.45
1:B:127:PHE:C	1:B:129:GLU:H	2.24	0.45
1:D:184:MET:HE2	1:D:184:MET:C	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:O	1:B:57:THR:HG22	2.16	0.44
1:B:63:LYS:HE3	1:B:67:CYS:SG	2.57	0.44
1:B:74:LEU:HD11	1:B:127:PHE:HE1	1.82	0.44
1:C:74:LEU:HD12	1:C:84:MET:HE1	1.98	0.44
1:C:157:ALA:HB1	1:D:157:ALA:HB1	1.99	0.44
1:B:122:ARG:O	1:B:126:MET:HG3	2.17	0.44
1:B:163:MET:CE	4:B:407:HOH:O	2.65	0.44
1:C:86:ARG:HH21	1:C:178:ALA:HB1	1.83	0.44
1:D:86:ARG:HH12	1:D:90:ASN:ND2	1.99	0.44
1:D:65:ASP:OD2	1:D:102:ARG:NH1	2.51	0.44
1:A:113:GLU:CD	1:B:168:ARG:HE	2.25	0.44
1:C:111:VAL:O	1:C:111:VAL:CG1	2.65	0.44
1:B:127:PHE:CD2	1:B:130:LEU:HB2	2.52	0.44
1:B:135:HIS:HA	1:B:143:MET:HE1	2.00	0.44
1:C:71:ILE:C	1:C:73:GLU:H	2.26	0.44
1:D:107:ARG:HH21	1:D:160:GLU:CD	2.24	0.44
1:D:51:LYS:O	1:D:55:ILE:HG12	2.17	0.44
1:C:127:PHE:HD2	1:C:130:LEU:HB3	1.81	0.44
1:C:138:VAL:O	1:C:139:LEU:C	2.61	0.44
1:D:92:TYR:HE1	2:D:301:BER:H202	1.83	0.43
1:B:144:SER:O	1:B:148:ARG:HB2	2.18	0.43
1:C:86:ARG:HA	1:C:181:PHE:CE1	2.53	0.43
1:A:107:ARG:O	1:A:111:VAL:HG12	2.18	0.43
1:C:62:LEU:HD22	1:C:102:ARG:HB3	2.01	0.43
1:C:89:TRP:O	1:C:93:ILE:HG12	2.18	0.43
1:A:58:LEU:HD23	1:A:109:LEU:HD21	2.01	0.43
1:C:26:ILE:HD13	4:C:404:HOH:O	2.18	0.43
1:B:162:THR:HG21	1:B:177:ILE:HA	2.00	0.43
1:C:85:THR:HG22	1:C:181:PHE:HE1	1.84	0.43
1:A:159:ALA:O	1:A:163:MET:HG3	2.19	0.42
1:D:86:ARG:NH1	1:D:90:ASN:ND2	2.54	0.42
1:B:26:ILE:HG21	1:B:112:SER:CB	2.49	0.42
1:B:127:PHE:N	1:B:128:PRO:HD3	2.34	0.42
1:D:92:TYR:CE2	1:D:163:MET:CE	3.02	0.42
1:D:140:MET:HE3	1:D:190:ARG:NH1	2.34	0.42
1:C:83:MET:HG2	1:C:87:PHE:HE2	1.84	0.42
1:D:59:TYR:CD2	1:D:115:LEU:HD23	2.54	0.42
1:B:103:HIS:HA	1:B:106:ILE:HG22	2.01	0.42
1:C:33:ILE:O	1:C:33:ILE:CG1	2.46	0.42
1:B:57:THR:HG23	1:B:58:LEU:N	2.34	0.42
1:B:86:ARG:HA	1:B:181:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:HE3	1:B:184:MET:HB3	1.88	0.42
1:C:112:SER:C	1:C:114:LYS:H	2.28	0.42
1:C:127:PHE:CD2	1:C:130:LEU:HB3	2.54	0.42
1:C:139:LEU:HD13	1:C:190:ARG:CA	2.48	0.42
1:D:69:SER:HA	1:D:72:MET:HE3	2.01	0.42
1:A:159:ALA:C	1:A:163:MET:HE3	2.44	0.42
1:B:76:ARG:O	1:B:77:SER:CB	2.67	0.42
1:B:135:HIS:HA	1:B:143:MET:CE	2.49	0.42
1:B:169:ASP:OD2	1:B:172:ARG:NH1	2.51	0.42
1:D:59:TYR:HE1	1:D:106:ILE:HD11	1.84	0.42
1:D:173:ALA:O	1:D:177:ILE:HG13	2.20	0.42
1:A:65:ASP:OD2	1:A:102:ARG:NH1	2.48	0.41
1:D:34:ALA:CB	1:D:41:GLU:HA	2.50	0.41
1:B:35:ARG:HG3	1:B:36:ASN:OD1	2.19	0.41
1:B:152:ASP:HB3	2:B:301:BER:H192	2.01	0.41
1:D:106:ILE:CD1	1:D:106:ILE:C	2.92	0.41
1:B:43:THR:O	1:B:46:ARG:CG	2.62	0.41
1:C:84:MET:HG3	1:C:133:LEU:HD21	2.03	0.41
1:A:127:PHE:CE2	1:A:130:LEU:HB2	2.56	0.41
1:A:127:PHE:CD2	1:A:130:LEU:HD23	2.56	0.41
1:C:15:GLU:O	1:C:19:GLN:HG2	2.20	0.41
1:C:85:THR:HG21	2:C:301:BER:H172	2.03	0.41
1:D:80:ASP:HB3	1:D:83:MET:HE3	2.02	0.41
1:A:64:GLN:NE2	1:A:126:MET:HE2	2.36	0.41
1:C:131:ARG:HG3	1:C:135:HIS:CE1	2.56	0.41
1:A:185:TRP:CE3	1:A:189:THR:HG21	2.56	0.40
1:B:26:ILE:HD12	1:B:114:LYS:HZ2	1.87	0.40
1:B:54:LEU:CA	1:B:57:THR:HG22	2.51	0.40
1:A:184:MET:HB3	1:A:184:MET:HE3	1.90	0.40
1:B:60:LEU:HD11	1:B:119:THR:CG2	2.33	0.40
1:D:60:LEU:HD23	1:D:119:THR:HG23	1.95	0.40
1:D:152:ASP:CG	2:D:301:BER:C19	2.94	0.40
1:C:128:PRO:HB3	1:C:131:ARG:HH21	1.83	0.40
1:C:169:ASP:N	1:C:170:PRO:HD3	2.37	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	182/194 (94%)	178 (98%)	4 (2%)	0	100	100
1	B	182/194 (94%)	172 (94%)	8 (4%)	2 (1%)	12	10
1	C	183/194 (94%)	173 (94%)	8 (4%)	2 (1%)	12	10
1	D	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
All	All	728/776 (94%)	695 (96%)	29 (4%)	4 (0%)	25	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	SER
1	C	72	MET
1	C	135	HIS
1	B	36	ASN

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	149/158 (94%)	138 (93%)	11 (7%)	11	11
1	B	149/158 (94%)	144 (97%)	5 (3%)	32	41
1	C	149/158 (94%)	134 (90%)	15 (10%)	6	5
1	D	148/158 (94%)	137 (93%)	11 (7%)	11	11
All	All	595/632 (94%)	553 (93%)	42 (7%)	12	12

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	26	ILE
1	A	43	THR
1	A	60	LEU
1	A	97	LEU
1	A	109	LEU
1	A	133	LEU
1	A	139	LEU
1	A	158	LEU
1	A	179	LEU
1	A	188	LEU
1	B	9	LYS
1	B	11	GLN
1	B	139	LEU
1	B	148	ARG
1	B	179	LEU
1	C	8	ASP
1	C	9	LYS
1	C	26	ILE
1	C	33	ILE
1	C	60	LEU
1	C	107	ARG
1	C	108	GLN
1	C	117	LYS
1	C	118	GLU
1	C	139	LEU
1	C	146	GLU
1	C	158	LEU
1	C	168	ARG
1	C	170	PRO
1	C	188	LEU
1	D	14	LEU
1	D	26	ILE
1	D	86	ARG
1	D	106	ILE
1	D	109	LEU
1	D	115	LEU
1	D	154	LEU
1	D	156	LEU
1	D	168	ARG
1	D	179	LEU
1	D	184	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	64	GLN
1	A	90	ASN
1	A	98	ASN
1	A	103	HIS
1	A	108	GLN
1	A	121	GLN
1	B	11	GLN
1	B	19	GLN
1	B	61	HIS
1	B	68	GLN
1	B	90	ASN
1	B	99	HIS
1	B	103	HIS
1	B	121	GLN
1	C	61	HIS
1	C	64	GLN
1	C	99	HIS
1	C	103	HIS
1	D	90	ASN
1	D	99	HIS
1	D	103	HIS

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](#)

8 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
3	SO4	B	302	-	4,4,4	0.40	0	6,6,6	0.47	0
2	BER	C	301	-	29,29,29	4.53	16 (55%)	41,43,43	3.87	21 (51%)
3	SO4	C	302	-	4,4,4	0.27	0	6,6,6	0.48	0
2	BER	A	301	-	29,29,29	4.61	17 (58%)	41,43,43	4.61	22 (53%)
3	SO4	D	302	-	4,4,4	0.42	0	6,6,6	0.37	0
2	BER	D	301	-	29,29,29	4.63	17 (58%)	41,43,43	4.68	23 (56%)
3	SO4	A	302	-	4,4,4	0.28	0	6,6,6	0.58	0
2	BER	B	301	-	29,29,29	4.66	17 (58%)	41,43,43	5.09	20 (48%)

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	BER	C	301	-	-	0/4/19/19	0/5/5/5
2	BER	D	301	-	-	4/4/19/19	0/5/5/5
2	BER	A	301	-	-	1/4/19/19	0/5/5/5
2	BER	B	301	-	-	4/4/19/19	0/5/5/5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	BER	C10-C4	-16.09	1.36	1.50
2	D	301	BER	C10-C4	-15.69	1.37	1.50
2	A	301	BER	C10-C4	-15.04	1.37	1.50
2	C	301	BER	C10-C4	-12.76	1.39	1.50
2	A	301	BER	C7-C10	-9.43	1.37	1.51
2	D	301	BER	C7-C10	-8.84	1.38	1.51
2	B	301	BER	C7-C10	-8.80	1.38	1.51
2	C	301	BER	C18-C15	8.55	1.51	1.38
2	C	301	BER	C15-C12	8.10	1.60	1.43
2	D	301	BER	C7-N1	-7.94	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	BER	C7-N1	-7.89	1.33	1.48
2	B	301	BER	C7-N1	-7.86	1.33	1.48
2	C	301	BER	C3-C1	6.52	1.51	1.39
2	C	301	BER	C7-N1	-6.46	1.36	1.48
2	C	301	BER	C3-C8	6.34	1.51	1.39
2	A	301	BER	C18-C15	6.29	1.48	1.38
2	D	301	BER	C1-N1	-5.84	1.31	1.39
2	B	301	BER	C1-N1	-5.62	1.31	1.39
2	B	301	BER	C13-C8	-5.57	1.29	1.42
2	C	301	BER	C6-C12	5.53	1.51	1.40
2	C	301	BER	O3-C15	5.15	1.48	1.38
2	A	301	BER	C1-N1	-5.03	1.32	1.39
2	D	301	BER	C18-C15	5.02	1.46	1.38
2	D	301	BER	C13-C8	-4.89	1.31	1.42
2	B	301	BER	C16-C18	-4.78	1.29	1.39
2	A	301	BER	C13-C8	-4.77	1.31	1.42
2	B	301	BER	C3-C8	4.75	1.48	1.39
2	B	301	BER	C3-C1	4.75	1.48	1.39
2	D	301	BER	C6-C12	4.56	1.49	1.40
2	C	301	BER	C13-C16	4.54	1.46	1.36
2	D	301	BER	C3-C1	4.51	1.47	1.39
2	D	301	BER	C3-C8	4.45	1.47	1.39
2	D	301	BER	C16-C18	-4.42	1.30	1.39
2	A	301	BER	C6-C12	4.38	1.49	1.40
2	A	301	BER	C3-C1	4.30	1.47	1.39
2	A	301	BER	C3-C8	4.00	1.46	1.39
2	C	301	BER	C12-C8	3.88	1.50	1.43
2	A	301	BER	C13-C16	3.87	1.45	1.36
2	B	301	BER	C6-C12	3.78	1.47	1.40
2	B	301	BER	C18-C15	3.74	1.44	1.38
2	A	301	BER	O1-C11	-3.63	1.32	1.38
2	A	301	BER	O4-C18	3.61	1.43	1.37
2	C	301	BER	C2-C1	3.61	1.48	1.42
2	C	301	BER	O4-C18	3.54	1.42	1.37
2	C	301	BER	C4-C2	3.48	1.50	1.42
2	B	301	BER	O4-C18	3.38	1.42	1.37
2	D	301	BER	O4-C18	3.23	1.42	1.37
2	B	301	BER	C13-C16	3.21	1.43	1.36
2	A	301	BER	C16-C18	-3.16	1.33	1.39
2	A	301	BER	C15-C12	3.06	1.49	1.43
2	D	301	BER	C13-C16	3.01	1.43	1.36
2	D	301	BER	C5-C2	-2.98	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	BER	C12-C8	2.92	1.48	1.43
2	D	301	BER	C15-C12	2.86	1.49	1.43
2	B	301	BER	C5-C2	-2.84	1.36	1.42
2	C	301	BER	C14-C11	2.76	1.46	1.39
2	A	301	BER	C5-C2	-2.71	1.36	1.42
2	B	301	BER	O1-C11	-2.69	1.33	1.38
2	B	301	BER	O2-C14	-2.65	1.33	1.38
2	A	301	BER	O2-C14	-2.63	1.33	1.38
2	D	301	BER	O1-C11	-2.62	1.33	1.38
2	B	301	BER	C15-C12	2.61	1.48	1.43
2	C	301	BER	C1-N1	-2.59	1.35	1.39
2	D	301	BER	C12-C8	2.43	1.47	1.43
2	C	301	BER	C13-C8	-2.39	1.36	1.42
2	B	301	BER	C12-C8	2.39	1.47	1.43
2	D	301	BER	O2-C14	-2.36	1.34	1.38

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	BER	C6-C12-C15	-16.60	106.44	121.55
2	B	301	BER	C18-C15-C12	-15.86	103.34	119.86
2	D	301	BER	C18-C15-C12	-15.10	104.13	119.86
2	A	301	BER	C6-C12-C15	-14.61	108.25	121.55
2	A	301	BER	C18-C15-C12	-12.78	106.55	119.86
2	D	301	BER	C6-C12-C15	-11.66	110.94	121.55
2	C	301	BER	C6-C12-C15	-10.84	111.68	121.55
2	C	301	BER	C18-C15-C12	-10.82	108.58	119.86
2	B	301	BER	C10-C7-N1	10.81	124.54	109.75
2	D	301	BER	C10-C7-N1	10.77	124.47	109.75
2	B	301	BER	C8-C3-C1	-9.84	110.17	120.87
2	D	301	BER	C8-C3-C1	-9.75	110.27	120.87
2	A	301	BER	C8-C3-C1	-9.44	110.61	120.87
2	A	301	BER	C10-C7-N1	8.88	121.89	109.75
2	C	301	BER	C10-C7-N1	7.99	120.67	109.75
2	B	301	BER	O3-C15-C18	-7.63	103.76	121.19
2	A	301	BER	C7-C10-C4	7.56	119.91	109.95
2	A	301	BER	O3-C15-C12	-6.79	103.97	117.32
2	B	301	BER	C7-C10-C4	6.62	118.67	109.95
2	D	301	BER	C7-C10-C4	6.58	118.61	109.95
2	D	301	BER	O3-C15-C18	-6.53	106.26	121.19
2	C	301	BER	C7-N1-C1	6.52	124.87	117.95
2	D	301	BER	C15-C12-C8	-6.51	106.56	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	BER	C8-C3-C1	-6.46	113.84	120.87
2	A	301	BER	C3-C1-C2	-6.10	112.58	122.51
2	C	301	BER	C7-C10-C4	6.05	117.92	109.95
2	A	301	BER	O3-C15-C18	-5.72	108.11	121.19
2	C	301	BER	C7-N1-C6	-5.21	112.57	118.46
2	C	301	BER	C16-C18-C15	5.18	123.38	119.80
2	B	301	BER	C6-C12-C8	-5.14	111.83	117.59
2	B	301	BER	O3-C15-C12	-4.92	107.66	117.32
2	C	301	BER	C12-C6-N1	-4.82	119.01	121.81
2	D	301	BER	C3-C1-C2	-4.59	115.03	122.51
2	B	301	BER	C3-C8-C12	4.58	124.12	119.28
2	D	301	BER	C6-C12-C8	-4.49	112.56	117.59
2	A	301	BER	C7-N1-C1	4.43	122.65	117.95
2	D	301	BER	O3-C15-C12	-4.09	109.29	117.32
2	A	301	BER	C11-C5-C2	-4.03	113.67	120.59
2	B	301	BER	C15-C12-C8	-3.98	111.27	118.68
2	D	301	BER	C11-C5-C2	-3.88	113.92	120.59
2	C	301	BER	C3-C1-C2	-3.88	116.18	122.51
2	D	301	BER	C5-C2-C1	-3.84	117.33	120.80
2	D	301	BER	C14-C9-C4	-3.70	114.32	120.27
2	B	301	BER	C11-C5-C2	-3.66	114.31	120.59
2	B	301	BER	C7-N1-C6	-3.61	114.38	118.46
2	B	301	BER	C14-C9-C4	-3.60	114.48	120.27
2	A	301	BER	O4-C18-C16	-3.56	118.30	124.30
2	B	301	BER	C3-C1-C2	-3.56	116.71	122.51
2	A	301	BER	C15-C12-C8	-3.51	112.14	118.68
2	D	301	BER	C17-O2-C14	3.42	109.89	105.32
2	B	301	BER	C9-C4-C2	3.35	122.43	118.87
2	D	301	BER	C7-N1-C1	3.31	121.47	117.95
2	B	301	BER	C7-N1-C1	3.30	121.45	117.95
2	C	301	BER	O2-C17-O1	-3.12	103.20	108.09
2	B	301	BER	C13-C8-C3	-3.10	117.08	122.00
2	A	301	BER	C16-C18-C15	3.00	121.88	119.80
2	C	301	BER	C11-C5-C2	-2.92	115.57	120.59
2	A	301	BER	C20-O4-C18	-2.85	113.33	117.51
2	A	301	BER	O4-C18-C15	2.82	119.83	116.44
2	A	301	BER	C17-O1-C11	2.77	109.03	105.32
2	D	301	BER	C16-C13-C8	-2.76	116.71	120.84
2	A	301	BER	C14-C9-C4	-2.74	115.86	120.27
2	D	301	BER	C17-O1-C11	2.68	108.91	105.32
2	C	301	BER	C3-C8-C12	-2.65	116.48	119.28
2	C	301	BER	C14-C9-C4	-2.62	116.06	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	BER	C4-C2-C5	2.60	124.00	118.91
2	D	301	BER	C4-C2-C5	2.52	123.84	118.91
2	A	301	BER	C6-C12-C8	-2.51	114.78	117.59
2	C	301	BER	C17-O2-C14	2.49	108.65	105.32
2	B	301	BER	C17-O2-C14	2.48	108.64	105.32
2	D	301	BER	C3-C8-C12	2.46	121.89	119.28
2	B	301	BER	C17-O1-C11	2.46	108.61	105.32
2	A	301	BER	C7-N1-C6	-2.40	115.74	118.46
2	C	301	BER	C13-C8-C12	2.38	122.20	119.12
2	D	301	BER	O4-C18-C15	2.34	119.25	116.44
2	C	301	BER	C20-O4-C18	-2.26	114.19	117.51
2	C	301	BER	O3-C15-C12	-2.21	112.97	117.32
2	C	301	BER	C17-O1-C11	2.21	108.28	105.32
2	C	301	BER	O2-C14-C11	-2.21	107.12	109.79
2	A	301	BER	C13-C8-C3	-2.20	118.50	122.00
2	A	301	BER	C3-C8-C12	2.17	121.57	119.28
2	D	301	BER	C9-C4-C2	2.17	121.17	118.87
2	B	301	BER	C5-C2-C1	-2.15	118.85	120.80
2	C	301	BER	C19-O3-C15	2.09	120.53	114.88
2	D	301	BER	O2-C14-C11	-2.08	107.27	109.79
2	D	301	BER	C7-N1-C6	-2.01	116.19	118.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	BER	C18-C15-O3-C19
2	B	301	BER	C16-C18-O4-C20
2	D	301	BER	C12-C15-O3-C19
2	B	301	BER	C15-C18-O4-C20
2	D	301	BER	C15-C18-O4-C20
2	B	301	BER	C18-C15-O3-C19
2	D	301	BER	C16-C18-O4-C20
2	B	301	BER	C12-C15-O3-C19
2	A	301	BER	C12-C15-O3-C19

There are no ring outliers.

6 monomers are involved in 30 short contacts:

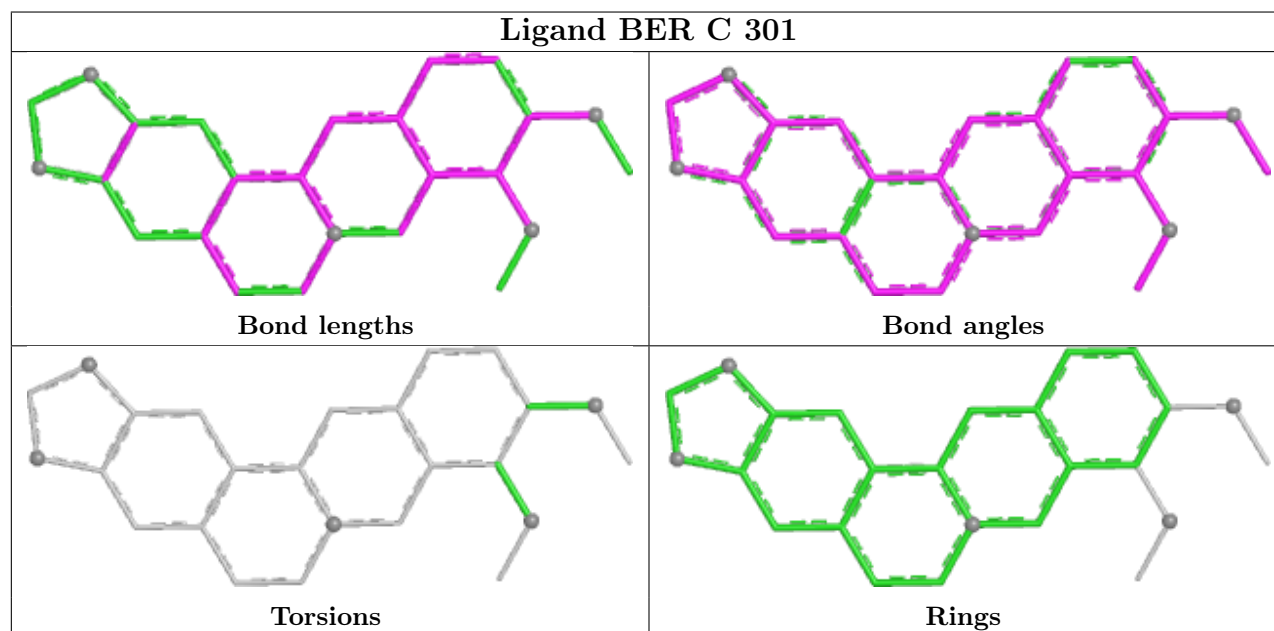
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	SO4	1	0

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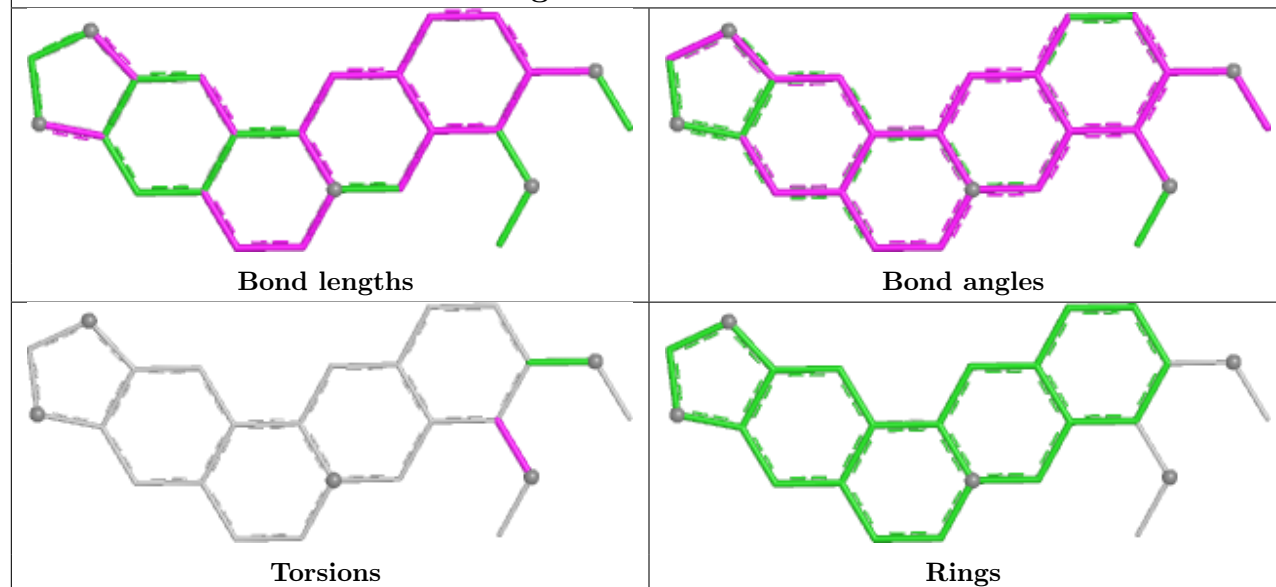
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	BER	3	0
3	C	302	SO4	1	0
2	A	301	BER	5	0
2	D	301	BER	11	0
2	B	301	BER	9	0

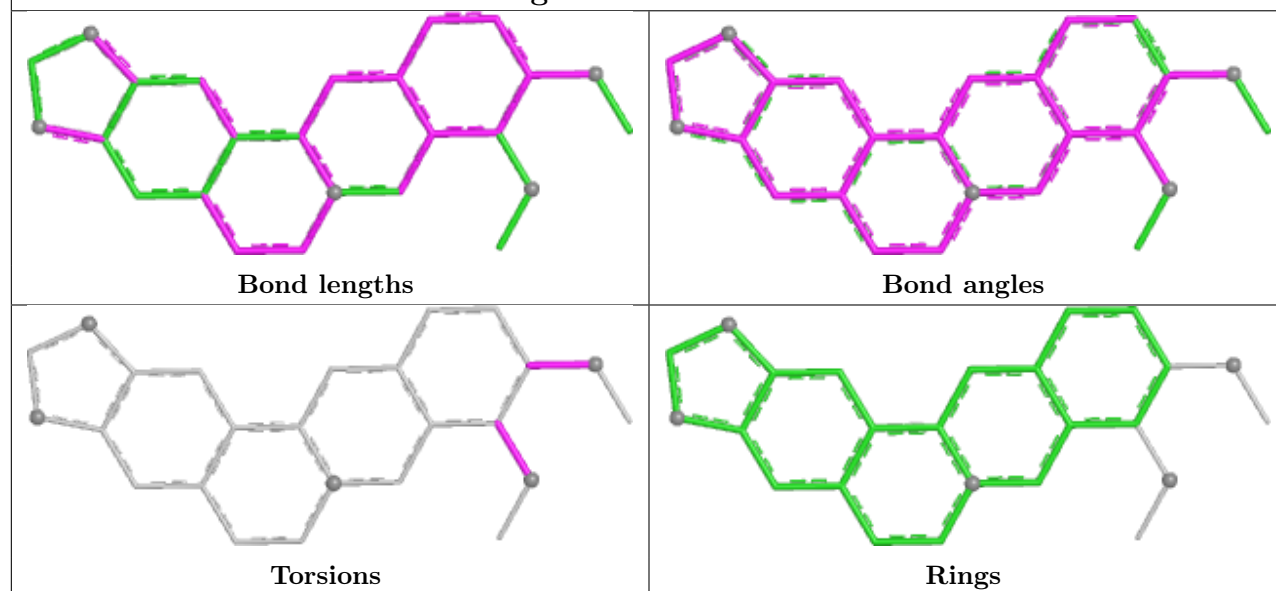
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

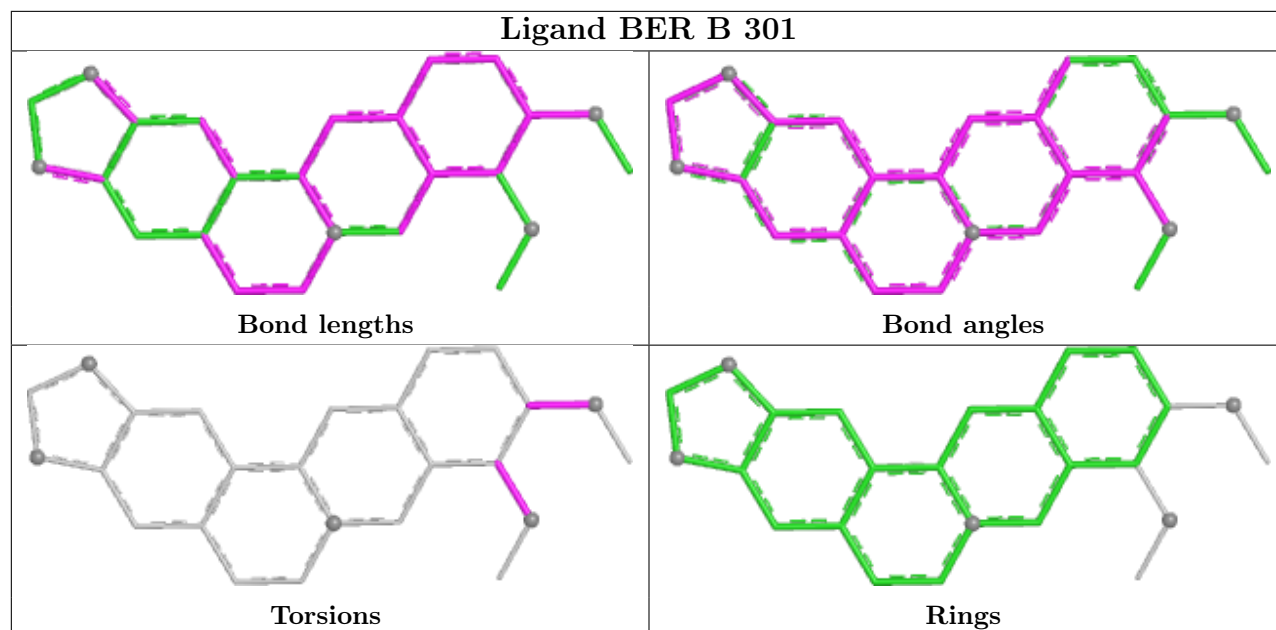


Ligand BER A 301



Ligand BER D 301





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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	184/194 (94%)	0.33	11 (5%) 29 35	21, 40, 69, 84	12 (6%)
1	B	184/194 (94%)	0.96	32 (17%) 5 6	23, 66, 101, 111	3 (1%)
1	C	185/194 (95%)	0.54	11 (5%) 29 36	23, 47, 78, 85	5 (2%)
1	D	183/194 (94%)	0.63	13 (7%) 23 29	24, 51, 86, 93	4 (2%)
All	All	736/776 (94%)	0.61	67 (9%) 16 20	21, 48, 90, 111	24 (3%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	ALA	6.5
1	D	34	ALA	4.4
1	B	39	VAL	4.3
1	B	32	VAL	3.7
1	D	130	LEU	3.6
1	D	70	MET	3.4
1	C	127	PHE	3.4
1	B	17	ALA	3.3
1	B	133	LEU	3.2
1	B	128	PRO	3.2
1	B	33	ILE	3.2
1	A	45	PHE	3.0
1	C	31	ALA	3.0
1	A	111	VAL	3.0
1	D	123	ALA	3.0
1	A	123	ALA	2.9
1	A	84	MET	2.8
1	D	132	ASP	2.8
1	C	129	GLU	2.8
1	A	135	HIS	2.7
1	B	119	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	PHE	2.7
1	C	7	GLU	2.6
1	C	123	ALA	2.5
1	C	47	TYR	2.5
1	A	190	ARG	2.5
1	B	74	LEU	2.5
1	A	87	PHE	2.5
1	C	36	ASN	2.5
1	B	25	GLY	2.4
1	B	78	ILE	2.4
1	B	27	ALA	2.4
1	B	31	ALA	2.4
1	D	91	SER	2.4
1	D	128	PRO	2.4
1	A	91	SER	2.3
1	D	11	GLN	2.3
1	B	28	ALA	2.3
1	A	125	ASP	2.3
1	B	111	VAL	2.3
1	B	132	ASP	2.3
1	B	168	ARG	2.3
1	D	39	VAL	2.2
1	B	44	LEU	2.2
1	B	42	GLY	2.2
1	B	71	ILE	2.2
1	B	84	MET	2.1
1	A	132	ASP	2.1
1	B	34	ALA	2.1
1	C	167	ALA	2.1
1	B	191	GLU	2.1
1	B	135	HIS	2.1
1	B	12	ALA	2.1
1	B	169	ASP	2.1
1	D	78	ILE	2.1
1	B	116	THR	2.1
1	D	116	THR	2.1
1	B	47	TYR	2.0
1	D	68	GLN	2.0
1	C	134	CYS	2.0
1	D	140	MET	2.0
1	B	76	ARG	2.0
1	B	79	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	75	ASP	2.0
1	C	38	GLY	2.0
1	C	87	PHE	2.0
1	B	134	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

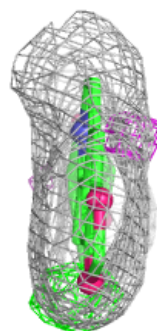
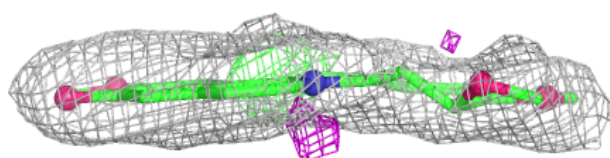
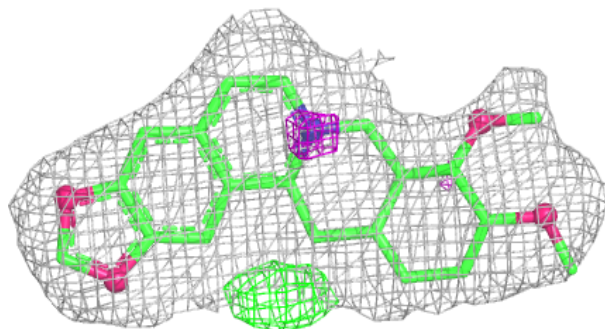
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BER	A	301	25/25	0.84	0.14	47,53,61,67	0
2	BER	C	301	25/25	0.85	0.13	45,49,54,58	0
2	BER	B	301	25/25	0.88	0.15	60,64,72,76	0
2	BER	D	301	25/25	0.88	0.14	57,62,71,73	0
3	SO4	B	302	5/5	0.90	0.10	79,80,81,82	0
3	SO4	C	302	5/5	0.93	0.11	62,65,67,67	0
3	SO4	D	302	5/5	0.93	0.10	59,60,61,64	0
3	SO4	A	302	5/5	0.97	0.07	46,50,54,55	0

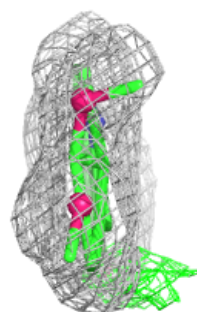
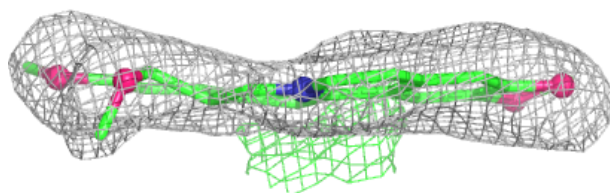
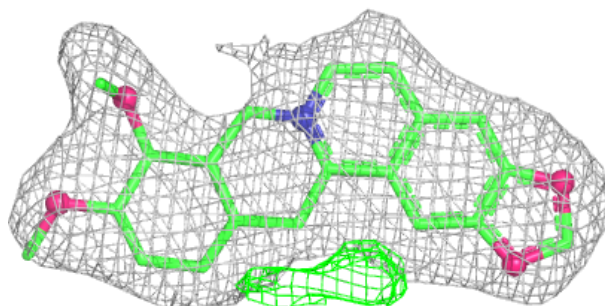
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BER A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

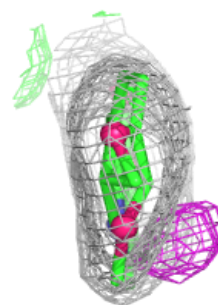
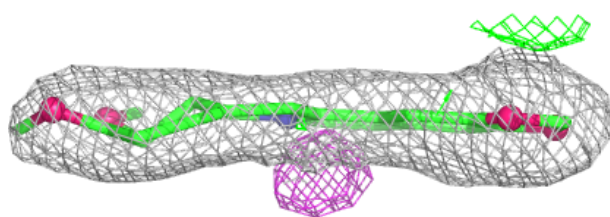
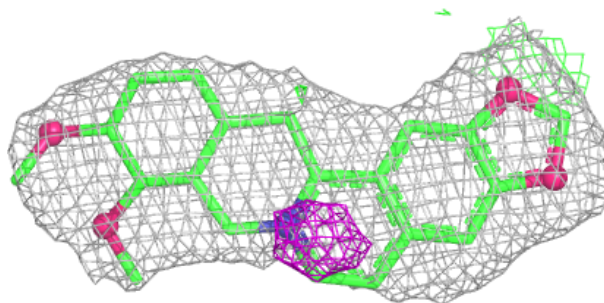
**Electron density around BER C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

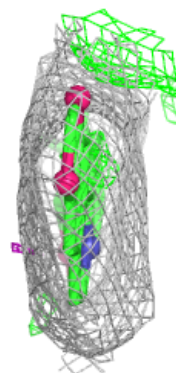
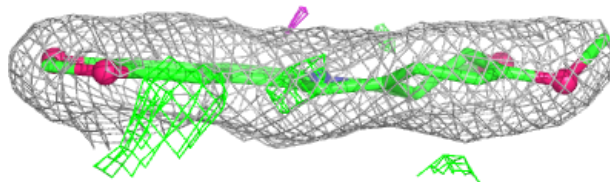
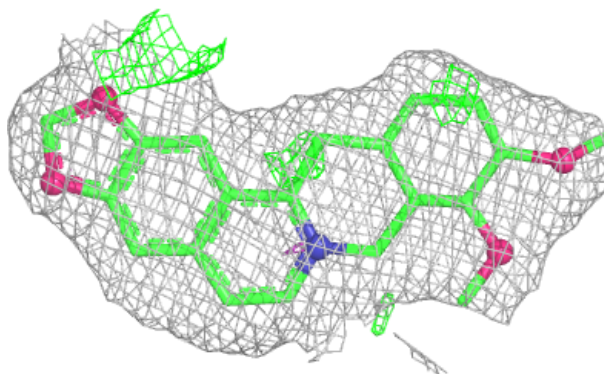


Electron density around BER B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BER D 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.