



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:30 PM UTC

PDB ID : 1EXI / pdb_00001exi
Title : CRYSTAL STRUCTURE OF TRANSCRIPTION ACTIVATOR BMRR,
FROM B. SUBTILIS, BOUND TO 21 BASE PAIR BMR OPERATOR AND
TPSB
Authors : Zheleznova-Heldwein, E.E.; Brennan, R.G.
Deposited on : 2000-05-02
Resolution : 3.12 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

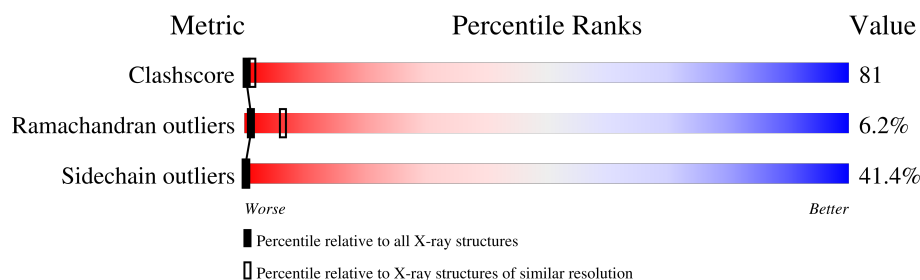
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 Å.

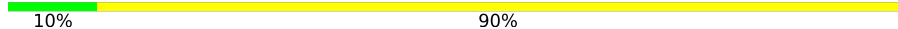
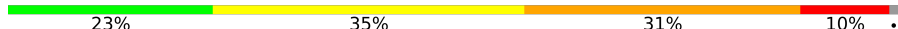
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)

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	M	21	
2	A	278	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2593 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 DNA chain called DNA (5'-D(*AP*CP*CP*CP*TP*CP*CP*CP*CP*TP*TP*AP*GP*GP*GP*GP*AP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	21	Total	C	N	O	P	0	0	0
			427	203	79	125	20			

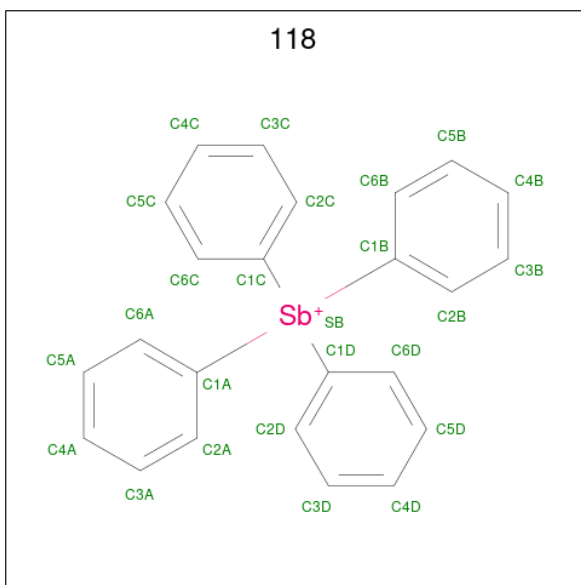
- Molecule 2 is a protein called MULTIDRUG-EFFLUX TRANSPORTER REGULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	275	Total	C	N	O	S	0	0	0
			2112	1354	334	416	8			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is TETRAPHENYLANTIMONIUM ION (CCD ID: 118) (formula: C₂₄H₂₀Sb).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	Sb	0	0
			25	24	1		
4	A	1	Total	C	Sb	0	0
			25	24	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	O	0	0
			1	1		
5	A	2	Total	O	0	0
			2	2		

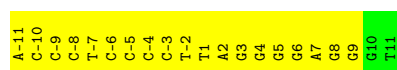
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

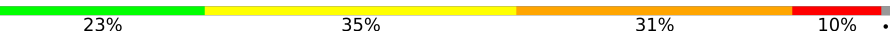
Note EDS was not executed.

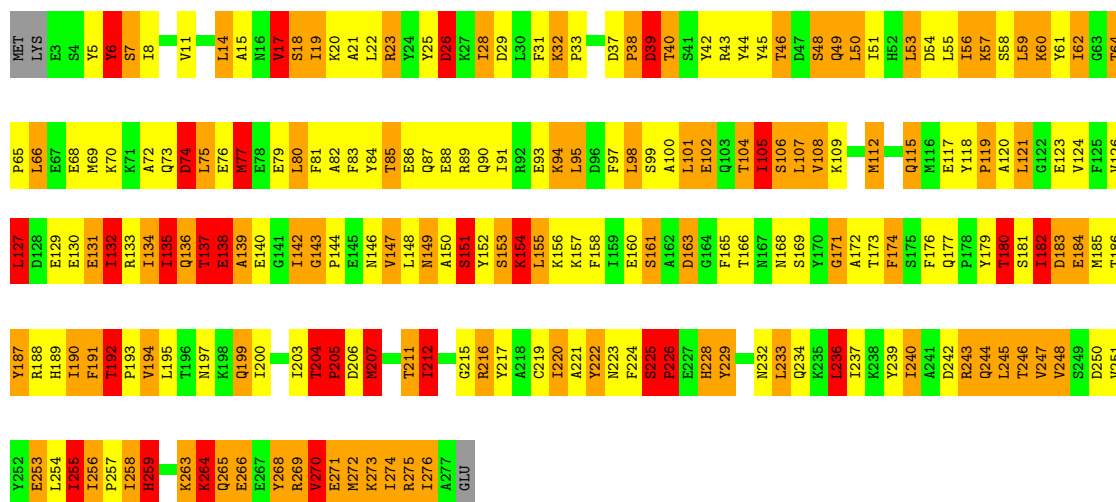
- Molecule 1: DNA (5'-D(*AP*CP*CP*CP*TP*CP*CP*CP*CP*TP*TP*AP*GP*GP*GP*GP*AP*GP*GP*GP*T)-3')

Chain M: 



- Molecule 2: MULTIDRUG-EFFLUX TRANSPORTER REGULATOR

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.15Å 110.15Å 144.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 3.12	Depositor
% Data completeness (in resolution range)	(Not available) (16.00-3.12)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.268 , 0.317	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2593	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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: 118, ZN

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	M	0.30	0/478	0.62	0/736
2	A	1.41	14/2159 (0.6%)	1.63	50/2942 (1.7%)
All	All	1.28	14/2637 (0.5%)	1.49	50/3678 (1.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	77	MET	SD-CE	9.85	2.04	1.79
2	A	212	ILE	N-CA	-9.08	1.38	1.46
2	A	135	ILE	CA-CB	8.16	1.66	1.54
2	A	56	ILE	CA-CB	-7.41	1.45	1.54
2	A	205	PRO	CA-C	6.47	1.61	1.52
2	A	211	THR	C-N	-6.38	1.26	1.33
2	A	46	THR	CA-C	6.33	1.60	1.52
2	A	270	VAL	CA-CB	-6.01	1.45	1.54
2	A	19	ILE	CA-C	-5.77	1.46	1.52
2	A	174	PHE	CA-C	-5.44	1.45	1.52
2	A	138	GLU	CG-CD	5.44	1.65	1.52
2	A	207	MET	SD-CE	5.30	1.92	1.79
2	A	192	THR	CA-C	-5.14	1.46	1.52
2	A	275	ARG	CA-C	-5.14	1.46	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	212	ILE	N-CA-C	-10.62	95.62	107.73
2	A	127	LEU	N-CA-C	10.21	121.72	108.34
2	A	149	ASN	N-CA-C	-10.19	103.01	114.62
2	A	265	GLN	OE1-CD-NE2	-10.16	112.44	122.60
2	A	15	ALA	N-CA-C	-9.96	90.35	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	168	ASN	N-CA-C	-9.33	99.48	112.45
2	A	26	ASP	N-CA-C	-9.24	100.13	111.40
2	A	259	HIS	N-CA-C	9.19	126.33	114.75
2	A	191	PHE	N-CA-C	8.90	123.66	109.86
2	A	264	LYS	N-CA-C	8.85	119.93	108.34
2	A	132	ILE	N-CA-C	8.79	127.62	109.34
2	A	62	ILE	CB-CA-C	-8.71	100.73	111.88
2	A	6	TYR	N-CA-C	8.67	123.59	109.72
2	A	271	GLU	N-CA-C	8.40	125.12	109.24
2	A	248	VAL	N-CA-C	8.14	121.02	113.20
2	A	7	SER	N-CA-C	-8.12	98.47	110.48
2	A	255	ILE	N-CA-C	7.88	120.86	108.89
2	A	108	VAL	CB-CA-C	-7.80	101.99	111.97
2	A	66	LEU	N-CA-C	-7.63	102.96	111.28
2	A	180	THR	N-CA-C	-7.12	102.71	111.40
2	A	105	ILE	CB-CA-C	-6.96	102.93	112.04
2	A	187	TYR	N-CA-C	6.95	120.45	110.10
2	A	263	LYS	CA-C-N	-6.89	111.09	122.39
2	A	263	LYS	C-N-CA	-6.89	111.09	122.39
2	A	118	TYR	N-CA-C	-6.72	99.62	109.50
2	A	265	GLN	CG-CD-NE2	6.70	126.44	116.40
2	A	204	THR	N-CA-C	-6.38	100.12	109.50
2	A	197	ASN	N-CA-C	-6.10	105.15	112.59
2	A	236	LEU	N-CA-C	-6.08	104.28	111.03
2	A	150	ALA	N-CA-C	-6.05	105.75	113.01
2	A	57	LYS	N-CA-C	-5.90	104.03	111.11
2	A	28	ILE	N-CA-C	-5.78	103.95	112.04
2	A	124	VAL	N-CA-C	5.74	116.47	109.30
2	A	171	GLY	N-CA-C	5.68	119.39	111.10
2	A	151	SER	N-CA-C	-5.62	106.38	113.18
2	A	137	THR	N-CA-C	-5.60	100.90	109.41
2	A	86	GLU	N-CA-C	-5.50	105.29	111.28
2	A	107	LEU	N-CA-C	-5.47	104.16	112.04
2	A	182	ILE	N-CA-C	-5.38	105.29	110.72
2	A	147	VAL	N-CA-C	5.33	120.43	109.34
2	A	39	ASP	N-CA-C	-5.31	105.92	112.72
2	A	17	VAL	N-CA-C	5.30	116.00	108.42
2	A	14	LEU	N-CA-C	5.18	116.73	111.14
2	A	77	MET	N-CA-C	5.17	121.80	110.80
2	A	143	GLY	N-CA-C	-5.17	101.80	112.34
2	A	233	LEU	N-CA-C	-5.14	105.57	111.07
2	A	131	GLU	N-CA-C	5.14	117.89	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	225	SER	N-CA-C	-5.09	98.56	109.81
2	A	204	THR	C-N-CD	-5.01	104.47	125.00
2	A	89	ARG	N-CA-C	-5.00	106.02	111.82

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	M	427	0	237	48	0
2	A	2112	0	1924	343	0
3	A	1	0	0	0	0
4	A	50	0	40	6	0
5	A	2	0	0	0	0
5	M	1	0	0	0	0
All	All	2593	0	2201	387	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 81.

All (387) 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:A:77:MET:SD	2:A:77:MET:CE	2.04	1.46
2:A:264:LYS:HA	2:A:264:LYS:HE2	1.15	1.14
2:A:240:ILE:HG23	2:A:245:LEU:HD22	1.29	1.13
2:A:59:LEU:HA	2:A:62:ILE:HD12	1.28	1.13
2:A:134:ILE:HG22	2:A:193:PRO:HA	1.29	1.09
2:A:264:LYS:HA	2:A:264:LYS:CE	1.87	1.00
2:A:139:ALA:HB2	2:A:190:ILE:HD12	1.47	0.96
2:A:264:LYS:HE2	2:A:264:LYS:CA	1.94	0.96
2:A:258:ILE:HG12	2:A:268:TYR:HA	1.49	0.95
2:A:101:LEU:HD23	2:A:101:LEU:H	1.32	0.95
2:A:257:PRO:HA	2:A:268:TYR:HB3	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:154:LYS:HG2	2:A:155:LEU:H	1.34	0.92
2:A:269:ARG:NH1	2:A:269:ARG:HB2	1.90	0.86
2:A:59:LEU:HA	2:A:62:ILE:CD1	2.05	0.85
1:M:3:DG:H2''	1:M:4:DG:H5'	1.58	0.84
2:A:59:LEU:HD22	2:A:62:ILE:HD11	1.60	0.83
1:M:-11:DA:H2''	1:M:-10:DC:H5'	1.61	0.83
2:A:219:CYS:HB3	2:A:273:LYS:CB	2.09	0.83
2:A:233:LEU:O	2:A:237:ILE:HD12	1.80	0.81
2:A:135:ILE:HG23	2:A:194:VAL:HG11	1.63	0.81
2:A:258:ILE:HD11	2:A:269:ARG:N	1.95	0.80
2:A:215:GLY:HA3	2:A:275:ARG:NE	1.95	0.80
2:A:243:ARG:HB2	2:A:245:LEU:HD12	1.63	0.80
2:A:17:VAL:HG11	2:A:22:LEU:HD23	1.64	0.79
2:A:46:THR:HG23	2:A:48:SER:HB3	1.65	0.79
2:A:247:VAL:HA	2:A:276:ILE:HG22	1.64	0.78
2:A:182:ILE:O	2:A:185:MET:HG2	1.82	0.78
2:A:98:LEU:HD12	2:A:98:LEU:C	2.09	0.78
2:A:82:ALA:O	2:A:85:THR:HG23	1.85	0.77
2:A:171:GLY:HA3	2:A:191:PHE:CZ	2.18	0.77
1:M:-8:DC:OP1	2:A:43:ARG:HG3	1.84	0.77
2:A:59:LEU:HD22	2:A:62:ILE:CD1	2.15	0.76
2:A:134:ILE:HG12	2:A:212:ILE:HD11	1.67	0.76
2:A:22:LEU:HD12	2:A:23:ARG:N	2.00	0.76
2:A:216:ARG:HB3	2:A:276:ILE:HD12	1.68	0.76
2:A:239:TYR:O	2:A:243:ARG:HG2	1.86	0.76
2:A:26:ASP:O	2:A:32:LYS:HD2	1.84	0.75
2:A:66:LEU:HA	2:A:69:MET:HE2	1.68	0.75
2:A:224:PHE:CE2	2:A:226:PRO:HD3	2.20	0.75
2:A:217:TYR:CE2	2:A:275:ARG:HB2	2.21	0.74
2:A:240:ILE:HG23	2:A:245:LEU:CD2	2.15	0.74
2:A:153:SER:O	2:A:157:LYS:HG2	1.88	0.73
2:A:223:ASN:ND2	2:A:269:ARG:HH12	1.86	0.73
2:A:98:LEU:HA	2:A:101:LEU:HG	1.70	0.73
2:A:174:PHE:O	2:A:250:ASP:HB3	1.88	0.73
2:A:139:ALA:HB2	2:A:190:ILE:HG23	1.71	0.72
2:A:269:ARG:HB2	2:A:269:ARG:CZ	2.20	0.72
2:A:248:VAL:CG2	2:A:275:ARG:HG2	2.19	0.72
1:M:-2:DT:C2	1:M:1:DT:H72	2.25	0.71
2:A:80:LEU:O	2:A:83:PHE:HB3	1.91	0.71
2:A:121:LEU:HD11	2:A:222:TYR:HA	1.73	0.71
1:M:-9:DC:C2	1:M:-8:DC:C5	2.78	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:-7:DT:C1'	1:M:-6:DC:H5'	2.20	0.71
2:A:142:ILE:O	2:A:187:TYR:HB2	1.89	0.71
2:A:245:LEU:H	2:A:245:LEU:CD1	2.04	0.71
2:A:204:THR:OG1	2:A:205:PRO:HD2	1.91	0.70
2:A:98:LEU:HD12	2:A:99:SER:N	2.06	0.70
2:A:172:ALA:HB1	2:A:190:ILE:HG22	1.74	0.70
2:A:176:PHE:C	2:A:177:GLN:HG2	2.16	0.70
2:A:31:PHE:CZ	2:A:53:LEU:HD11	2.26	0.70
2:A:173:THR:HG23	2:A:188:ARG:HB3	1.74	0.70
2:A:216:ARG:O	2:A:275:ARG:HA	1.91	0.70
2:A:37:ASP:OD2	2:A:38:PRO:HD2	1.92	0.69
2:A:134:ILE:HG22	2:A:193:PRO:CA	2.16	0.69
2:A:154:LYS:CG	2:A:155:LEU:H	2.04	0.69
2:A:104:THR:O	2:A:108:VAL:HG23	1.93	0.68
2:A:40:THR:HG23	2:A:42:TYR:CD1	2.29	0.68
4:A:503:118:H6A	4:A:503:118:H6C	1.75	0.68
2:A:240:ILE:HA	2:A:245:LEU:CD1	2.23	0.68
2:A:172:ALA:HA	2:A:190:ILE:HA	1.74	0.68
2:A:50:LEU:O	2:A:53:LEU:HB2	1.93	0.68
2:A:173:THR:HG22	2:A:189:HIS:HB2	1.76	0.68
2:A:154:LYS:H	2:A:154:LYS:HD2	1.59	0.67
2:A:180:THR:HB	2:A:184:GLU:CD	2.20	0.67
1:M:-7:DT:H1'	1:M:-6:DC:H5'	1.75	0.67
2:A:225:SER:OG	2:A:228:HIS:HB2	1.93	0.67
2:A:239:TYR:CE2	2:A:243:ARG:HG3	2.29	0.67
2:A:247:VAL:HA	2:A:276:ILE:CG2	2.25	0.67
2:A:246:THR:O	2:A:276:ILE:HG22	1.95	0.66
1:M:-8:DC:H3'	2:A:43:ARG:HH12	1.59	0.66
2:A:155:LEU:HD12	2:A:192:THR:HB	1.77	0.66
2:A:181:SER:O	2:A:184:GLU:HB2	1.95	0.66
2:A:219:CYS:HB3	2:A:273:LYS:HB3	1.75	0.66
1:M:-11:DA:H2''	1:M:-10:DC:C5'	2.26	0.66
2:A:180:THR:HG22	2:A:181:SER:N	2.09	0.66
2:A:5:TYR:CE2	4:A:503:118:H2D	2.30	0.66
2:A:134:ILE:HA	2:A:194:VAL:HG13	1.75	0.66
2:A:258:ILE:CG1	2:A:268:TYR:HA	2.24	0.66
2:A:256:ILE:HD12	2:A:269:ARG:O	1.96	0.66
2:A:18:SER:O	2:A:21:ALA:HB3	1.96	0.65
2:A:135:ILE:HG23	2:A:194:VAL:CG1	2.25	0.65
2:A:50:LEU:HD23	2:A:50:LEU:N	2.11	0.65
2:A:240:ILE:HA	2:A:245:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:DG:H2''	1:M:6:DG:OP2	1.94	0.65
2:A:136:GLN:HB3	2:A:191:PHE:CA	2.27	0.64
2:A:255:ILE:HD11	2:A:268:TYR:CB	2.26	0.64
2:A:264:LYS:HE2	2:A:264:LYS:C	2.22	0.64
4:A:503:118:H6A	4:A:503:118:C6C	2.27	0.64
2:A:173:THR:CG2	2:A:189:HIS:HB2	2.27	0.64
1:M:3:DG:H2'	1:M:4:DG:C8	2.33	0.64
2:A:156:LYS:O	2:A:160:GLU:HG2	1.98	0.64
2:A:69:MET:O	2:A:72:ALA:HB3	1.97	0.64
2:A:163:ASP:C	2:A:165:PHE:H	2.05	0.64
2:A:8:ILE:HD11	2:A:22:LEU:CD1	2.28	0.64
2:A:154:LYS:HD2	2:A:154:LYS:N	2.13	0.64
2:A:257:PRO:CA	2:A:268:TYR:HB3	2.25	0.64
2:A:259:HIS:CE1	2:A:266:GLU:HA	2.33	0.64
2:A:50:LEU:HD23	2:A:50:LEU:H	1.63	0.63
1:M:-4:DC:H2''	1:M:-3:DC:O5'	1.99	0.63
2:A:255:ILE:HD13	2:A:256:ILE:N	2.13	0.63
2:A:152:TYR:O	2:A:154:LYS:HD3	1.99	0.63
2:A:199:GLN:HA	2:A:199:GLN:NE2	2.14	0.62
2:A:255:ILE:HD11	2:A:268:TYR:CG	2.34	0.62
2:A:53:LEU:O	2:A:56:ILE:HG12	2.00	0.62
2:A:172:ALA:CB	2:A:190:ILE:HG22	2.29	0.62
1:M:-10:DC:H1'	1:M:-9:DC:H5'	1.80	0.62
2:A:98:LEU:HA	2:A:101:LEU:CD2	2.29	0.62
2:A:121:LEU:CD1	2:A:222:TYR:HA	2.30	0.62
2:A:139:ALA:CB	2:A:190:ILE:HD12	2.27	0.61
2:A:127:LEU:HD13	2:A:127:LEU:N	2.14	0.61
2:A:138:GLU:HA	2:A:189:HIS:HD2	1.65	0.61
2:A:220:ILE:CG2	2:A:236:LEU:HD22	2.30	0.61
2:A:50:LEU:HA	2:A:53:LEU:CD1	2.31	0.61
2:A:58:SER:O	2:A:61:TYR:HB3	2.00	0.61
2:A:246:THR:C	2:A:276:ILE:HG22	2.26	0.61
1:M:-9:DC:H5'	1:M:-9:DC:C6	2.36	0.60
2:A:33:PRO:HA	2:A:45:TYR:CE1	2.36	0.60
2:A:81:PHE:O	2:A:85:THR:HG22	2.01	0.60
2:A:264:LYS:HD3	2:A:265:GLN:H	1.65	0.60
2:A:101:LEU:HD23	2:A:101:LEU:N	2.11	0.60
2:A:219:CYS:HB3	2:A:273:LYS:HB2	1.82	0.60
2:A:132:ILE:O	2:A:211:THR:HA	2.00	0.60
2:A:143:GLY:H	2:A:146:ASN:CG	2.08	0.60
2:A:127:LEU:HD22	2:A:127:LEU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:22:LEU:HA	2:A:25:TYR:CD2	2.37	0.59
2:A:135:ILE:O	2:A:155:LEU:HD11	2.02	0.59
2:A:98:LEU:O	2:A:101:LEU:HG	2.03	0.59
2:A:144:PRO:HA	2:A:187:TYR:CE1	2.38	0.58
2:A:134:ILE:CG1	2:A:212:ILE:HD11	2.33	0.58
1:M:-3:DC:C4	1:M:-2:DT:H73	2.38	0.58
2:A:176:PHE:CZ	2:A:240:ILE:HD13	2.38	0.58
2:A:206:ASP:OD2	2:A:207:MET:HG2	2.03	0.58
2:A:37:ASP:HB3	2:A:40:THR:HG22	1.85	0.58
2:A:33:PRO:HA	2:A:45:TYR:CD1	2.39	0.58
2:A:199:GLN:HE21	2:A:200:ILE:N	2.02	0.58
2:A:17:VAL:CG1	2:A:22:LEU:HD23	2.33	0.58
2:A:126:VAL:C	2:A:127:LEU:HD13	2.29	0.58
2:A:97:PHE:CD2	2:A:98:LEU:N	2.72	0.57
2:A:97:PHE:O	2:A:100:ALA:HB3	2.04	0.57
2:A:131:GLU:C	2:A:132:ILE:HG13	2.27	0.57
2:A:174:PHE:CZ	2:A:251:VAL:HB	2.39	0.57
2:A:19:ILE:HD12	2:A:19:ILE:N	2.19	0.57
2:A:73:GLN:CG	2:A:74:ASP:H	2.17	0.57
2:A:98:LEU:HA	2:A:101:LEU:CG	2.33	0.57
2:A:155:LEU:CD1	2:A:192:THR:HB	2.34	0.57
2:A:220:ILE:HG12	2:A:221:ALA:N	2.19	0.57
2:A:274:ILE:HD13	2:A:275:ARG:H	1.69	0.57
2:A:133:ARG:HB3	2:A:194:VAL:HG22	1.85	0.57
2:A:134:ILE:HG12	2:A:212:ILE:CD1	2.33	0.57
2:A:75:LEU:HB2	2:A:79:GLU:HB2	1.87	0.57
2:A:171:GLY:HA3	2:A:191:PHE:CE2	2.39	0.57
2:A:139:ALA:HB2	2:A:190:ILE:CG2	2.35	0.57
1:M:-8:DC:H2''	1:M:-7:DT:OP2	2.04	0.57
2:A:75:LEU:HB2	2:A:79:GLU:CB	2.35	0.57
2:A:40:THR:HG23	2:A:42:TYR:CG	2.40	0.56
2:A:104:THR:HG22	2:A:105:ILE:N	2.20	0.56
2:A:136:GLN:HB3	2:A:191:PHE:HA	1.87	0.56
2:A:220:ILE:CD1	2:A:232:ASN:HB3	2.36	0.56
1:M:-10:DC:H5'	1:M:-10:DC:H6	1.70	0.56
1:M:-9:DC:H5'	1:M:-9:DC:H6	1.71	0.56
2:A:134:ILE:CD1	2:A:212:ILE:HD11	2.36	0.56
1:M:-10:DC:H5'	1:M:-10:DC:C6	2.41	0.56
2:A:65:PRO:HG2	2:A:68:GLU:H	1.71	0.56
2:A:136:GLN:HB3	2:A:191:PHE:N	2.21	0.56
2:A:148:LEU:C	2:A:149:ASN:HD22	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:-8:DC:H2'	2:A:23:ARG:HH21	1.72	0.55
2:A:33:PRO:HB3	2:A:45:TYR:CZ	2.42	0.55
2:A:37:ASP:OD1	2:A:40:THR:HG22	2.07	0.55
2:A:82:ALA:HA	2:A:85:THR:CG2	2.37	0.55
2:A:42:TYR:HB3	2:A:44:TYR:CE1	2.42	0.54
2:A:43:ARG:HG3	2:A:43:ARG:HH11	1.72	0.54
2:A:177:GLN:HB2	2:A:179:TYR:CE2	2.42	0.54
2:A:90:GLN:O	2:A:93:GLU:HB3	2.08	0.54
2:A:247:VAL:CA	2:A:276:ILE:HG22	2.36	0.54
2:A:37:ASP:C	2:A:39:ASP:H	2.16	0.54
1:M:-3:DC:C5	1:M:-2:DT:H73	2.43	0.54
2:A:224:PHE:HB2	2:A:270:VAL:CG2	2.38	0.54
2:A:239:TYR:C	2:A:239:TYR:CD2	2.86	0.54
2:A:132:ILE:HG22	2:A:134:ILE:HG23	1.90	0.54
2:A:25:TYR:HE1	2:A:66:LEU:HD13	1.73	0.54
2:A:46:THR:HG22	2:A:49:GLN:CG	2.38	0.54
2:A:55:LEU:HD13	2:A:55:LEU:C	2.33	0.53
2:A:82:ALA:HA	2:A:85:THR:HG23	1.91	0.53
2:A:176:PHE:CD2	2:A:247:VAL:HG11	2.44	0.53
2:A:224:PHE:CE2	4:A:502:118:H6C	2.44	0.53
2:A:17:VAL:HG13	2:A:18:SER:N	2.24	0.53
2:A:82:ALA:C	2:A:85:THR:HG23	2.32	0.53
2:A:255:ILE:HD11	2:A:268:TYR:HB2	1.91	0.53
2:A:182:ILE:HG22	2:A:183:ASP:N	2.24	0.53
2:A:7:SER:O	2:A:11:VAL:HG23	2.09	0.53
2:A:172:ALA:N	2:A:191:PHE:CE2	2.77	0.52
1:M:-10:DC:H1'	1:M:-9:DC:C5'	2.40	0.52
2:A:105:ILE:HG22	2:A:106:SER:N	2.20	0.52
2:A:59:LEU:HB3	2:A:69:MET:CG	2.39	0.52
1:M:8:DG:H2''	1:M:9:DG:OP2	2.10	0.52
2:A:98:LEU:HA	2:A:101:LEU:HD21	1.91	0.52
2:A:154:LYS:HG2	2:A:155:LEU:N	2.16	0.51
2:A:225:SER:CB	2:A:228:HIS:HB2	2.41	0.51
1:M:-7:DT:H2''	1:M:-6:DC:O5'	2.10	0.51
1:M:-10:DC:C2	1:M:-9:DC:C5	2.98	0.51
2:A:50:LEU:HA	2:A:53:LEU:HD13	1.92	0.51
2:A:157:LYS:O	2:A:161:SER:HB3	2.11	0.51
2:A:119:PRO:CD	2:A:120:ALA:H	2.24	0.51
2:A:127:LEU:HD23	2:A:129:GLU:HG2	1.92	0.51
2:A:19:ILE:HD12	2:A:19:ILE:H	1.76	0.51
2:A:40:THR:CG2	2:A:42:TYR:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:LEU:HA	2:A:53:LEU:HD12	1.93	0.51
2:A:274:ILE:HD13	2:A:275:ARG:N	2.25	0.51
2:A:173:THR:OG1	2:A:250:ASP:HB2	2.11	0.51
2:A:127:LEU:N	2:A:127:LEU:HD22	2.24	0.51
2:A:257:PRO:HA	2:A:268:TYR:CB	2.31	0.51
1:M:-8:DC:H5''	2:A:42:TYR:HA	1.92	0.50
2:A:5:TYR:HE2	4:A:503:118:H2D	1.76	0.50
2:A:153:SER:C	2:A:157:LYS:HG2	2.35	0.50
2:A:271:GLU:HG2	2:A:271:GLU:O	2.11	0.50
2:A:46:THR:HG23	2:A:48:SER:CB	2.37	0.50
2:A:98:LEU:CA	2:A:101:LEU:HG	2.40	0.50
2:A:217:TYR:CZ	2:A:275:ARG:HB2	2.46	0.50
1:M:-5:DC:H2''	1:M:-4:DC:OP2	2.09	0.50
2:A:65:PRO:HG2	2:A:68:GLU:CB	2.41	0.50
2:A:99:SER:O	2:A:102:GLU:HB3	2.11	0.50
2:A:222:TYR:OH	2:A:229:TYR:HD1	1.95	0.50
2:A:224:PHE:CE2	4:A:502:118:C6C	2.94	0.50
2:A:19:ILE:H	2:A:19:ILE:CD1	2.24	0.50
2:A:40:THR:O	2:A:42:TYR:HD1	1.95	0.50
2:A:22:LEU:HA	2:A:25:TYR:HD2	1.77	0.50
2:A:269:ARG:HB2	2:A:269:ARG:HH11	1.72	0.50
2:A:154:LYS:N	2:A:154:LYS:CD	2.74	0.50
1:M:-7:DT:H4'	1:M:-6:DC:OP1	2.11	0.49
2:A:163:ASP:OD1	2:A:195:LEU:HB2	2.12	0.49
1:M:-9:DC:H2''	1:M:-8:DC:O5'	2.11	0.49
2:A:215:GLY:HA3	2:A:275:ARG:HE	1.76	0.49
1:M:-9:DC:H2''	1:M:-8:DC:OP2	2.08	0.49
1:M:-2:DT:N1	1:M:1:DT:H72	2.27	0.49
1:M:-10:DC:H2''	1:M:-9:DC:H5'	1.93	0.49
2:A:76:GLU:O	2:A:79:GLU:HG2	2.13	0.49
2:A:255:ILE:C	2:A:256:ILE:HG13	2.32	0.49
2:A:98:LEU:C	2:A:98:LEU:CD1	2.82	0.49
2:A:220:ILE:HD11	2:A:232:ASN:HB3	1.95	0.49
2:A:152:TYR:C	2:A:154:LYS:HD3	2.38	0.48
2:A:224:PHE:HB2	2:A:270:VAL:HG21	1.95	0.48
2:A:53:LEU:O	2:A:57:LYS:HG3	2.13	0.48
2:A:136:GLN:HB3	2:A:190:ILE:C	2.39	0.48
2:A:40:THR:HG23	2:A:42:TYR:HB2	1.96	0.48
2:A:94:LYS:O	2:A:97:PHE:HB3	2.14	0.48
2:A:101:LEU:H	2:A:101:LEU:CD2	2.10	0.48
2:A:6:TYR:O	2:A:44:TYR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:SER:O	2:A:51:ILE:HG22	2.13	0.48
2:A:73:GLN:CG	2:A:74:ASP:N	2.76	0.48
2:A:134:ILE:CA	2:A:194:VAL:HG13	2.42	0.48
2:A:22:LEU:HD12	2:A:23:ARG:H	1.74	0.48
2:A:46:THR:HG22	2:A:49:GLN:HG3	1.95	0.48
2:A:173:THR:HG22	2:A:189:HIS:H	1.78	0.48
2:A:233:LEU:C	2:A:237:ILE:HD12	2.37	0.48
2:A:119:PRO:HD2	2:A:120:ALA:H	1.77	0.47
2:A:245:LEU:H	2:A:245:LEU:HD13	1.78	0.47
2:A:137:THR:HG23	2:A:138:GLU:N	2.29	0.47
2:A:31:PHE:CZ	2:A:53:LEU:CD1	2.98	0.47
2:A:31:PHE:CZ	2:A:49:GLN:HB3	2.49	0.47
2:A:59:LEU:HD23	2:A:59:LEU:N	2.29	0.47
2:A:242:ASP:C	2:A:244:GLN:N	2.71	0.47
2:A:132:ILE:HB	2:A:212:ILE:CG1	2.44	0.47
1:M:8:DG:OP2	1:M:8:DG:H2'	2.13	0.47
2:A:69:MET:HA	2:A:72:ALA:CB	2.44	0.47
2:A:239:TYR:C	2:A:239:TYR:HD2	2.23	0.47
2:A:256:ILE:O	2:A:268:TYR:HB3	2.15	0.47
2:A:59:LEU:N	2:A:59:LEU:CD2	2.77	0.47
2:A:137:THR:HG22	2:A:190:ILE:HD11	1.97	0.47
2:A:135:ILE:CG2	2:A:194:VAL:HG11	2.40	0.47
2:A:182:ILE:CG2	2:A:183:ASP:N	2.77	0.47
2:A:59:LEU:HB3	2:A:69:MET:SD	2.55	0.47
2:A:83:PHE:C	2:A:83:PHE:CD2	2.93	0.47
2:A:97:PHE:CG	2:A:98:LEU:N	2.79	0.47
1:M:-3:DC:C6	1:M:-2:DT:H71	2.50	0.46
2:A:91:ILE:C	2:A:93:GLU:H	2.23	0.46
2:A:143:GLY:H	2:A:146:ASN:HB2	1.79	0.46
2:A:45:TYR:N	2:A:45:TYR:CD2	2.83	0.46
2:A:243:ARG:CB	2:A:245:LEU:HD12	2.41	0.46
1:M:-8:DC:H3'	2:A:43:ARG:NH1	2.28	0.46
2:A:182:ILE:C	2:A:184:GLU:N	2.74	0.46
2:A:199:GLN:NE2	2:A:199:GLN:CA	2.79	0.46
2:A:8:ILE:HD11	2:A:22:LEU:HD13	1.97	0.46
2:A:248:VAL:HG23	2:A:275:ARG:HG2	1.94	0.46
2:A:69:MET:HA	2:A:72:ALA:HB3	1.96	0.45
1:M:2:DA:C2	1:M:3:DG:C4	3.04	0.45
2:A:46:THR:H	2:A:49:GLN:HG3	1.82	0.45
2:A:139:ALA:CB	2:A:190:ILE:HG23	2.45	0.45
2:A:144:PRO:HA	2:A:187:TYR:HE1	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:242:ASP:C	2:A:244:GLN:H	2.23	0.45
1:M:7:DA:H2''	1:M:8:DG:OP2	2.17	0.45
2:A:19:ILE:N	2:A:19:ILE:CD1	2.79	0.45
2:A:121:LEU:HA	2:A:121:LEU:HD13	1.57	0.45
2:A:146:ASN:N	2:A:146:ASN:HD22	2.15	0.45
2:A:255:ILE:CG1	2:A:256:ILE:N	2.79	0.45
1:M:-5:DC:H2''	1:M:-4:DC:O5'	2.15	0.45
2:A:82:ALA:CA	2:A:85:THR:HG23	2.45	0.45
2:A:143:GLY:H	2:A:146:ASN:CB	2.30	0.45
2:A:182:ILE:C	2:A:184:GLU:H	2.24	0.45
2:A:46:THR:CG2	2:A:48:SER:HB3	2.41	0.45
2:A:136:GLN:HG2	2:A:191:PHE:HB3	1.98	0.45
2:A:245:LEU:HD12	2:A:245:LEU:H	1.81	0.45
2:A:55:LEU:O	2:A:58:SER:HB2	2.15	0.45
2:A:255:ILE:HG12	2:A:256:ILE:H	1.81	0.45
2:A:14:LEU:HA	2:A:14:LEU:HD23	1.69	0.45
1:M:3:DG:OP1	1:M:3:DG:H4'	2.15	0.45
2:A:42:TYR:HB3	2:A:44:TYR:HE1	1.81	0.45
2:A:176:PHE:O	2:A:177:GLN:HG2	2.17	0.44
2:A:68:GLU:C	2:A:70:LYS:N	2.74	0.44
1:M:-4:DC:H2''	1:M:-3:DC:C6	2.52	0.44
2:A:149:ASN:C	2:A:151:SER:N	2.74	0.44
2:A:64:THR:HB	2:A:65:PRO:HD2	1.99	0.44
2:A:132:ILE:HB	2:A:212:ILE:HG12	1.99	0.44
2:A:255:ILE:HD13	2:A:255:ILE:C	2.42	0.44
1:M:-9:DC:H3'	2:A:8:ILE:HG21	1.98	0.44
2:A:153:SER:OG	2:A:154:LYS:HD2	2.18	0.44
2:A:169:SER:CB	2:A:193:PRO:HG2	2.48	0.44
2:A:253:GLU:HA	2:A:272:MET:HA	1.99	0.44
2:A:276:ILE:HD12	2:A:276:ILE:O	2.17	0.44
2:A:77:MET:C	2:A:79:GLU:N	2.75	0.44
2:A:109:LYS:O	2:A:112:MET:HB2	2.18	0.44
2:A:115:GLN:OE1	2:A:115:GLN:HA	2.17	0.44
2:A:181:SER:H	2:A:184:GLU:HB2	1.82	0.44
1:M:-10:DC:H2''	1:M:-9:DC:C5'	2.48	0.44
2:A:46:THR:C	2:A:48:SER:N	2.75	0.44
2:A:75:LEU:HD12	2:A:80:LEU:CA	2.47	0.44
2:A:182:ILE:HD12	2:A:182:ILE:HA	1.82	0.44
2:A:28:ILE:O	2:A:29:ASP:HB2	2.17	0.43
2:A:101:LEU:O	2:A:102:GLU:C	2.62	0.43
2:A:163:ASP:C	2:A:165:PHE:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:-7:DT:O4'	1:M:-6:DC:H5'	2.17	0.43
2:A:54:ASP:O	2:A:57:LYS:HB2	2.18	0.43
2:A:19:ILE:O	2:A:20:LYS:C	2.61	0.43
2:A:45:TYR:HA	2:A:49:GLN:OE1	2.18	0.43
2:A:158:PHE:CZ	2:A:203:ILE:HA	2.54	0.43
2:A:240:ILE:HA	2:A:245:LEU:HD11	1.97	0.43
2:A:245:LEU:CD1	2:A:245:LEU:N	2.78	0.43
2:A:255:ILE:CD1	2:A:256:ILE:N	2.79	0.43
2:A:56:ILE:CG1	2:A:57:LYS:N	2.81	0.43
2:A:59:LEU:CA	2:A:62:ILE:HD12	2.20	0.43
2:A:105:ILE:C	2:A:107:LEU:N	2.77	0.43
2:A:152:TYR:O	2:A:153:SER:C	2.62	0.43
2:A:199:GLN:HE21	2:A:199:GLN:C	2.27	0.43
1:M:-4:DC:H2''	1:M:-3:DC:H6	1.84	0.42
2:A:59:LEU:HB3	2:A:69:MET:HG2	2.02	0.42
2:A:146:ASN:N	2:A:146:ASN:ND2	2.67	0.42
2:A:69:MET:C	2:A:72:ALA:HB3	2.45	0.42
2:A:264:LYS:CD	2:A:265:GLN:H	2.32	0.42
2:A:105:ILE:C	2:A:107:LEU:H	2.27	0.42
2:A:169:SER:CB	2:A:254:LEU:HD21	2.49	0.42
2:A:75:LEU:HD12	2:A:80:LEU:HA	2.01	0.42
2:A:268:TYR:CD1	2:A:268:TYR:N	2.87	0.42
1:M:-3:DC:O5'	1:M:-3:DC:H6	2.03	0.42
2:A:40:THR:HG23	2:A:42:TYR:CB	2.48	0.42
2:A:101:LEU:HA	2:A:104:THR:HB	2.02	0.42
2:A:173:THR:CG2	2:A:189:HIS:H	2.32	0.42
2:A:73:GLN:HG3	2:A:74:ASP:H	1.85	0.41
2:A:182:ILE:HD12	2:A:185:MET:SD	2.60	0.41
2:A:80:LEU:O	2:A:80:LEU:HD12	2.20	0.41
1:M:1:DT:H4'	1:M:1:DT:OP1	2.20	0.41
1:M:6:DG:H2''	1:M:7:DA:OP2	2.20	0.41
2:A:95:LEU:HD23	2:A:95:LEU:HA	1.82	0.41
2:A:132:ILE:HD12	2:A:212:ILE:HB	2.02	0.41
2:A:258:ILE:HD11	2:A:269:ARG:H	1.82	0.41
2:A:182:ILE:HD11	2:A:229:TYR:CE2	2.55	0.41
2:A:33:PRO:HB3	2:A:45:TYR:CE2	2.56	0.41
2:A:43:ARG:HG3	2:A:43:ARG:NH1	2.35	0.41
2:A:44:TYR:CD1	2:A:44:TYR:N	2.89	0.41
2:A:50:LEU:H	2:A:50:LEU:CD2	2.20	0.41
2:A:239:TYR:CD2	2:A:243:ARG:HG3	2.56	0.41
2:A:149:ASN:C	2:A:151:SER:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:60:LYS:HE2	2:A:60:LYS:HB2	1.84	0.40
2:A:70:LYS:O	2:A:73:GLN:HG2	2.20	0.40
2:A:216:ARG:C	2:A:217:TYR:CD1	2.99	0.40
1:M:-3:DC:H3'	1:M:-2:DT:H71	2.02	0.40
2:A:59:LEU:CB	2:A:69:MET:HG2	2.51	0.40
2:A:199:GLN:HA	2:A:199:GLN:HE21	1.86	0.40
2:A:31:PHE:HZ	2:A:49:GLN:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	273/278 (98%)	195 (71%)	61 (22%)	17 (6%)	1 6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	49	GLN
2	A	74	ASP
2	A	77	MET
2	A	95	LEU
2	A	140	GLU
2	A	147	VAL
2	A	153	SER
2	A	229	TYR
2	A	154	LYS
2	A	139	ALA
2	A	205	PRO
2	A	48	SER
2	A	222	TYR
2	A	142	ILE

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Mol	Chain	Res	Type
2	A	226	PRO
2	A	38	PRO
2	A	119	PRO

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
2	A	210/255 (82%)	123 (59%)	87 (41%)	0 0

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	TYR
2	A	17	VAL
2	A	18	SER
2	A	23	ARG
2	A	26	ASP
2	A	32	LYS
2	A	39	ASP
2	A	40	THR
2	A	50	LEU
2	A	53	LEU
2	A	59	LEU
2	A	60	LYS
2	A	64	THR
2	A	74	ASP
2	A	75	LEU
2	A	80	LEU
2	A	84	TYR
2	A	85	THR
2	A	87	GLN
2	A	88	GLU
2	A	94	LYS
2	A	98	LEU
2	A	101	LEU

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Mol	Chain	Res	Type
2	A	102	GLU
2	A	104	THR
2	A	105	ILE
2	A	106	SER
2	A	112	MET
2	A	115	GLN
2	A	117	GLU
2	A	121	LEU
2	A	123	GLU
2	A	127	LEU
2	A	130	GLU
2	A	132	ILE
2	A	134	ILE
2	A	135	ILE
2	A	136	GLN
2	A	137	THR
2	A	138	GLU
2	A	151	SER
2	A	154	LYS
2	A	155	LEU
2	A	161	SER
2	A	163	ASP
2	A	166	THR
2	A	180	THR
2	A	182	ILE
2	A	183	ASP
2	A	184	GLU
2	A	186	THR
2	A	190	ILE
2	A	192	THR
2	A	194	VAL
2	A	199	GLN
2	A	204	THR
2	A	205	PRO
2	A	207	MET
2	A	212	ILE
2	A	216	ARG
2	A	220	ILE
2	A	225	SER
2	A	226	PRO
2	A	228	HIS
2	A	234	GLN

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Mol	Chain	Res	Type
2	A	236	LEU
2	A	240	ILE
2	A	243	ARG
2	A	244	GLN
2	A	245	LEU
2	A	246	THR
2	A	247	VAL
2	A	253	GLU
2	A	255	ILE
2	A	256	ILE
2	A	258	ILE
2	A	259	HIS
2	A	263	LYS
2	A	264	LYS
2	A	266	GLU
2	A	268	TYR
2	A	269	ARG
2	A	270	VAL
2	A	272	MET
2	A	273	LYS
2	A	274	ILE
2	A	276	ILE

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

Mol	Chain	Res	Type
2	A	73	GLN
2	A	149	ASN
2	A	189	HIS
2	A	199	GLN
2	A	223	ASN
2	A	259	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	118	A	502	-	28,28,28	5.04	6 (21%)	24,38,38	0.45	0
4	118	A	503	-	28,28,28	3.89	6 (21%)	24,38,38	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	118	A	502	-	-	-	0/4/4/4
4	118	A	503	-	-	-	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	118	SB-C1A	-17.81	1.74	2.10
4	A	502	118	SB-C1D	-14.25	1.81	2.10
4	A	503	118	SB-C1B	-12.26	1.85	2.10
4	A	502	118	SB-C1C	-10.94	1.88	2.10
4	A	503	118	SB-C1D	-10.55	1.88	2.10
4	A	503	118	SB-C1A	-9.89	1.90	2.10
4	A	502	118	SB-C1B	-5.60	1.99	2.10
4	A	503	118	SB-C1C	-5.57	1.99	2.10
4	A	502	118	C5A-C4A	2.80	1.44	1.38
4	A	502	118	C3B-C4B	2.50	1.43	1.38
4	A	503	118	C4B-C5B	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	118	C3B-C2B	-2.29	1.35	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

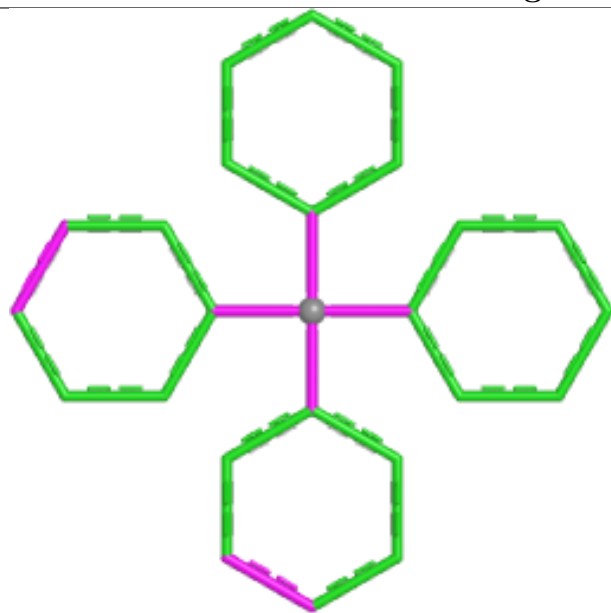
There are no ring outliers.

2 monomers are involved in 6 short contacts:

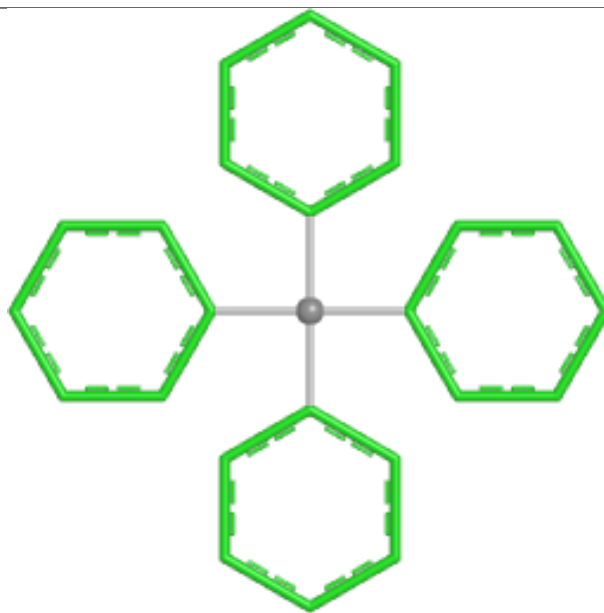
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	118	2	0
4	A	503	118	4	0

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.

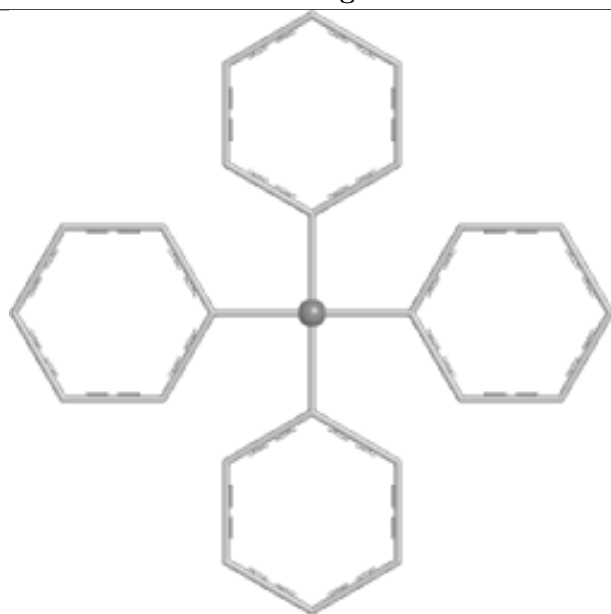
Ligand 118 A 502



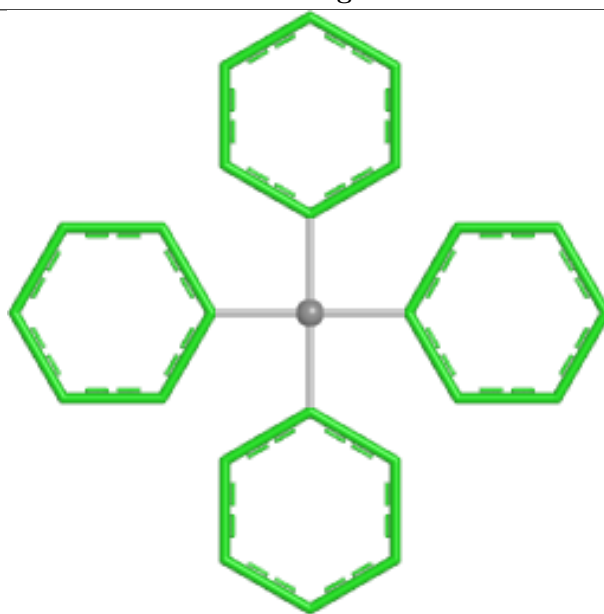
Bond lengths



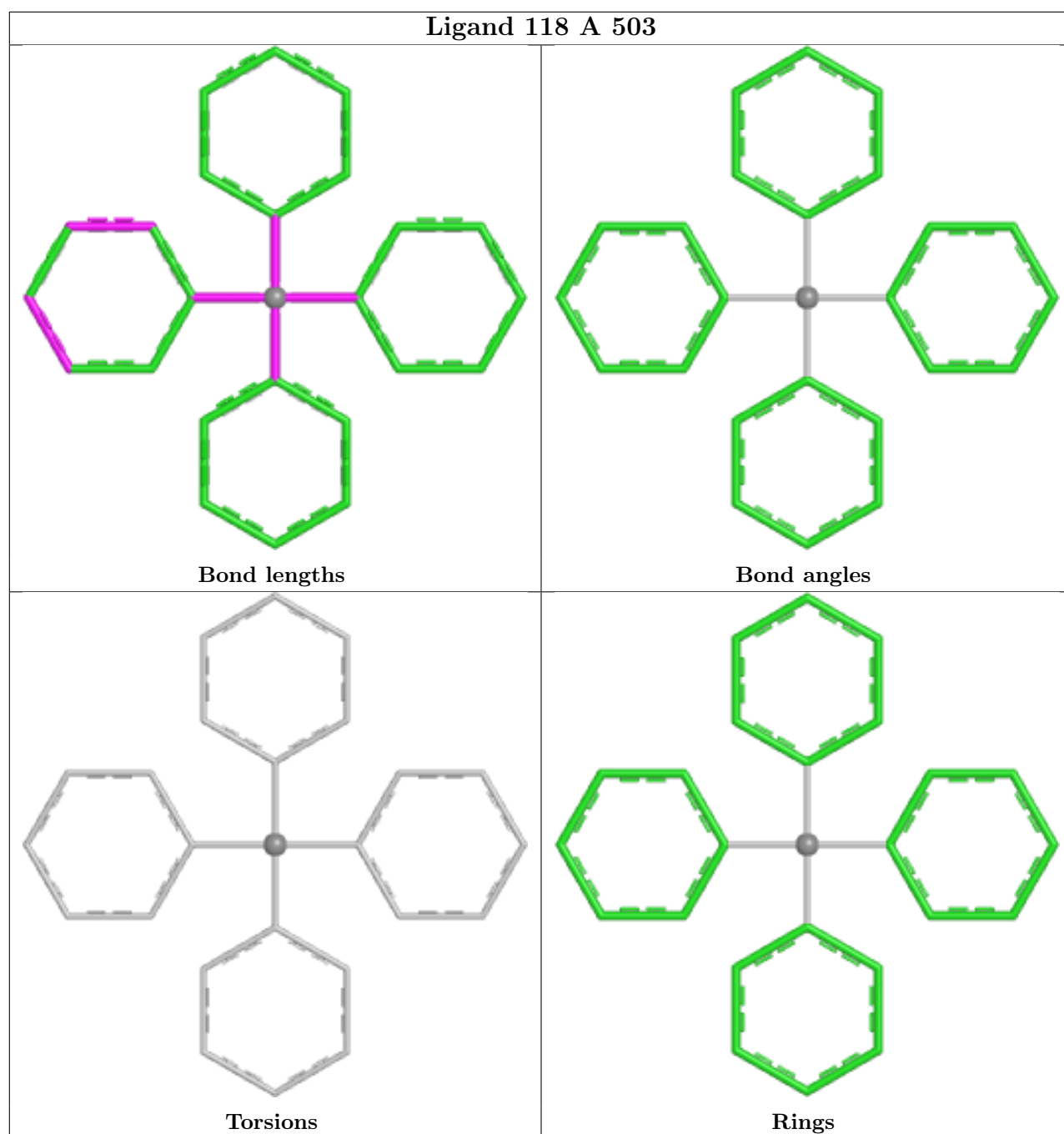
Bond angles



Torsions



Rings



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.