Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 04:12 PM EST

PDB ID	:	1EXI
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)

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

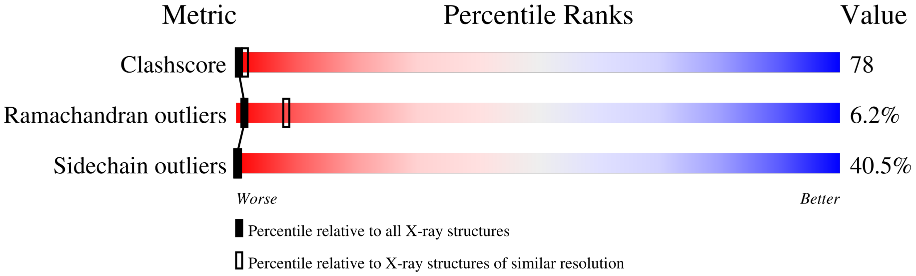
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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.

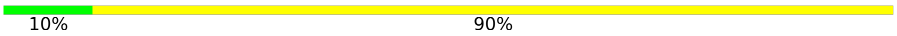
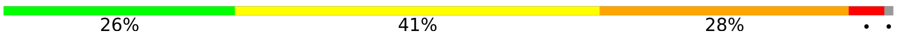
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	M	21	
2	A	278	

2 Entry composition (i)

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
			Total	C	N	O	P			
1	M	21	427	203	79	125	20	0	0	0

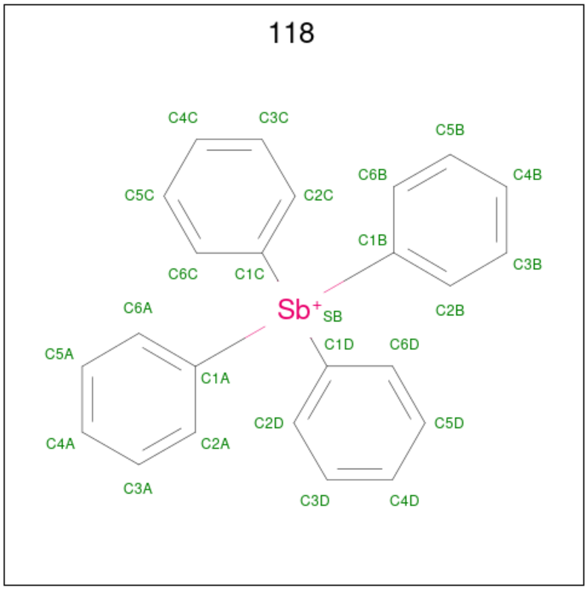
- Molecule 2 is a protein called MULTIDRUG-EFFLUX TRANSPORTER REGULATOR.

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is TETRAPHENYLANTIMONIUM ION (three-letter code: 118) (formula: $C_{24}H_{20}Sb$).



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

- Molecule 5 is water.

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

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.

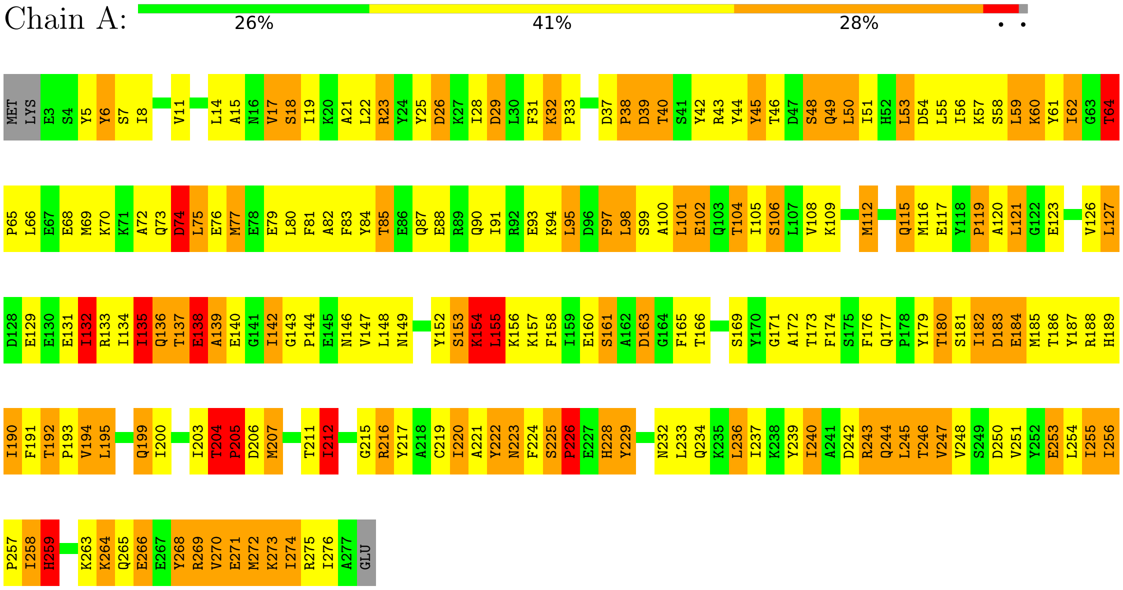
Note EDS was not executed.

- 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 ⓘ

5.1 Standard geometry ⓘ

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	0.43	0/478	0.74	0/736
2	A	1.09	3/2159 (0.1%)	1.12	9/2942 (0.3%)
All	All	1.00	3/2637 (0.1%)	1.06	9/3678 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	138	GLU	CG-CD	9.13	1.65	1.51
2	A	135	ILE	CA-CB	5.16	1.66	1.54
2	A	45	TYR	CE2-CZ	5.03	1.45	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	15	ALA	N-CA-C	-7.65	90.35	111.00
2	A	204	THR	C-N-CD	-7.33	104.47	120.60
2	A	155	LEU	CA-CB-CG	6.34	129.87	115.30
2	A	132	ILE	N-CA-C	6.15	127.62	111.00
2	A	64	THR	C-N-CD	-6.05	107.28	120.60
2	A	212	ILE	N-CA-C	-5.70	95.62	111.00
2	A	259	HIS	N-CA-C	5.68	126.33	111.00
2	A	62	ILE	CB-CA-C	-5.44	100.73	111.60
2	A	271	GLU	N-CA-C	5.23	125.12	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	427	0	237	48	0
2	A	2112	0	1924	329	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	373	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 78.

All (373) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:LEU:HA	2:A:69:MET:HE2	1.65	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: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:98:LEU:HD12	2:A:98:LEU:C	2.09	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:176:PHE:C	2:A:177:GLN:HG2	2.16	0.65
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:180:THR:HB	2:A:184:GLU:CD	2.20	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
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:264:LYS:HE2	2:A:264:LYS:C	2.22	0.60
2:A:163:ASP:C	2:A:165:PHE:H	2.05	0.59
2:A:127:LEU:HD22	2:A:127:LEU:H	1.67	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:97:PHE:O	2:A:100:ALA:HB3	2.04	0.57
2:A:97:PHE:CD2	2:A:98:LEU:N	2.72	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:105:ILE:HG22	2:A:106:SER:N	2.20	0.56
2:A:220:ILE:CD1	2:A:232:ASN:HB3	2.36	0.56
2:A:246:THR:C	2:A:276:ILE:HG22	2.26	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:143:GLY:H	2:A:146:ASN:CG	2.08	0.55
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
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:132:ILE:HG22	2:A:134:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:131:GLU:C	2:A:132:ILE:HG13	2.27	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:126:VAL:C	2:A:127:LEU:HD13	2.29	0.53
2:A:17:VAL:HG13	2:A:18:SER:N	2.24	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: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
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:148:LEU:C	2:A:149:ASN:HD22	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:37:ASP:C	2:A:39:ASP:H	2.16	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:239:TYR:C	2:A:239:TYR:CD2	2.86	0.49
2:A:55:LEU:HD13	2:A:55:LEU:C	2.33	0.49
2:A:220:ILE:HD11	2:A:232:ASN:HB3	1.95	0.49
2:A:224:PHE:HB2	2:A:270:VAL:HG21	1.95	0.48
2:A:255:ILE:C	2:A:256:ILE:HG13	2.32	0.48
2:A:53:LEU:O	2:A:57:LYS:HG3	2.13	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
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:82:ALA:C	2:A:85:THR:HG23	2.32	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:MET:HA	2:A:72:ALA:CB	2.44	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: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: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:153:SER:C	2:A:157:LYS:HG2	2.35	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
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: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:104:THR:CG2	2:A:105:ILE:N	2.77	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
1:M:-4:DC:H2”	1:M:-3:DC:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:152:TYR:C	2:A:154:LYS:HD3	2.38	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: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
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:45:TYR:HA	2:A:49:GLN:OE1	2.18	0.43
2:A:136:GLN:HB3	2:A:190:ILE:C	2.39	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:233:LEU:C	2:A:237:ILE:HD12	2.37	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:242:ASP:C	2:A:244:GLN:N	2.71	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:239:TYR:C	2:A:239:TYR:HD2	2.23	0.42
2:A:154:LYS:CG	2:A:155:LEU:N	2.77	0.42
2:A:264:LYS:CD	2:A:265:GLN:H	2.32	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:83:PHE:C	2:A:83:PHE:CD2	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:ILE:C	2:A:93:GLU:H	2.23	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:242:ASP:C	2:A:244:GLN:H	2.23	0.41
2:A:182:ILE:C	2:A:184:GLU:H	2.24	0.41
2:A:60:LYS:HE2	2:A:60:LYS:HB2	1.84	0.40
2:A:77:MET:C	2:A:79:GLU:N	2.75	0.40
2:A:70:LYS:O	2:A:73:GLN:HG2	2.20	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

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
2	A	273/278 (98%)	195 (71%)	61 (22%)	17 (6%)	1 8

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
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%)	125 (60%)	85 (40%)	0 0

All (85) 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	29	ASP
2	A	32	LYS
2	A	39	ASP

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Mol	Chain	Res	Type
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	84	TYR
2	A	85	THR
2	A	87	GLN
2	A	88	GLU
2	A	97	PHE
2	A	98	LEU
2	A	101	LEU
2	A	102	GLU
2	A	104	THR
2	A	106	SER
2	A	112	MET
2	A	115	GLN
2	A	116	MET
2	A	117	GLU
2	A	121	LEU
2	A	123	GLU
2	A	127	LEU
2	A	132	ILE
2	A	135	ILE
2	A	136	GLN
2	A	137	THR
2	A	138	GLU
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

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Mol	Chain	Res	Type
2	A	194	VAL
2	A	195	LEU
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	223	ASN
2	A	225	SER
2	A	226	PRO
2	A	228	HIS
2	A	234	GLN
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

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

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Mol	Chain	Res	Type
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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	5.97	6 (21%)	24,38,38	0.40	0
4	118	A	503	-	28,28,28	4.58	5 (17%)	24,38,38	0.40	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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	118	SB-C1A	-21.37	1.74	2.10
4	A	502	118	SB-C1D	-17.08	1.81	2.10
4	A	503	118	SB-C1B	-14.69	1.85	2.10
4	A	502	118	SB-C1C	-13.10	1.88	2.10
4	A	503	118	SB-C1D	-12.63	1.88	2.10
4	A	503	118	SB-C1A	-11.84	1.90	2.10
4	A	502	118	SB-C1B	-6.67	1.99	2.10
4	A	503	118	SB-C1C	-6.64	1.99	2.10
4	A	502	118	C5A-C4A	2.41	1.44	1.38
4	A	502	118	C3B-C4B	2.16	1.43	1.38
4	A	503	118	C4B-C5B	2.01	1.43	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

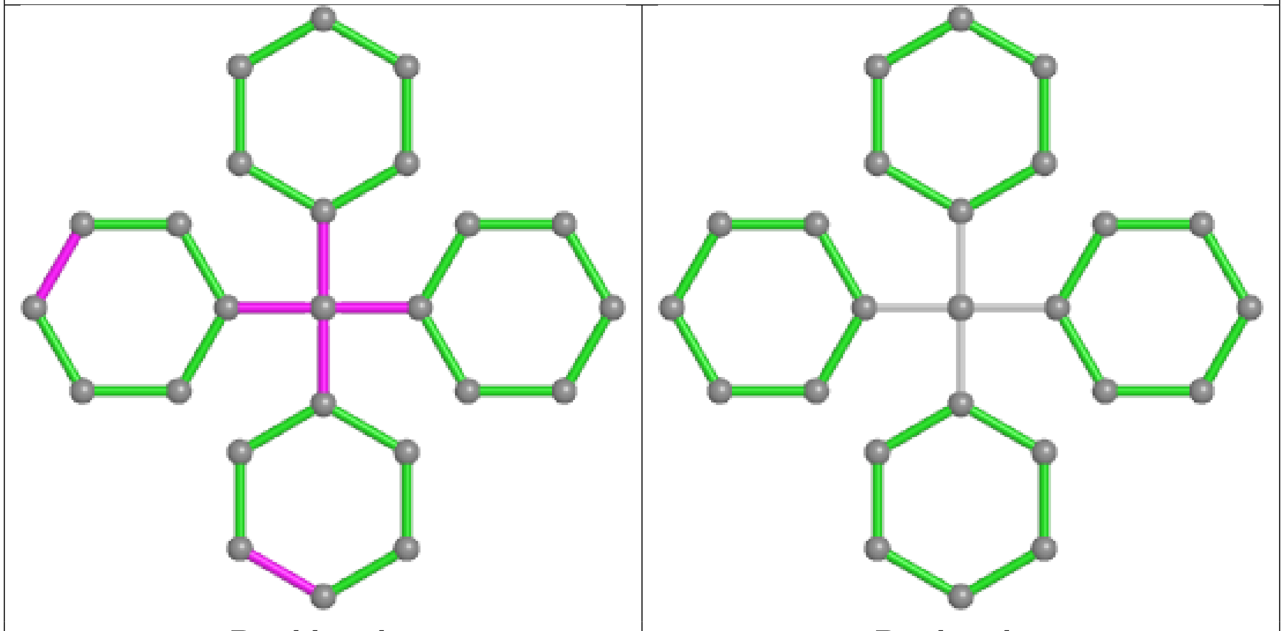
There are no ring outliers.

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

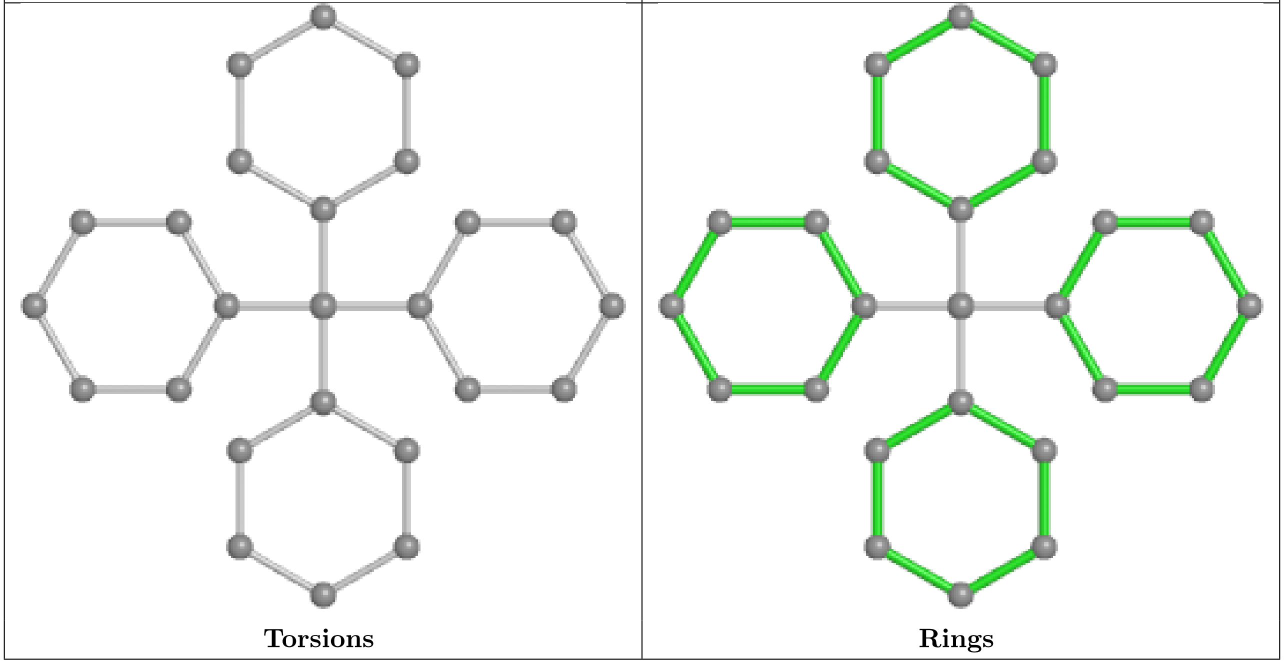
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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



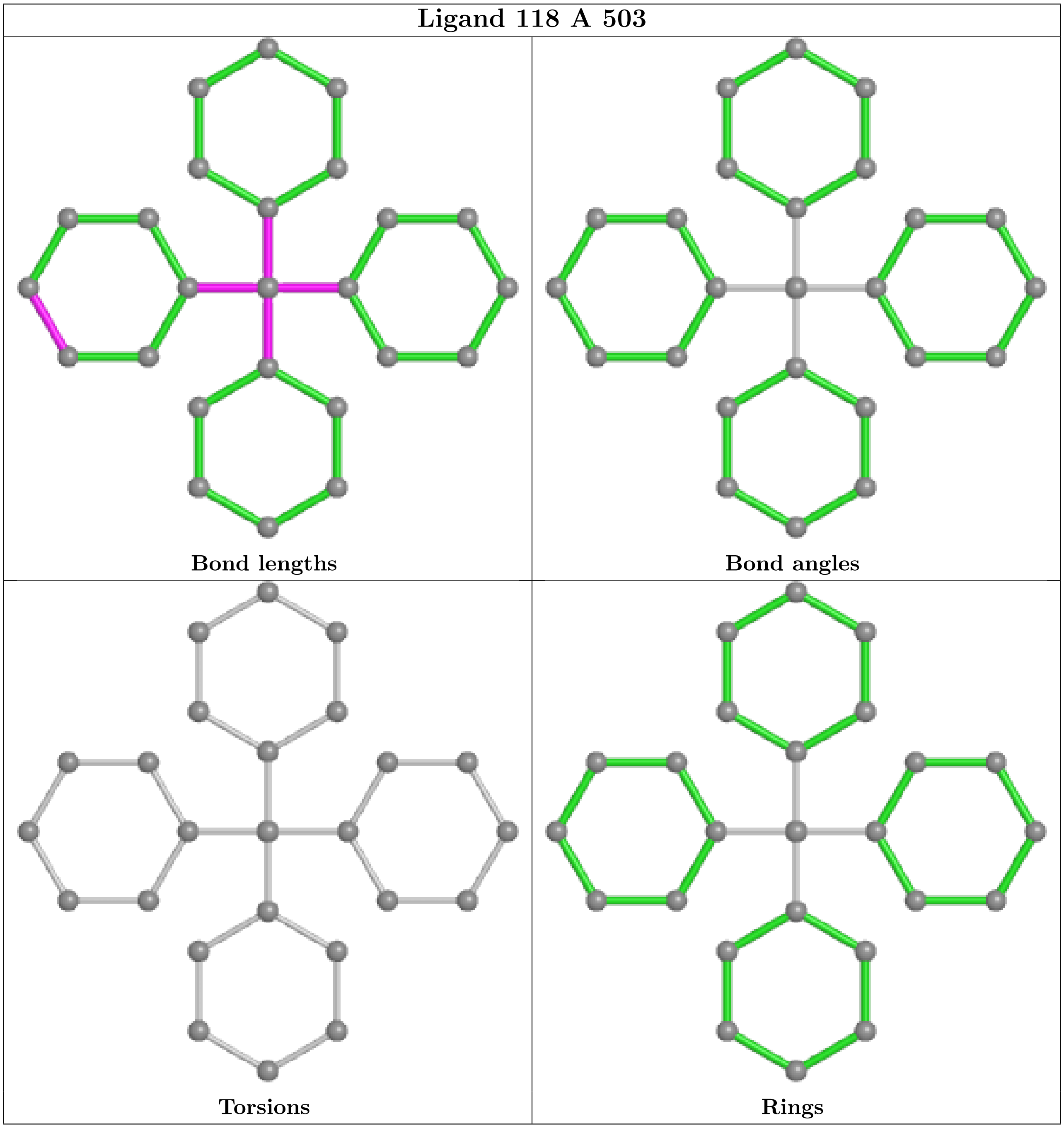
Bond lengths

Bond angles



Torsions

Rings



Ligand 118 A 503

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.