Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 07:39 PM EDT

PDB ID	:	2ZW7
Title	:	Crystal structure of bleomycin N-acetyltransferase complexed with bleomycin A2 and coenzyme A
Authors	:	Oda, K.; Matoba, Y.; Sugiyama, M.
Deposited on	:	2008-12-01
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

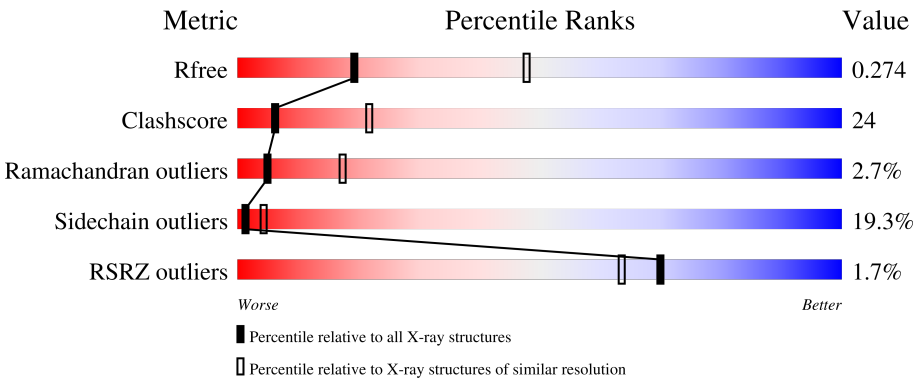
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	301	45% 42% 10% • •
1	B	301	3% 49% 40% 8% •

2 Entry composition (i)

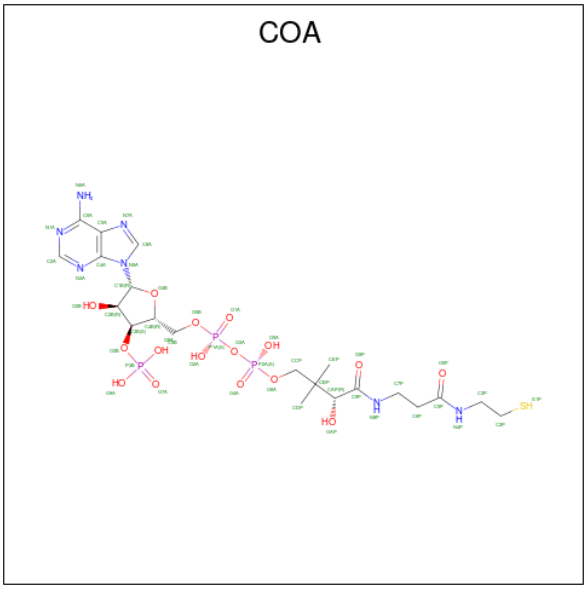
There are 4 unique types of molecules in this entry. The entry contains 4669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bleomycin acetyltransferase.

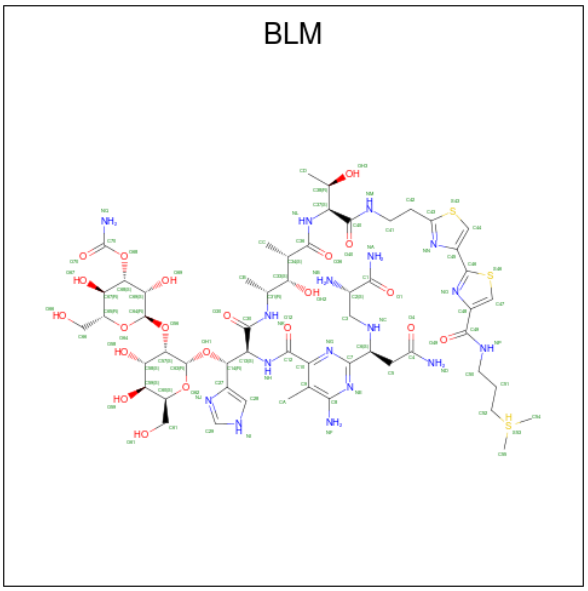
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	293	2209	1386	418	400	2	3	0	0	0
1	B	293	2209	1386	418	400	2	3	0	0	0

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0

- Molecule 3 is BLEOMYCIN A2 (three-letter code: BLM) (formula: $C_{55}H_{85}N_{17}O_{21}S_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	96	55	17	21	3	0	0
			Total	C	N	O	S		
3	B	1	96	55	17	21	3	0	0

- Molecule 4 is water.

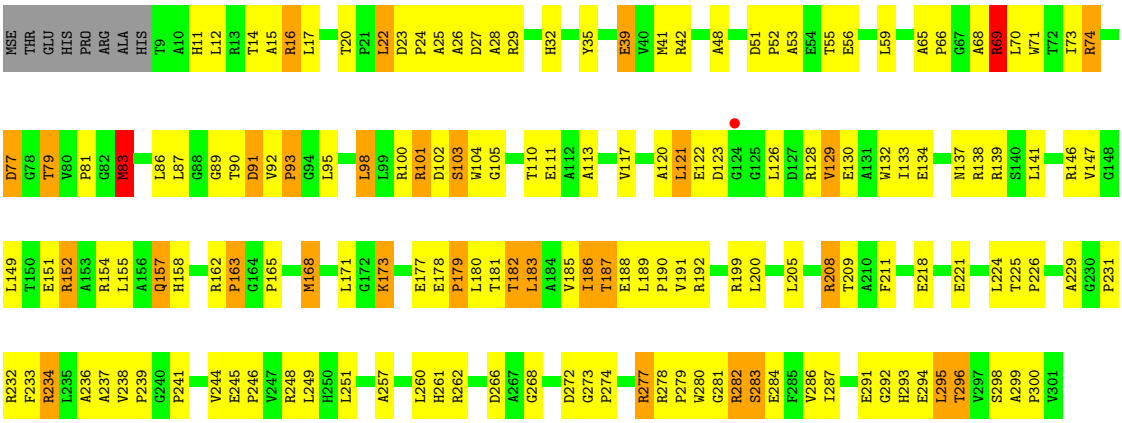
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	6	6	6	0	0
			Total	O		
4	B	5	5	5	0	0

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.

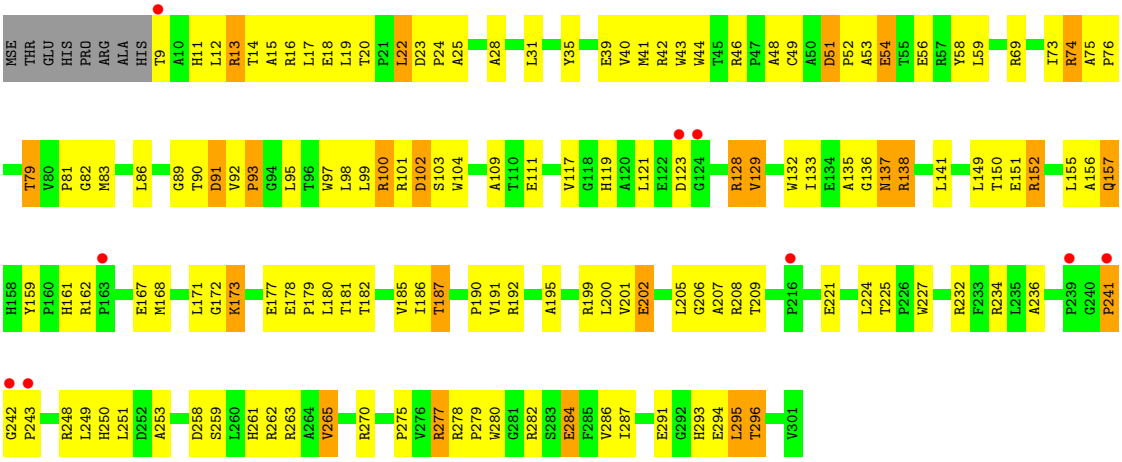
• Molecule 1: Bleomycin acetyltransferase

Chain A:



• Molecule 1: Bleomycin acetyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	70.05Å 70.05Å 534.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 44.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.7 (30.00-2.80) 89.1 (44.92-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.207 , 0.258 0.227 , 0.274	Depositor DCC
R_{free} test set	897 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4669	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BLM, COA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.37	0/2267	0.63	1/3101 (0.0%)
1	B	0.35	0/2267	0.61	0/3101
All	All	0.36	0/4534	0.62	1/6202 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	MSE	CG-SE-CE	5.01	109.92	98.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2209	0	2178	125	0
1	B	2209	0	2178	112	0
2	A	48	0	32	4	0
3	A	96	0	85	3	0
3	B	96	0	85	4	0
4	A	6	0	0	0	0
4	B	5	0	0	1	0
All	All	4669	0	4558	225	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 24.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:MSE:HE1	1:B:98:LEU:HD21	1.34	1.02
1:B:41:MSE:HG3	1:B:48:ALA:HA	1.47	0.97
1:A:149:LEU:HD23	1:A:173:LYS:HB2	1.46	0.96
1:B:149:LEU:HD23	1:B:173:LYS:HB2	1.52	0.92
1:A:157:GLN:HE21	1:A:168:MSE:HE1	1.35	0.89
1:B:90:THR:O	1:B:91:ASP:HB3	1.73	0.88
1:A:229:ALA:HA	1:A:232:ARG:HH12	1.43	0.82
1:B:41:MSE:CE	1:B:98:LEU:HD21	2.09	0.81
1:A:251:LEU:HD22	1:B:185:VAL:HG22	1.62	0.81
1:B:35:TYR:HA	1:B:41:MSE:HE3	1.62	0.79
1:A:65:ALA:HB3	1:A:68:ALA:HB2	1.64	0.78
1:A:41:MSE:HG3	1:A:48:ALA:HA	1.66	0.78
1:B:12:LEU:HB2	1:B:19:LEU:HB2	1.66	0.77
1:A:149:LEU:CD2	1:A:173:LYS:HB2	2.16	0.76
1:A:83:MSE:HE3	1:A:98:LEU:HD23	1.69	0.74
1:A:244:VAL:HG21	1:A:291:GLU:HB3	1.69	0.74
1:A:35:TYR:OH	1:A:83:MSE:HE2	1.88	0.73
1:B:296:THR:HG22	4:B:407:HOH:O	1.88	0.73
1:B:41:MSE:HE1	1:B:98:LEU:CD2	2.15	0.72
1:A:221:GLU:HG3	1:A:234:ARG:HD3	1.71	0.72
1:A:221:GLU:OE2	1:A:234:ARG:NH1	2.24	0.71
1:A:83:MSE:HE3	1:A:98:LEU:CD2	2.20	0.70
1:B:224:LEU:HD12	1:B:232:ARG:HA	1.72	0.70
1:A:229:ALA:HA	1:A:232:ARG:NH1	2.07	0.70
1:A:224:LEU:HD12	1:A:232:ARG:HA	1.73	0.69
1:A:186:ILE:HD12	1:A:232:ARG:HE	1.56	0.69
1:B:286:VAL:HG22	1:B:296:THR:HB	1.73	0.69
1:B:41:MSE:HG3	1:B:48:ALA:CA	2.23	0.67
1:B:13:ARG:HG2	1:B:18:GLU:OE2	1.95	0.67
1:A:51:ASP:OD2	1:A:53:ALA:HB3	1.95	0.66
1:B:95:LEU:HD11	1:B:117:VAL:HG22	1.76	0.66
1:B:261:HIS:O	1:B:265:VAL:HG12	1.96	0.66
1:B:42:ARG:HG2	1:B:43:TRP:CD1	2.30	0.65
1:A:180:LEU:HD21	1:B:259:SER:HB3	1.77	0.65
1:B:278:ARG:HB3	1:B:279:PRO:HD2	1.78	0.64
1:B:25:ALA:HA	1:B:56:GLU:OE1	1.97	0.64
1:A:186:ILE:HG21	1:A:234:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.63	0.63
1:B:19:LEU:HD21	1:B:73:ILE:HG12	1.81	0.62
1:A:11:HIS:HD2	1:A:20:THR:HG22	1.63	0.62
1:A:182:THR:HG21	1:B:224:LEU:HD22	1.81	0.62
1:B:22:LEU:HD23	1:B:24:PRO:HD3	1.81	0.62
1:A:257:ALA:HA	1:A:260:LEU:HD12	1.82	0.61
1:A:152:ARG:NH2	1:A:177:GLU:OE1	2.30	0.61
1:B:51:ASP:OD2	1:B:53:ALA:HB3	2.00	0.61
1:A:117:VAL:HG21	1:A:147:VAL:HG11	1.81	0.61
1:A:294:GLU:C	1:A:295:LEU:HD23	2.21	0.61
1:B:15:ALA:HB3	1:B:111:GLU:OE2	2.01	0.60
1:A:277:ARG:HH21	1:A:282:ARG:N	2.00	0.60
1:A:151:GLU:N	1:A:171:LEU:HD23	2.17	0.60
1:B:49:CYS:HB3	1:B:54:GLU:HB3	1.82	0.60
1:A:182:THR:CG2	1:B:224:LEU:HB3	2.32	0.59
1:B:132:TRP:O	3:B:403:BLM:H3E	2.02	0.59
1:A:133:ILE:HG22	1:A:134:GLU:O	2.03	0.58
1:B:73:ILE:CG2	1:B:81:PRO:HG2	2.34	0.58
1:A:86:LEU:HD23	1:A:95:LEU:HD23	1.84	0.58
1:A:95:LEU:HD21	1:A:129:VAL:HG11	1.86	0.58
1:A:208:ARG:HD3	1:A:226:PRO:HA	1.86	0.58
1:A:14:THR:OG1	1:A:17:LEU:HB2	2.05	0.57
1:A:66:PRO:O	1:A:89:GLY:N	2.37	0.57
1:A:22:LEU:HD11	1:A:59:LEU:HD13	1.87	0.57
1:A:251:LEU:CD2	1:B:185:VAL:HG22	2.34	0.57
1:A:104:TRP:NE1	2:A:401:COA:H10	2.20	0.57
1:A:224:LEU:CD1	1:A:232:ARG:HA	2.35	0.57
1:B:40:VAL:HG12	1:B:98:LEU:HD11	1.87	0.57
1:B:250:HIS:C	1:B:251:LEU:HD23	2.25	0.56
1:A:157:GLN:HG3	1:A:158:HIS:N	2.19	0.56
1:A:17:LEU:HD13	1:A:73:ILE:HG23	1.88	0.56
1:A:51:ASP:HB2	1:A:52:PRO:HD2	1.87	0.56
1:A:246:PRO:HB3	1:A:292:GLY:O	2.04	0.56
1:A:244:VAL:CG2	1:A:291:GLU:HB3	2.35	0.56
1:A:261:HIS:CE1	1:A:274:PRO:HA	2.41	0.56
1:B:195:ALA:O	1:B:199:ARG:HG3	2.05	0.56
1:A:187:THR:HB	1:B:249:LEU:CD2	2.35	0.56
1:B:46:ARG:NH2	1:B:54:GLU:OE1	2.39	0.55
1:B:151:GLU:N	1:B:171:LEU:HD23	2.20	0.55
1:A:86:LEU:HD11	1:A:120:ALA:HB2	1.88	0.55
1:A:113:ALA:O	1:A:117:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD11	1:A:168:MSE:HE2	1.89	0.55
1:B:73:ILE:HB	1:B:82:GLY:O	2.07	0.55
1:B:11:HIS:HD2	1:B:20:THR:HG22	1.73	0.54
1:B:86:LEU:HD23	1:B:95:LEU:HD23	1.89	0.54
1:A:278:ARG:HB3	1:A:279:PRO:HD2	1.89	0.54
1:A:105:GLY:HA2	2:A:401:COA:C4B	2.38	0.54
1:A:69:ARG:O	1:A:69:ARG:HG2	2.07	0.54
1:B:208:ARG:NH2	1:B:227:TRP:O	2.41	0.54
1:B:95:LEU:HD11	1:B:117:VAL:CG2	2.38	0.53
1:A:182:THR:HG21	1:B:224:LEU:HB3	1.91	0.53
1:A:71:TRP:O	1:A:83:MSE:HG2	2.08	0.53
1:A:132:TRP:HE3	1:A:168:MSE:HE3	1.72	0.53
1:A:187:THR:HB	1:B:187:THR:HG21	1.90	0.53
1:B:18:GLU:O	1:B:74:ARG:HB2	2.08	0.53
1:A:277:ARG:HH21	1:A:281:GLY:C	2.12	0.53
1:A:105:GLY:HA2	2:A:401:COA:H4B	1.91	0.52
1:B:279:PRO:HG2	1:B:280:TRP:CE3	2.45	0.52
1:A:133:ILE:CG2	1:A:137:ASN:HB3	2.39	0.51
1:A:279:PRO:HG2	1:A:280:TRP:CE3	2.44	0.51
1:B:250:HIS:O	1:B:251:LEU:HD23	2.10	0.51
1:B:135:ALA:HB2	1:B:167:GLU:HB3	1.93	0.51
1:A:41:MSE:HG3	1:A:48:ALA:CA	2.37	0.51
1:A:95:LEU:HD12	1:A:149:LEU:HD11	1.92	0.51
1:B:190:PRO:HD2	1:B:293:HIS:CE1	2.46	0.51
1:B:275:PRO:HA	1:B:284:GLU:O	2.11	0.51
1:A:23:ASP:HB3	1:A:26:ALA:HB3	1.93	0.51
1:B:202:GLU:HG3	1:B:207:ALA:O	2.11	0.51
1:A:120:ALA:O	1:A:126:LEU:HB2	2.11	0.50
1:A:226:PRO:HB2	1:B:128:ARG:HD2	1.92	0.50
1:B:151:GLU:CA	1:B:171:LEU:HD23	2.42	0.50
1:B:19:LEU:CD2	1:B:73:ILE:HG12	2.42	0.50
1:B:241:PRO:HD2	1:B:242:GLY:H	1.77	0.50
1:A:90:THR:HB	3:A:402:BLM:HAB	1.93	0.50
1:A:249:LEU:CD2	1:B:187:THR:HB	2.42	0.50
1:A:295:LEU:HD23	1:A:295:LEU:N	2.27	0.50
1:A:69:ARG:HD2	1:A:86:LEU:HD12	1.93	0.49
1:A:24:PRO:O	1:A:28:ALA:HB2	2.12	0.49
1:B:205:LEU:HD21	1:B:287:ILE:HD12	1.93	0.49
1:B:75:ALA:HB1	1:B:76:PRO:HD2	1.94	0.49
1:B:136:GLY:O	1:B:138:ARG:N	2.45	0.49
1:A:22:LEU:HG	1:A:23:ASP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:OD1	1:A:77:ASP:N	2.37	0.49
1:A:133:ILE:HG21	1:A:141:LEU:HG	1.95	0.49
1:B:155:LEU:HG	1:B:168:MSE:HB2	1.93	0.49
1:B:150:THR:O	1:B:152:ARG:HD3	2.13	0.49
1:A:11:HIS:CD2	1:A:20:THR:HG22	2.45	0.49
1:A:182:THR:HG21	1:B:224:LEU:CD2	2.42	0.49
1:A:205:LEU:HD21	1:A:287:ILE:HD12	1.94	0.49
1:B:73:ILE:HG21	1:B:81:PRO:HG2	1.93	0.49
1:A:101:ARG:HA	1:A:101:ARG:HD2	1.52	0.49
1:A:138:ARG:HG3	1:A:139:ARG:H	1.78	0.49
1:A:178:GLU:OE1	1:A:179:PRO:HD2	2.12	0.48
1:B:14:THR:OG1	1:B:17:LEU:HB2	2.12	0.48
1:A:165:PRO:HB3	1:A:300:PRO:HG2	1.94	0.48
1:B:224:LEU:HD12	1:B:232:ARG:CA	2.41	0.48
1:A:73:ILE:O	1:A:81:PRO:HD2	2.14	0.48
1:B:206:GLY:HA3	1:B:263:ARG:NH1	2.29	0.48
1:A:32:HIS:ND1	1:A:55:THR:OG1	2.40	0.48
1:B:9:THR:HB	1:B:69:ARG:HH21	1.79	0.48
1:B:133:ILE:HG21	1:B:141:LEU:HG	1.96	0.48
1:B:191:VAL:HA	1:B:291:GLU:HG2	1.95	0.47
1:A:20:THR:OG1	1:A:74:ARG:NH1	2.48	0.47
1:A:105:GLY:C	2:A:401:COA:O4B	2.53	0.47
1:A:249:LEU:HD22	1:B:187:THR:HB	1.95	0.47
1:A:185:VAL:HG22	1:B:251:LEU:HD22	1.95	0.47
1:B:11:HIS:CD2	1:B:20:THR:HG22	2.50	0.47
1:B:51:ASP:HB2	1:B:52:PRO:HD2	1.97	0.47
1:B:119:HIS:CE1	1:B:123:ASP:HB2	2.50	0.47
1:A:83:MSE:CE	1:A:98:LEU:CD2	2.93	0.47
1:A:183:LEU:HD12	1:B:253:ALA:C	2.35	0.47
1:B:133:ILE:CG2	1:B:137:ASN:HB3	2.45	0.47
1:A:186:ILE:CD1	1:A:232:ARG:HE	2.23	0.46
1:B:294:GLU:C	1:B:295:LEU:HD23	2.36	0.46
1:B:117:VAL:HG13	1:B:129:VAL:HG21	1.97	0.46
1:B:99:LEU:HD11	1:B:109:ALA:HB2	1.98	0.46
1:B:151:GLU:HA	1:B:171:LEU:HD23	1.98	0.45
1:B:19:LEU:CD2	1:B:73:ILE:HA	2.47	0.45
1:B:157:GLN:NE2	3:B:403:BLM:O4	2.50	0.45
1:A:110:THR:OG1	1:A:146:ARG:NH1	2.47	0.45
1:B:98:LEU:O	1:B:99:LEU:HD23	2.17	0.45
1:B:24:PRO:O	1:B:28:ALA:HB2	2.17	0.44
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PRO:CB	1:A:300:PRO:HG2	2.48	0.44
1:B:282:ARG:HG2	1:B:282:ARG:NH1	2.33	0.44
1:A:121:LEU:HD11	1:A:128:ARG:HA	1.98	0.44
1:B:155:LEU:HD12	1:B:156:ALA:O	2.17	0.44
1:B:201:VAL:HG23	1:B:207:ALA:HB3	1.99	0.44
3:B:403:BLM:HAA	3:B:403:BLM:O12	2.17	0.44
1:A:133:ILE:HD12	1:A:133:ILE:N	2.32	0.44
1:A:286:VAL:HG22	1:A:296:THR:HB	1.99	0.44
1:A:188:GLU:O	1:A:189:LEU:HD23	2.18	0.44
1:A:283:SER:O	1:A:298:SER:HA	2.18	0.44
1:B:221:GLU:HB2	1:B:234:ARG:HD3	1.99	0.44
1:A:22:LEU:HD23	1:A:24:PRO:HD3	2.00	0.44
1:B:278:ARG:HG3	1:B:280:TRP:CZ2	2.53	0.44
1:A:191:VAL:O	1:A:237:ALA:HA	2.17	0.43
1:A:299:ALA:HB1	1:A:300:PRO:HD2	1.99	0.43
1:A:42:ARG:HG2	1:A:42:ARG:NH1	2.33	0.43
1:A:157:GLN:NE2	3:A:402:BLM:HD2	2.16	0.43
3:A:402:BLM:HAA	3:A:402:BLM:O12	2.17	0.43
1:A:117:VAL:HG21	1:A:147:VAL:CG1	2.49	0.43
1:B:95:LEU:HD21	1:B:129:VAL:HG11	2.01	0.43
1:A:186:ILE:HG22	1:A:234:ARG:HG2	1.99	0.43
1:B:95:LEU:HD12	1:B:149:LEU:HD11	2.00	0.43
1:A:211:PHE:CZ	1:A:221:GLU:HB2	2.53	0.43
1:B:159:TYR:O	1:B:162:ARG:HB2	2.18	0.43
1:B:102:ASP:OD2	1:B:102:ASP:N	2.48	0.43
1:A:266:ASP:C	1:A:268:GLY:H	2.22	0.42
1:B:133:ILE:HG23	1:B:137:ASN:HB3	2.00	0.42
1:B:152:ARG:NH1	1:B:172:GLY:O	2.51	0.42
1:B:46:ARG:HD3	1:B:58:TYR:CE1	2.54	0.42
1:A:16:ARG:NH1	1:A:111:GLU:OE1	2.44	0.42
1:A:27:ASP:O	1:A:28:ALA:C	2.57	0.42
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.85	0.42
1:A:272:ASP:OD1	1:A:273:GLY:N	2.52	0.42
1:B:92:VAL:HA	1:B:93:PRO:HD2	1.85	0.42
1:B:178:GLU:HA	1:B:179:PRO:HD2	1.87	0.42
1:A:14:THR:O	1:A:15:ALA:C	2.57	0.42
1:B:97:TRP:O	1:B:98:LEU:HB2	2.19	0.42
1:B:241:PRO:CD	1:B:242:GLY:H	2.32	0.42
1:B:14:THR:O	1:B:15:ALA:C	2.58	0.42
1:B:101:ARG:HG2	1:B:104:TRP:CZ3	2.55	0.42
1:A:279:PRO:C	1:A:281:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:O	1:A:42:ARG:HG3	2.20	0.42
1:A:100:ARG:HG3	1:A:103:SER:OG	2.20	0.42
1:A:25:ALA:HA	1:A:56:GLU:OE1	2.20	0.41
1:B:35:TYR:CA	1:B:41:MSE:HE3	2.43	0.41
1:A:92:VAL:HA	1:A:93:PRO:HD2	1.71	0.41
1:A:231:PRO:HG2	1:B:182:THR:O	2.20	0.41
1:A:92:VAL:HG11	1:A:130:GLU:CD	2.41	0.41
1:A:122:GLU:HG3	1:A:123:ASP:N	2.36	0.41
1:A:190:PRO:HA	1:A:236:ALA:O	2.20	0.41
1:A:90:THR:O	1:A:91:ASP:C	2.59	0.41
1:A:224:LEU:HD11	1:A:233:PHE:CE2	2.56	0.41
1:A:190:PRO:HD2	1:A:293:HIS:CE1	2.54	0.41
1:A:272:ASP:OD2	1:A:286:VAL:HB	2.20	0.41
1:B:295:LEU:HD23	1:B:295:LEU:N	2.36	0.41
1:A:17:LEU:HD13	1:A:73:ILE:CG2	2.50	0.41
1:B:31:LEU:HD12	1:B:59:LEU:CD1	2.51	0.41
3:B:403:BLM:H3X	3:B:403:BLM:H5E	1.75	0.41
1:B:100:ARG:H	1:B:100:ARG:HG3	1.57	0.40
1:B:23:ASP:O	1:B:24:PRO:C	2.60	0.40
1:B:43:TRP:CG	1:B:137:ASN:ND2	2.89	0.40
1:B:159:TYR:HB3	1:B:161:HIS:CD2	2.56	0.40
1:A:162:ARG:HB3	1:A:163:PRO:HD2	2.03	0.40
1:B:190:PRO:HA	1:B:236:ALA:O	2.22	0.40
1:B:277:ARG:HD2	1:B:278:ARG:O	2.21	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
1	A	291/301 (97%)	256 (88%)	27 (9%)	8 (3%)	5 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	291/301 (97%)	261 (90%)	22 (8%)	8 (3%)	5 17
All	All	582/602 (97%)	517 (89%)	49 (8%)	16 (3%)	5 17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	PRO
1	A	69	ARG
1	A	79	THR
1	A	241	PRO
1	B	91	ASP
1	A	179	PRO
1	B	79	THR
1	A	93	PRO
1	B	209	THR
1	A	91	ASP
1	B	137	ASN
1	B	93	PRO
1	B	243	PRO
1	B	89	GLY
1	B	241	PRO
1	A	163	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	215/218 (99%)	170 (79%)	45 (21%)	1 3
1	B	215/218 (99%)	177 (82%)	38 (18%)	2 5
All	All	430/436 (99%)	347 (81%)	83 (19%)	1 4

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	16	ARG
1	A	22	LEU
1	A	29	ARG
1	A	39	GLU
1	A	69	ARG
1	A	70	LEU
1	A	74	ARG
1	A	77	ASP
1	A	79	THR
1	A	83	MSE
1	A	98	LEU
1	A	101	ARG
1	A	102	ASP
1	A	103	SER
1	A	121	LEU
1	A	129	VAL
1	A	152	ARG
1	A	154	ARG
1	A	157	GLN
1	A	168	MSE
1	A	173	LYS
1	A	181	THR
1	A	182	THR
1	A	183	LEU
1	A	186	ILE
1	A	187	THR
1	A	192	ARG
1	A	199	ARG
1	A	200	LEU
1	A	208	ARG
1	A	209	THR
1	A	218	GLU
1	A	225	THR
1	A	234	ARG
1	A	238	VAL
1	A	245	GLU
1	A	248	ARG
1	A	262	ARG
1	A	277	ARG
1	A	282	ARG
1	A	283	SER
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	296	THR
1	B	13	ARG
1	B	16	ARG
1	B	22	LEU
1	B	39	GLU
1	B	44	TRP
1	B	51	ASP
1	B	54	GLU
1	B	74	ARG
1	B	79	THR
1	B	83	MSE
1	B	100	ARG
1	B	102	ASP
1	B	103	SER
1	B	121	LEU
1	B	128	ARG
1	B	129	VAL
1	B	138	ARG
1	B	152	ARG
1	B	157	GLN
1	B	173	LYS
1	B	177	GLU
1	B	180	LEU
1	B	181	THR
1	B	186	ILE
1	B	187	THR
1	B	192	ARG
1	B	200	LEU
1	B	202	GLU
1	B	225	THR
1	B	248	ARG
1	B	258	ASP
1	B	262	ARG
1	B	265	VAL
1	B	270	ARG
1	B	277	ARG
1	B	284	GLU
1	B	295	LEU
1	B	296	THR

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

Mol	Chain	Res	Type
1	A	11	HIS
1	A	157	GLN
1	A	166	HIS
1	A	261	HIS
1	B	11	HIS
1	B	161	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	COA	A	401	-	41,50,50	1.26	4 (9%)	52,75,75	1.81	12 (23%)
3	BLM	A	402	-	88,101,101	1.76	11 (12%)	108,143,143	2.34	25 (23%)
3	BLM	B	403	-	88,101,101	1.74	10 (11%)	108,143,143	2.41	24 (22%)

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	COA	A	401	-	-	9/44/64/64	0/3/3/3
3	BLM	A	402	-	-	18/86/142/142	0/6/6/6
3	BLM	B	403	-	-	26/86/142/142	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	BLM	C8-NE	8.32	1.46	1.35
3	B	403	BLM	C8-NE	7.85	1.46	1.35
3	B	403	BLM	C7-NE	-7.18	1.21	1.34
3	B	403	BLM	C10-NG	7.01	1.49	1.34
3	A	402	BLM	C7-NE	-6.99	1.22	1.34
3	A	402	BLM	C10-NG	6.80	1.48	1.34
3	A	402	BLM	C10-C12	-4.42	1.43	1.50
3	B	403	BLM	C10-C12	-4.33	1.44	1.50
3	A	402	BLM	C9-C8	4.25	1.53	1.43
3	B	403	BLM	C9-C8	4.18	1.53	1.43
2	A	401	COA	P3B-O3B	3.54	1.66	1.59
3	A	402	BLM	C47-S46	3.18	1.75	1.70
2	A	401	COA	O4B-C1B	2.99	1.45	1.41
3	B	403	BLM	C47-S46	2.68	1.74	1.70
3	B	403	BLM	C12-NH	2.66	1.40	1.34
3	A	402	BLM	C27-C14	2.57	1.53	1.51
3	A	402	BLM	C12-NH	2.56	1.39	1.34
3	B	403	BLM	C27-C14	2.49	1.53	1.51
3	A	402	BLM	C1-NA	2.40	1.39	1.32
2	A	401	COA	C8A-N7A	-2.34	1.30	1.34
3	B	403	BLM	C1-NA	2.34	1.38	1.32
3	B	403	BLM	C70-NQ	2.31	1.38	1.33
3	A	402	BLM	C70-NQ	2.14	1.37	1.33
2	A	401	COA	C9P-N8P	2.04	1.38	1.33
3	A	402	BLM	O68-C68	-2.01	1.41	1.44

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	BLM	C45-C44-S43	-14.67	108.43	112.53
3	A	402	BLM	C45-C44-S43	-12.55	109.03	112.53
3	A	402	BLM	C12-C10-NG	-8.04	108.49	115.99
3	B	403	BLM	C12-C10-NG	-7.79	108.73	115.99
2	A	401	COA	P2A-O3A-P1A	-6.96	108.96	132.83
3	B	403	BLM	C68-O68-C70	6.76	126.77	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	BLM	C6-C5-C4	5.76	123.69	112.24
3	A	402	BLM	C68-O68-C70	5.49	124.95	117.12
3	A	402	BLM	C9-C10-C12	5.45	133.73	123.14
3	B	403	BLM	C6-C5-C4	5.32	122.83	112.24
3	B	403	BLM	C9-C10-C12	5.22	133.30	123.14
3	A	402	BLM	C9-C10-NG	-5.18	117.78	123.31
3	B	403	BLM	C9-C10-NG	-5.00	117.97	123.31
3	A	402	BLM	O68-C68-C69	4.76	118.56	107.70
3	B	403	BLM	O68-C68-C69	4.75	118.52	107.70
3	A	402	BLM	O68-C70-O70	4.43	128.17	123.69
2	A	401	COA	N3A-C2A-N1A	-4.40	121.80	128.68
3	A	402	BLM	C3-C2-C1	3.91	115.54	108.66
3	B	403	BLM	O70-C70-NQ	-3.84	119.18	125.51
3	A	402	BLM	O70-C70-NQ	-3.82	119.21	125.51
3	A	402	BLM	O1-C1-NA	-3.81	116.37	123.00
3	B	403	BLM	O68-C70-O70	3.65	127.39	123.69
3	B	403	BLM	O1-C1-NA	-3.43	117.03	123.00
3	B	403	BLM	C54-S53-C52	3.12	107.16	101.63
2	A	401	COA	O9A-P3B-O7A	-3.02	98.88	110.68
3	A	402	BLM	C55-S53-C52	3.00	106.95	101.63
2	A	401	COA	O8A-P3B-O3B	2.98	119.35	105.99
3	A	402	BLM	NF-C8-NE	2.90	121.14	117.03
3	A	402	BLM	C54-S53-C52	2.81	106.61	101.63
3	B	403	BLM	O1-C1-C2	2.79	124.38	120.30
3	A	402	BLM	O1-C1-C2	2.75	124.34	120.30
3	B	403	BLM	C7-NE-C8	2.73	122.42	118.11
3	A	402	BLM	C47-S46-C46	-2.69	87.88	91.12
3	B	403	BLM	C55-S53-C52	2.68	106.39	101.63
3	A	402	BLM	C63-OH1-C14	2.68	119.35	114.99
3	B	403	BLM	NF-C8-NE	2.67	120.81	117.03
2	A	401	COA	O2A-P1A-O5B	2.67	120.15	107.75
2	A	401	COA	O9A-P3B-O8A	-2.60	97.69	107.64
3	A	402	BLM	C7-NE-C8	2.57	122.18	118.11
3	B	403	BLM	C28-NI-C29	2.50	109.68	105.78
3	A	402	BLM	C64-O64-C65	2.46	118.52	113.69
3	A	402	BLM	C28-NI-C29	2.42	109.55	105.78
3	B	403	BLM	C47-S46-C46	-2.40	88.23	91.12
3	A	402	BLM	CA-C9-C8	-2.35	117.84	121.27
3	A	402	BLM	CB-C31-C33	-2.33	109.57	112.30
3	A	402	BLM	O56-C57-C58	2.32	113.45	107.28
2	A	401	COA	C6P-C5P-N4P	2.31	120.30	116.42
2	A	401	COA	O8A-P3B-O7A	2.30	119.69	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	BLM	C27-C28-NI	-2.26	104.73	108.67
3	A	402	BLM	C27-C28-NI	-2.22	104.80	108.67
3	B	403	BLM	CA-C9-C8	-2.22	118.03	121.27
3	B	403	BLM	C63-O62-C60	2.22	118.04	113.69
3	B	403	BLM	C63-OH1-C14	2.21	118.59	114.99
2	A	401	COA	P1A-O5B-C5B	-2.21	108.74	121.68
2	A	401	COA	P2A-O6A-CCP	-2.17	109.02	121.56
3	B	403	BLM	CB-C31-NK	-2.16	105.97	109.70
2	A	401	COA	O6A-P2A-O4A	-2.10	100.85	109.07
3	B	403	BLM	C48-C49-NP	-2.08	112.67	115.59
3	B	403	BLM	O56-C57-C58	2.08	112.81	107.28
2	A	401	COA	C4A-C5A-N7A	-2.01	107.31	109.40
3	A	402	BLM	C63-O62-C60	2.00	117.62	113.69

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	COA	CCP-O6A-P2A-O3A
2	A	401	COA	CAP-CBP-CCP-O6A
2	A	401	COA	S1P-C2P-C3P-N4P
3	A	402	BLM	NA-C1-C2-C3
3	A	402	BLM	O1-C1-C2-C3
3	A	402	BLM	C7-C6-NC-C3
3	A	402	BLM	C40-C37-C38-OH3
3	A	402	BLM	C40-C37-C38-CD
3	A	402	BLM	C50-C51-C52-S53
3	A	402	BLM	C51-C52-S53-C55
3	A	402	BLM	C51-C52-S53-C54
3	A	402	BLM	NQ-C70-O68-C68
3	A	402	BLM	O70-C70-O68-C68
3	B	403	BLM	C2-C3-NC-C6
3	B	403	BLM	C5-C6-NC-C3
3	B	403	BLM	C7-C6-NC-C3
3	B	403	BLM	CC-C34-C36-O36
3	B	403	BLM	CC-C34-C36-NL
3	B	403	BLM	NL-C37-C38-OH3
3	B	403	BLM	C40-C37-C38-OH3
3	B	403	BLM	C51-C52-S53-C54
3	B	403	BLM	NQ-C70-O68-C68
3	B	403	BLM	O70-C70-O68-C68
3	B	403	BLM	C59-C60-C61-O61

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Mol	Chain	Res	Type	Atoms
3	B	403	BLM	O62-C60-C61-O61
3	A	402	BLM	O62-C60-C61-O61
3	B	403	BLM	ND-C4-C5-C6
3	B	403	BLM	NL-C37-C40-O40
3	B	403	BLM	NL-C37-C40-NM
3	A	402	BLM	NL-C37-C38-OH3
3	A	402	BLM	NL-C37-C38-CD
3	B	403	BLM	C51-C52-S53-C55
3	B	403	BLM	O4-C4-C5-C6
3	A	402	BLM	C59-C60-C61-O61
3	A	402	BLM	C4-C5-C6-NC
3	B	403	BLM	C38-C37-C40-O40
3	A	402	BLM	C1-C2-C3-NC
2	A	401	COA	CEP-CBP-CCP-O6A
3	B	403	BLM	C38-C37-C40-NM
2	A	401	COA	P1A-O3A-P2A-O4A
2	A	401	COA	P1A-O3A-P2A-O5A
3	B	403	BLM	NK-C31-C33-OH2
3	B	403	BLM	NL-C37-C38-CD
2	A	401	COA	CCP-O6A-P2A-O5A
3	B	403	BLM	C69-C68-O68-C70
3	A	402	BLM	NB-C2-C3-NC
3	B	403	BLM	NH-C13-C14-C27
2	A	401	COA	CDP-CBP-CCP-O6A
3	B	403	BLM	C40-C37-C38-CD
2	A	401	COA	C3B-O3B-P3B-O7A
3	A	402	BLM	C5-C6-NC-C3
3	B	403	BLM	NH-C13-C14-OH1
3	B	403	BLM	C50-C51-C52-S53

There are no ring outliers.

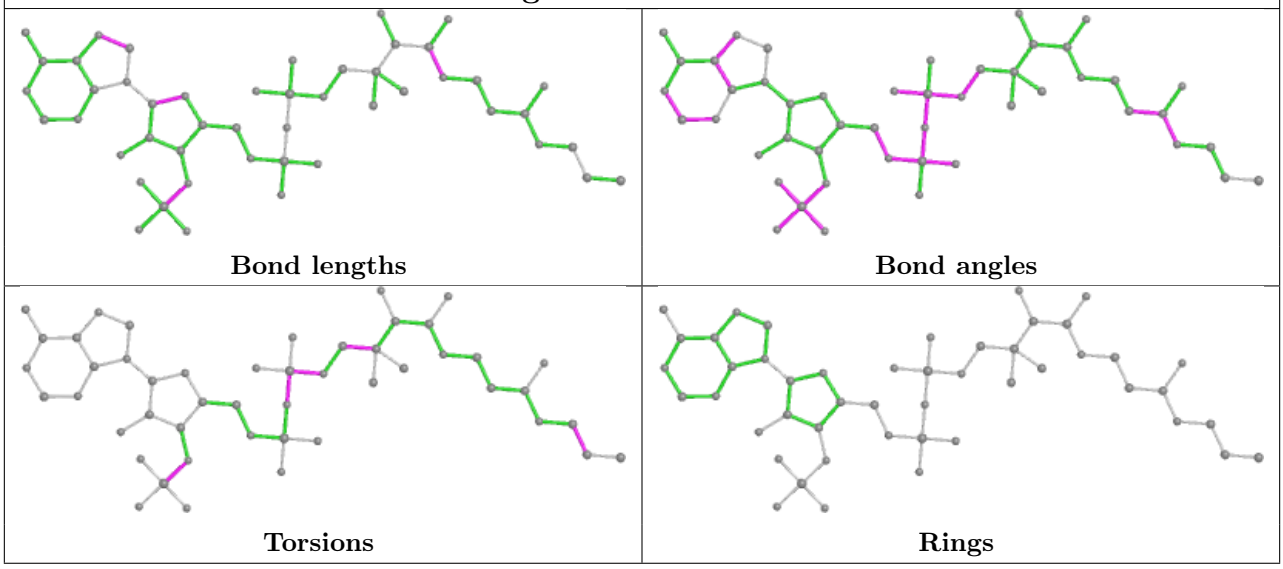
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	COA	4	0
3	A	402	BLM	3	0
3	B	403	BLM	4	0

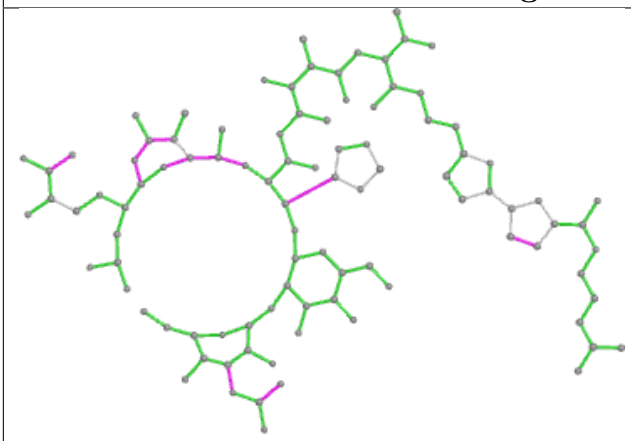
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

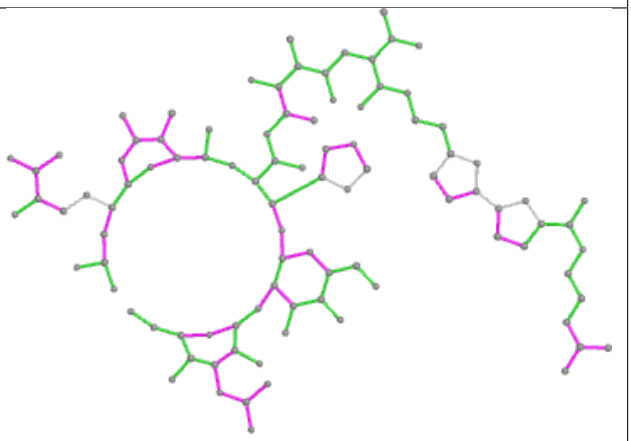
Ligand COA A 401



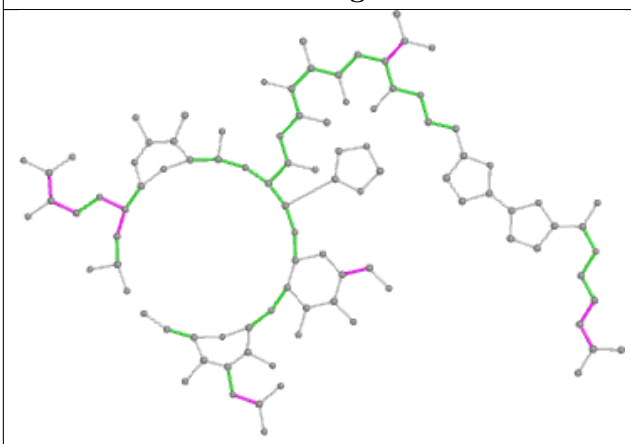
Ligand BLM A 402



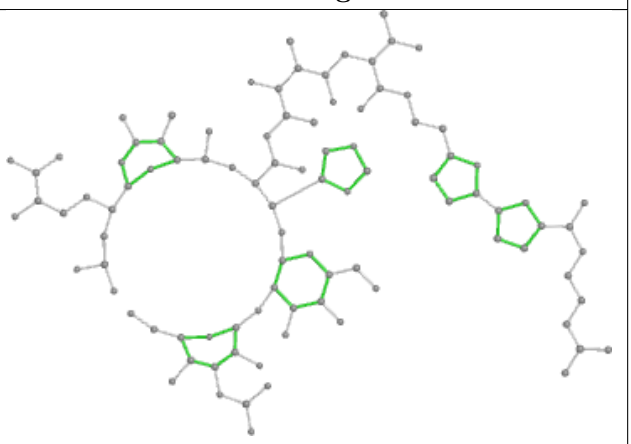
Bond lengths



Bond angles

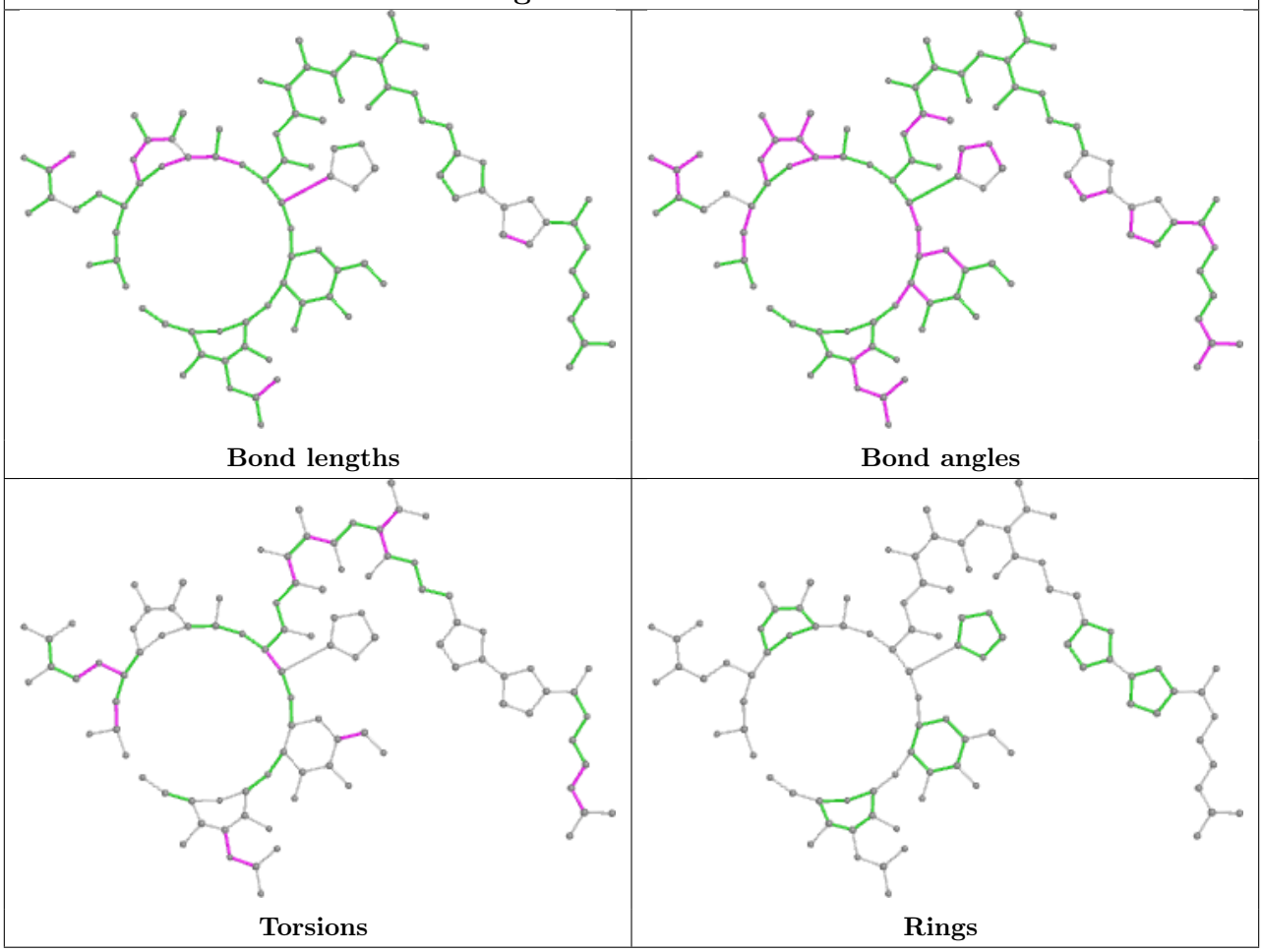


Torsions



Rings

Ligand BLM B 403



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	290/301 (96%)	-0.30	1 (0%)	94	93	6, 23, 51, 70	0
1	B	290/301 (96%)	-0.14	9 (3%)	49	39	6, 25, 57, 74	0
All	All	580/602 (96%)	-0.22	10 (1%)	70	63	6, 24, 54, 74	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	PRO	5.0
1	B	9	THR	3.6
1	B	124	GLY	3.5
1	B	239	PRO	3.3
1	B	241	PRO	2.6
1	B	123	ASP	2.5
1	B	242	GLY	2.4
1	B	163	PRO	2.4
1	B	216	PRO	2.2
1	A	124	GLY	2.1

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)

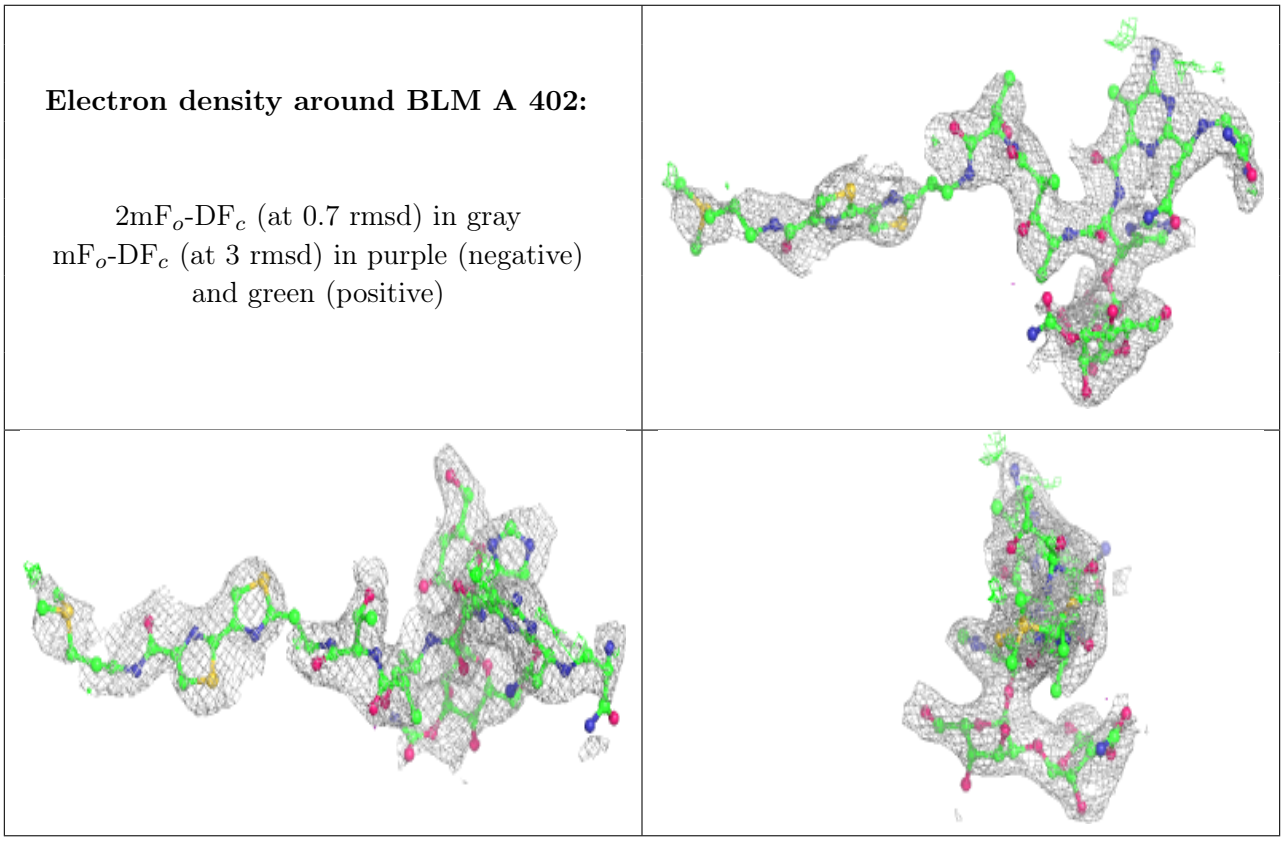
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BLM	A	402	96/96	0.84	0.24	52,75,90,92	0
3	BLM	B	403	96/96	0.89	0.21	20,52,71,90	0
2	COA	A	401	48/48	0.95	0.16	11,29,45,50	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.

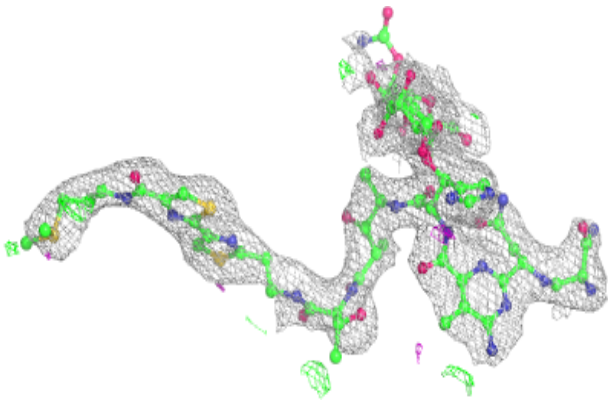
Electron density around BLM A 402:

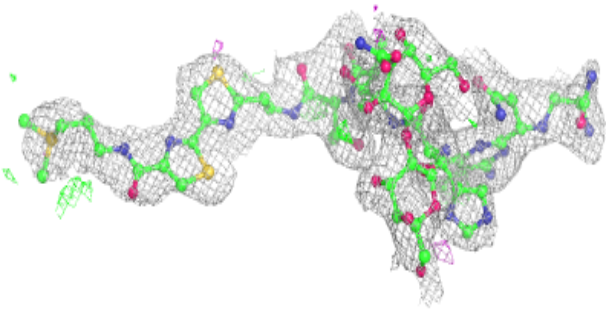
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

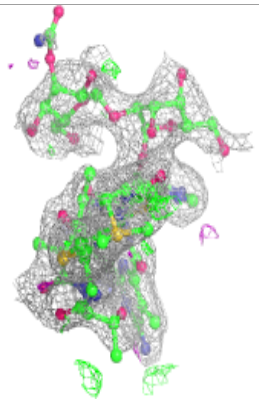


Electron density around BLM B 403:

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

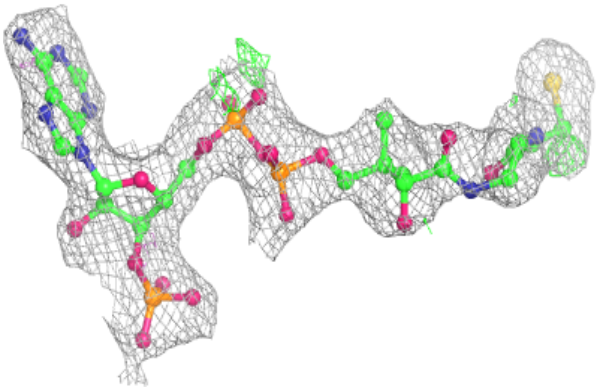


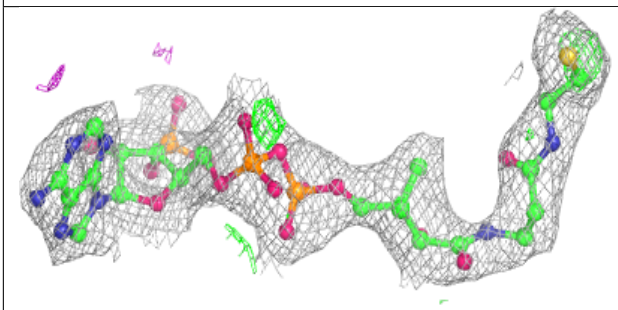


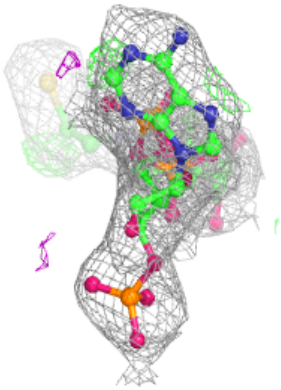


Electron density around COA A 401:

$2mF_o$-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.