Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 02:38 PM EST

PDB ID	:	2OLV
Title	:	Structural Insight Into the Transglycosylation Step Of Bacterial Cell Wall Biosynthesis : Donor Ligand Complex
Authors	:	Lovering, A.L.; De Castro, L.; Lim, D.; Strynadka, N.C.J.
Deposited on	:	2007-01-19
Resolution	:	2.80 Å(reported)

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

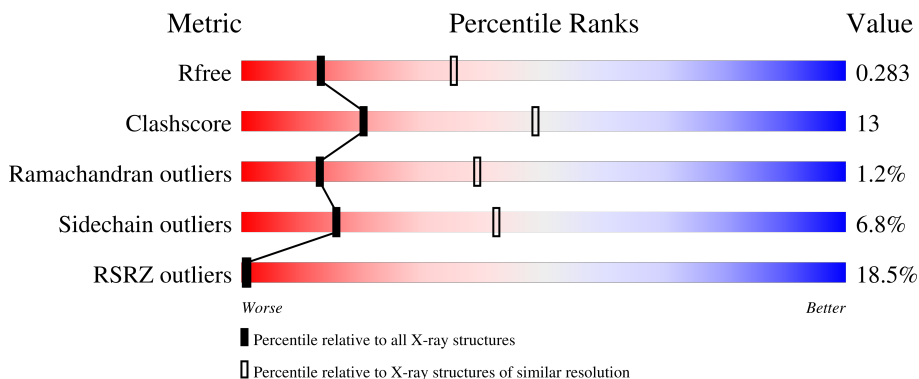|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.283
Clashscore		13
Ramachandran outliers		1.2%
Sidechain outliers		6.8%
RSRZ outliers		18.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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	669	18% ... 66% / 24% / • / 8%
1	B	669	15% ... 69% / 21% / • / 8%

2　Entry composition　ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9878 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total 4851	C 3038	N 837	O 964	Se 12	0	0	0
1	B	618	Total 4859	C 3042	N 839	O 966	Se 12	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MSE	-	SEE REMARK 999	UNP Q2YY56
A	106	MSE	MET	modified residue	UNP Q2YY56
A	257	MSE	MET	modified residue	UNP Q2YY56
A	285	PRO	ALA	variant	UNP Q2YY56
A	311	MSE	MET	modified residue	UNP Q2YY56
A	335	MSE	MET	modified residue	UNP Q2YY56
A	413	MSE	MET	modified residue	UNP Q2YY56
A	439	THR	VAL	variant	UNP Q2YY56
A	548	MSE	MET	modified residue	UNP Q2YY56
A	555	MSE	MET	modified residue	UNP Q2YY56
A	559	MSE	MET	modified residue	UNP Q2YY56
A	580	MSE	MET	modified residue	UNP Q2YY56
A	618	MSE	MET	modified residue	UNP Q2YY56
A	622	MSE	MET	modified residue	UNP Q2YY56
A	652	MSE	MET	modified residue	UNP Q2YY56
B	59	MSE	-	SEE REMARK 999	UNP Q2YY56
B	106	MSE	MET	modified residue	UNP Q2YY56
B	257	MSE	MET	modified residue	UNP Q2YY56
B	285	PRO	ALA	variant	UNP Q2YY56
B	311	MSE	MET	modified residue	UNP Q2YY56
B	335	MSE	MET	modified residue	UNP Q2YY56
B	413	MSE	MET	modified residue	UNP Q2YY56
B	439	THR	VAL	variant	UNP Q2YY56
B	548	MSE	MET	modified residue	UNP Q2YY56
B	555	MSE	MET	modified residue	UNP Q2YY56

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Chain	Residue	Modelled	Actual	Comment	Reference
B	559	MSE	MET	modified residue	UNP Q2YY56
B	580	MSE	MET	modified residue	UNP Q2YY56
B	618	MSE	MET	modified residue	UNP Q2YY56
B	622	MSE	MET	modified residue	UNP Q2YY56
B	652	MSE	MET	modified residue	UNP Q2YY56

- Molecule 2 is MOENOMYCIN (three-letter code: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).
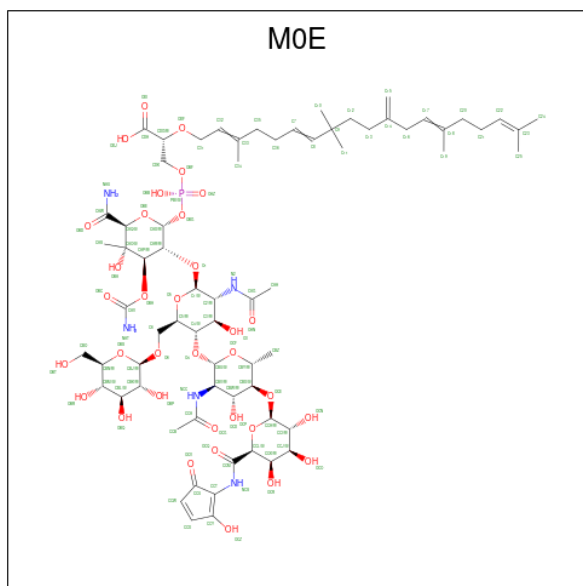
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			84	44	5	34	1		
2	B	1	Total	C	N	O	P	0	0
			84	44	5	34	1		

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 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: Penicillin-binding protein 2

Chain A:

- Molecule 1: Penicillin-binding protein 2

Chain B:
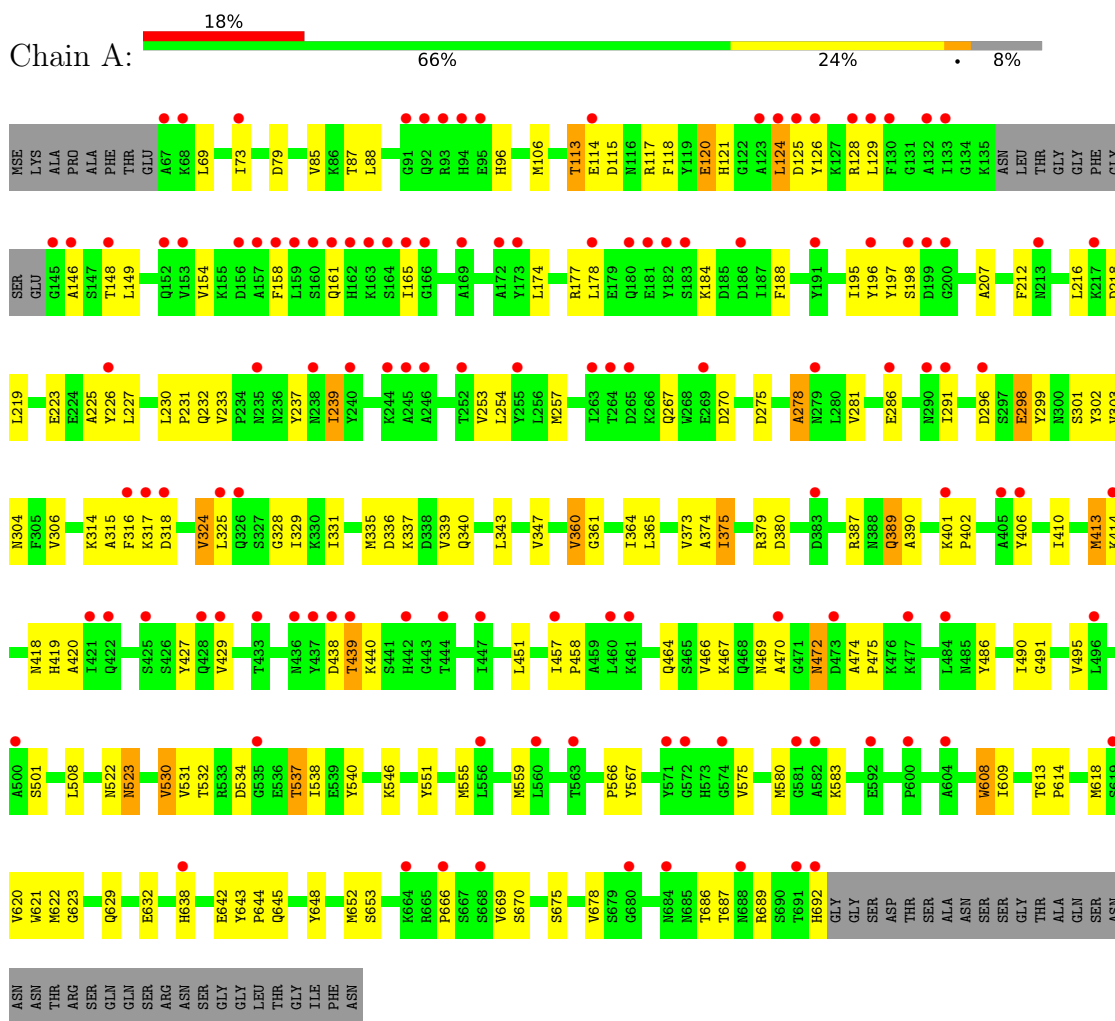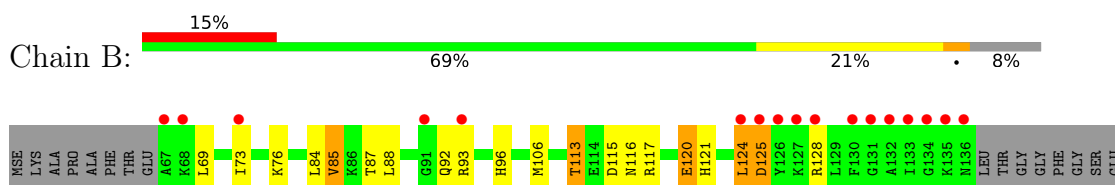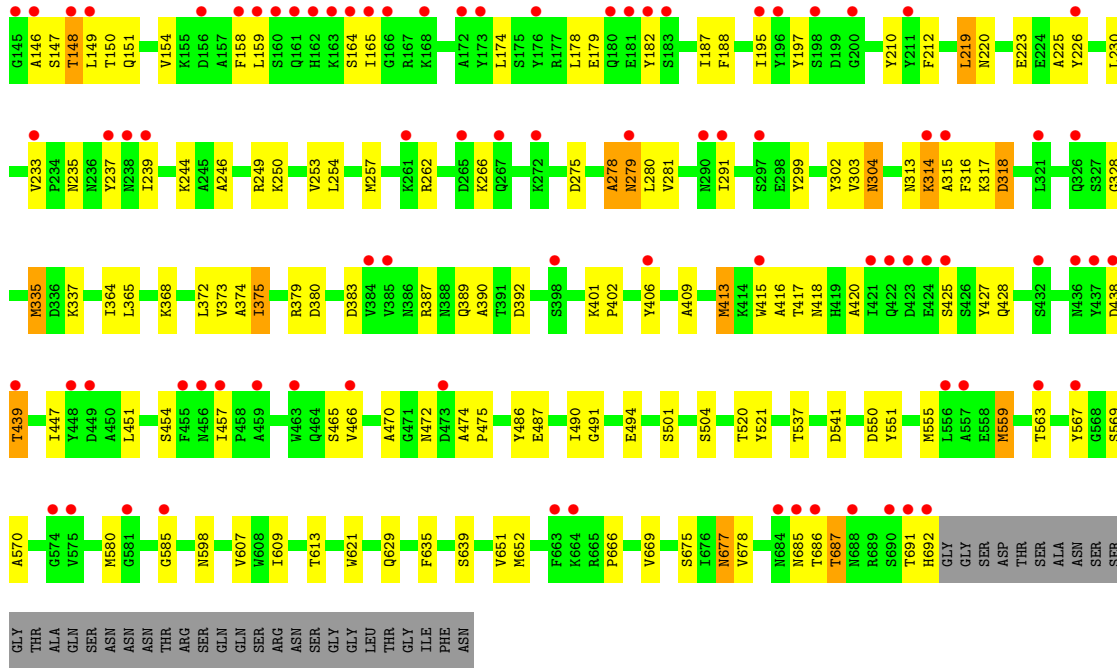
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	79.56Å 212.21Å 91.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 2.80 44.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.15-2.80) 99.9 (44.14-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.231 , 0.280 0.236 , 0.283	Depositor DCC
R_{free} test set	1955 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	58.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 74.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9878	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M0E

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	0.56	0/4943	0.63	0/6662
1	B	0.54	0/4951	0.65	1/6673 (0.0%)
All	All	0.55	0/9894	0.64	1/13335 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

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	B	372	LEU	CB-CG-CD1	-5.87	101.03	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLU	Peptide
1	A	608	TRP	Peptide
1	B	120	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4851	0	4666	124	1
1	B	4859	0	4672	109	0
2	A	84	0	62	6	0
2	B	84	0	62	5	0
All	All	9878	0	9462	242	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG12	1:A:257:MSE:HE2	1.18	1.14
1:A:254:LEU:HA	1:A:257:MSE:HE3	1.45	0.97
1:B:253:VAL:HG12	1:B:257:MSE:HE2	1.52	0.89
1:B:254:LEU:HA	1:B:257:MSE:HE3	1.56	0.88
1:A:551:TYR:HB2	1:A:555:MSE:HE3	1.55	0.87
1:B:413:MSE:HE1	1:B:470:ALA:HB2	1.55	0.87
1:B:551:TYR:HB2	1:B:555:MSE:HE3	1.59	0.85
1:B:85:VAL:HG11	1:B:335:MSE:HE1	1.59	0.84
1:A:438:ASP:O	1:A:439:THR:HG22	1.76	0.84
1:B:438:ASP:O	1:B:439:THR:HG22	1.79	0.82
1:A:225:ALA:HB2	1:A:257:MSE:HE1	1.59	0.82
1:A:233:VAL:HG22	1:A:237:TYR:CE1	2.15	0.81
1:A:302:TYR:HB3	1:A:335:MSE:HE2	1.63	0.80
1:A:451:LEU:HD22	1:A:559:MSE:HE2	1.64	0.77
1:A:118:PHE:O	1:A:184:LYS:NZ	2.18	0.77
1:A:233:VAL:O	1:A:233:VAL:HG23	1.85	0.76
1:B:69:LEU:HD21	1:B:178:LEU:HD11	1.67	0.76
2:A:901:M0E:HAH2	2:A:901:M0E:OBC	1.87	0.75
1:B:225:ALA:HB2	1:B:257:MSE:HE1	1.67	0.75
1:A:413:MSE:HE1	1:A:470:ALA:HB2	1.69	0.73
1:A:451:LEU:CD2	1:A:559:MSE:HE2	2.19	0.73
1:B:128:ARG:HH21	1:B:146:ALA:HB1	1.54	0.72
1:A:336:ASP:OD2	1:A:339:VAL:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:HB2	1:A:686:THR:HG22	1.74	0.69
1:A:225:ALA:CB	1:A:257:MSE:HE1	2.23	0.69
1:A:532:THR:OG1	1:A:534:ASP:OD2	2.05	0.69
1:A:375:ILE:HD11	1:A:390:ALA:HB3	1.74	0.68
1:B:316:PHE:O	1:B:318:ASP:N	2.24	0.68
1:B:233:VAL:HG22	1:B:237:TYR:CE1	2.29	0.68
1:B:420:ALA:HB2	1:B:687:THR:OG1	1.94	0.67
1:A:106:MSE:HE3	1:A:216:LEU:HD22	1.77	0.67
1:A:73:ILE:HG23	1:A:328:GLY:CA	2.25	0.67
1:A:666:PRO:HG2	1:A:669:VAL:HG13	1.78	0.66
1:A:420:ALA:HB2	1:A:687:THR:HG23	1.77	0.65
1:A:207:ALA:HB1	1:A:227:LEU:HD22	1.79	0.65
1:A:406:TYR:CD2	1:A:451:LEU:HD13	2.33	0.64
1:B:239:ILE:HG22	1:B:246:ALA:CB	2.26	0.64
1:B:417:THR:HG22	1:B:559:MSE:SE	2.48	0.64
1:B:451:LEU:HD22	1:B:559:MSE:HE2	1.81	0.63
1:A:125:ASP:O	1:A:126:TYR:CD1	2.52	0.62
1:A:360:VAL:HG13	1:A:622:MSE:HE2	1.81	0.62
1:B:375:ILE:HD11	1:B:390:ALA:HB3	1.80	0.62
1:B:128:ARG:NH2	1:B:146:ALA:HB1	2.15	0.61
1:A:302:TYR:CB	1:A:335:MSE:HE2	2.28	0.61
1:B:148:THR:HG23	1:B:151:GLN:HG2	1.81	0.61
1:B:416:ALA:HB2	1:B:677:ASN:HB3	1.83	0.60
1:B:598:ASN:ND2	1:B:629:GLN:OE1	2.31	0.60
1:B:239:ILE:HD12	1:B:280:LEU:HD22	1.82	0.60
1:B:555:MSE:HE1	1:B:678:VAL:HG22	1.84	0.60
1:A:233:VAL:HG22	1:A:237:TYR:CD1	2.37	0.59
1:B:154:VAL:HG11	1:B:174:LEU:HB2	1.84	0.59
1:B:115:ASP:HB3	1:B:149:LEU:HD13	1.84	0.59
1:A:299:TYR:O	1:A:303:VAL:HG23	2.02	0.59
1:B:120:GLU:N	1:B:120:GLU:OE1	2.36	0.58
1:B:406:TYR:CD2	1:B:451:LEU:HD13	2.38	0.58
1:A:580:MSE:HB3	1:A:613:THR:HG22	1.85	0.58
1:A:389:GLN:HG3	1:A:621:TRP:CZ3	2.39	0.58
1:B:427:TYR:HB2	1:B:457:ILE:HD13	1.84	0.58
1:B:666:PRO:HG2	1:B:669:VAL:HG13	1.84	0.57
1:A:120:GLU:N	1:A:120:GLU:OE1	2.38	0.57
1:A:429:VAL:HG22	1:A:464:GLN:NE2	2.19	0.57
1:A:316:PHE:O	1:A:318:ASP:N	2.38	0.57
1:B:92:GLN:HE22	1:B:291:ILE:HD11	1.69	0.57
2:B:901:M0E:OCV	2:B:901:M0E:OCQ	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ILE:HD12	1:A:645:GLN:HG2	1.87	0.56
1:A:618:MSE:HE2	1:A:620:VAL:CG2	2.35	0.56
1:B:124:LEU:N	1:B:148:THR:HG21	2.21	0.56
1:B:580:MSE:HB3	1:B:613:THR:HG22	1.87	0.56
1:A:73:ILE:HD13	1:A:96:HIS:ND1	2.20	0.56
1:A:254:LEU:CA	1:A:257:MSE:HE3	2.30	0.56
1:B:147:SER:HB2	1:B:151:GLN:HE21	1.71	0.56
1:A:531:VAL:HG22	1:A:537:THR:HB	1.88	0.55
1:B:73:ILE:HD12	1:B:96:HIS:ND1	2.21	0.55
1:B:418:ASN:HB2	1:B:686:THR:HG22	1.88	0.55
1:A:73:ILE:HG23	1:A:73:ILE:O	2.07	0.55
1:A:467:LYS:HG2	1:A:472:ASN:HA	1.89	0.55
1:B:249:ARG:O	1:B:253:VAL:HG23	2.07	0.55
1:B:84:LEU:HD12	1:B:85:VAL:H	1.71	0.55
1:B:226:TYR:CZ	1:B:230:LEU:HD13	2.42	0.55
1:A:413:MSE:CE	1:A:470:ALA:HB2	2.34	0.54
1:A:413:MSE:HE2	1:A:469:ASN:HB2	1.89	0.54
1:A:154:VAL:HG11	1:A:174:LEU:HB2	1.87	0.54
2:A:901:M0E:OCQ	2:A:901:M0E:OCV	2.25	0.54
1:B:85:VAL:HG22	1:B:299:TYR:CZ	2.42	0.54
1:A:115:ASP:HB3	1:A:149:LEU:HD13	1.89	0.54
1:A:364:ILE:HG22	1:A:373:VAL:CG2	2.37	0.53
1:A:530:VAL:HG13	1:A:540:TYR:CE1	2.43	0.53
1:A:618:MSE:HE2	1:A:620:VAL:HG22	1.90	0.53
1:A:486:TYR:CD1	1:A:490:ILE:HD11	2.44	0.53
1:A:125:ASP:O	1:A:126:TYR:CG	2.62	0.53
1:B:302:TYR:CZ	1:B:335:MSE:HB2	2.44	0.53
1:A:233:VAL:O	1:A:233:VAL:CG2	2.57	0.53
1:B:73:ILE:CD1	1:B:96:HIS:ND1	2.72	0.53
1:A:302:TYR:O	1:A:306:VAL:HG23	2.09	0.52
1:B:124:LEU:H	1:B:148:THR:HG21	1.73	0.52
1:A:429:VAL:HG22	1:A:464:GLN:HE22	1.73	0.52
1:B:563:THR:HG22	1:B:570:ALA:HB3	1.92	0.52
1:A:73:ILE:HG23	1:A:328:GLY:HA2	1.91	0.52
1:A:113:THR:HG22	1:A:114:GLU:HG2	1.92	0.52
2:A:901:M0E:H62	2:A:901:M0E:HBU	1.93	0.51
1:A:324:VAL:HG13	1:A:329:ILE:HD13	1.93	0.51
1:A:575:VAL:HG23	1:A:580:MSE:SE	2.59	0.51
1:A:410:ILE:HD13	1:A:555:MSE:SE	2.61	0.50
1:B:304:ASN:HB2	1:B:383:ASP:OD1	2.11	0.50
1:A:555:MSE:O	1:A:559:MSE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD11	1:B:174:LEU:HD12	1.93	0.50
1:B:438:ASP:O	1:B:439:THR:CG2	2.57	0.50
1:B:239:ILE:HG22	1:B:246:ALA:HB3	1.94	0.50
1:B:691:THR:HG22	1:B:692:HIS:N	2.27	0.50
1:A:226:TYR:CZ	1:A:230:LEU:HD13	2.46	0.50
1:A:418:ASN:HB2	1:A:686:THR:CG2	2.40	0.49
1:B:314:LYS:HG3	1:B:315:ALA:N	2.25	0.49
1:A:302:TYR:CZ	1:A:335:MSE:HB2	2.47	0.49
2:B:901:M0E:OBC	2:B:901:M0E:HAH2	2.13	0.49
1:B:106:MSE:HE2	1:B:219:LEU:HD21	1.95	0.49
1:B:364:ILE:HD11	1:B:651:VAL:HG11	1.94	0.49
1:A:567:TYR:CZ	1:A:692:HIS:HB2	2.47	0.49
1:B:313:ASN:O	1:B:314:LYS:C	2.49	0.49
1:A:457:ILE:HB	1:A:458:PRO:HD3	1.94	0.48
1:A:420:ALA:HB2	1:A:687:THR:CG2	2.43	0.48
2:A:901:M0E:HBJ	2:A:901:M0E:O5	2.13	0.48
1:B:88:LEU:HD11	1:B:303:VAL:HG11	1.96	0.48
1:B:150:THR:HG21	1:B:179:GLU:OE2	2.14	0.48
1:A:88:LEU:HD21	1:A:303:VAL:HG11	1.96	0.48
1:A:124:LEU:HD12	1:A:125:ASP:H	1.79	0.48
1:A:302:TYR:CD1	1:A:335:MSE:HE3	2.49	0.48
1:A:254:LEU:HD23	1:A:257:MSE:CE	2.44	0.47
1:A:316:PHE:CD2	1:A:324:VAL:HG21	2.48	0.47
1:A:73:ILE:HG23	1:A:328:GLY:N	2.28	0.47
1:B:365:LEU:HD12	1:B:365:LEU:C	2.35	0.47
1:B:373:VAL:HG13	1:B:374:ALA:N	2.28	0.47
1:A:124:LEU:H	1:A:148:THR:HG21	1.80	0.47
1:A:197:TYR:O	1:A:198:SER:HB3	2.14	0.47
1:A:306:VAL:CG1	1:A:331:ILE:HG21	2.45	0.47
1:A:427:TYR:HB2	1:A:457:ILE:HD12	1.96	0.47
1:A:195:ILE:HD12	1:A:231:PRO:CG	2.45	0.46
1:B:555:MSE:O	1:B:559:MSE:HB2	2.15	0.46
1:B:580:MSE:CE	1:B:652:MSE:HE3	2.46	0.46
1:A:414:LYS:HD3	1:A:678:VAL:HG11	1.98	0.46
1:A:555:MSE:HE1	1:A:678:VAL:HG22	1.97	0.46
1:B:73:ILE:CG2	1:B:328:GLY:CA	2.94	0.46
1:B:113:THR:OG1	1:B:253:VAL:HG13	2.15	0.46
1:B:254:LEU:HD23	1:B:257:MSE:HE3	1.97	0.46
1:B:124:LEU:HD12	1:B:125:ASP:H	1.81	0.46
1:A:613:THR:HB	1:A:614:PRO:CD	2.46	0.46
1:B:147:SER:HB2	1:B:151:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASP:O	1:B:504:SER:HA	2.15	0.46
1:B:474:ALA:N	1:B:475:PRO:CD	2.78	0.46
1:A:85:VAL:HG13	1:A:299:TYR:CE1	2.51	0.46
1:A:302:TYR:CE1	1:A:335:MSE:HB2	2.51	0.46
1:A:418:ASN:O	1:A:419:HIS:C	2.54	0.46
1:A:196:TYR:CE1	1:A:198:SER:HA	2.52	0.45
1:A:340:GLN:HA	1:A:374:ALA:HB1	1.97	0.45
1:A:418:ASN:HD21	1:A:675:SER:HB3	1.80	0.45
1:A:73:ILE:HD12	1:A:96:HIS:HB3	1.98	0.45
1:B:69:LEU:HD12	1:B:182:TYR:CZ	2.51	0.45
1:B:73:ILE:HG23	1:B:328:GLY:HA2	1.98	0.45
2:B:901:M0E:HAH2	2:B:901:M0E:CAV	2.46	0.45
1:A:232:GLN:O	2:A:901:M0E:H1	2.16	0.45
1:B:117:ARG:O	1:B:121:HIS:HB2	2.16	0.45
1:A:566:PRO:O	1:A:567:TYR:HB2	2.16	0.45
1:B:409:ALA:HA	1:B:466:VAL:HG22	1.98	0.45
1:A:79:ASP:HB3	1:A:85:VAL:HG21	1.99	0.44
1:A:551:TYR:HB2	1:A:669:VAL:HG12	1.99	0.44
1:B:291:ILE:O	1:B:291:ILE:HG23	2.17	0.44
1:B:491:GLY:O	1:B:494:GLU:HG2	2.16	0.44
1:A:466:VAL:O	1:A:470:ALA:HB3	2.17	0.44
1:B:220:ASN:OD1	1:B:220:ASN:C	2.56	0.44
1:B:226:TYR:CE2	1:B:230:LEU:HD13	2.52	0.44
1:B:609:ILE:HG23	1:B:609:ILE:O	2.18	0.44
1:A:508:LEU:HD12	1:A:608:TRP:CZ3	2.52	0.44
1:A:638:HIS:O	1:A:642:GLU:HB2	2.18	0.44
1:B:212:PHE:CE2	1:B:223:GLU:HG2	2.53	0.44
1:A:117:ARG:O	1:A:121:HIS:HB2	2.18	0.44
1:A:522:ASN:O	1:A:523:ASN:C	2.55	0.44
1:A:643:TYR:N	1:A:644:PRO:HD2	2.32	0.44
1:B:195:ILE:HG13	1:B:197:TYR:CE1	2.53	0.44
1:A:302:TYR:HA	1:A:375:ILE:CG2	2.48	0.44
1:A:361:GLY:HA3	1:A:389:GLN:HB3	1.99	0.43
1:A:401:LYS:N	1:A:402:PRO:CD	2.82	0.43
1:B:486:TYR:CD1	1:B:490:ILE:HD11	2.53	0.43
1:A:343:LEU:O	1:A:347:VAL:HG23	2.18	0.43
1:A:648:TYR:CZ	1:A:652:MSE:HG3	2.54	0.43
2:A:901:M0E:H62	2:A:901:M0E:CBU	2.48	0.43
1:B:116:ASN:OD1	1:B:262:ARG:NH1	2.51	0.43
1:B:389:GLN:HG3	1:B:621:TRP:CZ3	2.53	0.43
1:A:438:ASP:O	1:A:439:THR:CG2	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:TYR:CZ	1:B:692:HIS:HB2	2.53	0.43
1:B:76:LYS:HG2	1:B:87:THR:HG23	2.00	0.43
1:A:230:LEU:N	1:A:231:PRO:CD	2.81	0.43
1:B:85:VAL:HG11	1:B:335:MSE:CE	2.38	0.42
1:B:230:LEU:HD12	1:B:237:TYR:HB2	2.00	0.42
1:B:416:ALA:O	1:B:447:ILE:HD11	2.19	0.42
1:A:296:ASP:C	1:A:298:GLU:N	2.73	0.42
1:A:530:VAL:HG13	1:A:540:TYR:HE1	1.83	0.42
1:A:296:ASP:O	1:A:298:GLU:N	2.52	0.42
1:B:88:LEU:N	1:B:88:LEU:CD2	2.83	0.42
1:B:225:ALA:CB	1:B:257:MSE:HE1	2.44	0.42
1:B:279:ASN:HD22	1:B:279:ASN:HA	1.68	0.42
1:A:226:TYR:CZ	1:A:239:ILE:HG23	2.55	0.42
1:A:275:ASP:O	1:A:278:ALA:HB2	2.20	0.42
1:B:150:THR:HG23	1:B:187:ILE:HD13	2.01	0.42
1:B:69:LEU:HD21	1:B:178:LEU:CD1	2.43	0.42
1:B:92:GLN:NE2	1:B:291:ILE:HD11	2.34	0.42
1:A:88:LEU:HD12	1:A:325:LEU:HD22	2.01	0.42
1:A:314:LYS:HG3	1:A:315:ALA:N	2.34	0.42
1:B:233:VAL:CG2	1:B:237:TYR:CE1	2.99	0.42
1:A:281:VAL:O	1:A:281:VAL:HG13	2.19	0.42
2:B:901:M0E:OCQ	2:B:901:M0E:OCD	2.38	0.41
1:B:401:LYS:N	1:B:402:PRO:CD	2.84	0.41
1:B:418:ASN:HD21	1:B:675:SER:HB2	1.85	0.41
1:A:491:GLY:O	1:A:495:VAL:HG23	2.20	0.41
1:B:281:VAL:HG13	1:B:281:VAL:O	2.20	0.41
1:B:551:TYR:HB2	1:B:669:VAL:HG12	2.03	0.41
1:B:373:VAL:CG1	1:B:374:ALA:N	2.82	0.41
1:B:413:MSE:HE1	1:B:470:ALA:CB	2.40	0.41
1:B:451:LEU:CD2	1:B:559:MSE:HE2	2.47	0.41
1:A:538:ILE:HD12	1:A:538:ILE:N	2.36	0.41
1:B:124:LEU:HD22	1:B:151:GLN:HE22	1.85	0.41
1:B:84:LEU:HD12	1:B:85:VAL:N	2.33	0.41
1:B:607:VAL:HG22	1:B:635:PHE:CE1	2.56	0.41
1:A:439:THR:HG23	1:A:440:LYS:N	2.36	0.41
1:B:93:ARG:NH1	1:B:210:TYR:CE2	2.88	0.41
1:B:401:LYS:NZ	1:B:454:SER:O	2.54	0.41
1:B:585:GLY:O	1:B:607:VAL:HA	2.20	0.41
1:A:113:THR:CG2	1:A:114:GLU:HG2	2.50	0.41
1:A:128:ARG:HH21	1:A:146:ALA:HB1	1.85	0.40
1:A:364:ILE:HG22	1:A:373:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ALA:N	1:A:475:PRO:CD	2.83	0.40
1:A:575:VAL:HG11	1:A:653:SER:HA	2.04	0.40
1:B:235:ASN:HB2	2:B:901:M0E:HCB1	2.03	0.40
1:B:375:ILE:HD11	1:B:390:ALA:CB	2.50	0.40
1:A:364:ILE:CG2	1:A:373:VAL:CG2	2.99	0.40
1:B:490:ILE:HA	1:B:494:GLU:HG3	2.03	0.40
1:A:621:TRP:CZ2	1:A:623:GLY:HA3	2.57	0.40
1:B:415:TRP:HZ2	1:B:465:SER:HG	1.68	0.40
1:A:69:LEU:HD21	1:A:178:LEU:HD11	2.03	0.40
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.97	0.40
1:A:212:PHE:CE2	1:A:223:GLU:HG2	2.57	0.40
1:A:418:ASN:HD21	1:A:675:SER:CB	2.35	0.40
1:B:275:ASP:O	1:B:278:ALA:HB2	2.21	0.40
1:B:364:ILE:O	1:B:373:VAL:HG12	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TYR:OH	1:A:126:TYR:OH[2_465]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	613/669 (92%)	538 (88%)	67 (11%)	8 (1%)	12	36
1	B	614/669 (92%)	554 (90%)	53 (9%)	7 (1%)	14	41
All	All	1227/1338 (92%)	1092 (89%)	120 (10%)	15 (1%)	13	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	PHE
1	A	278	ALA
1	A	317	LYS
1	A	337	LYS
1	A	439	THR
1	B	158	PHE
1	B	278	ALA
1	B	439	THR
1	B	314	LYS
1	B	317	LYS
1	A	523	ASN
1	B	164	SER
1	B	165	ILE
1	A	165	ILE
1	A	291	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	520/546 (95%)	486 (94%)	34 (6%)	17	44
1	B	521/546 (95%)	484 (93%)	37 (7%)	14	39
All	All	1041/1092 (95%)	970 (93%)	71 (7%)	16	42

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	A	113	THR
1	A	124	LEU
1	A	161	GLN
1	A	177	ARG
1	A	188	PHE
1	A	218	ASP
1	A	219	LEU
1	A	239	ILE

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Mol	Chain	Res	Type
1	A	267	GLN
1	A	270	ASP
1	A	286	GLU
1	A	298	GLU
1	A	301	SER
1	A	304	ASN
1	A	324	VAL
1	A	360	VAL
1	A	365	LEU
1	A	375	ILE
1	A	379	ARG
1	A	380	ASP
1	A	387	ARG
1	A	389	GLN
1	A	413	MSE
1	A	472	ASN
1	A	501	SER
1	A	530	VAL
1	A	537	THR
1	A	546	LYS
1	A	583	LYS
1	A	629	GLN
1	A	632	GLU
1	A	670	SER
1	A	689	ARG
1	B	85	VAL
1	B	113	THR
1	B	124	LEU
1	B	125	ASP
1	B	148	THR
1	B	188	PHE
1	B	219	LEU
1	B	244	LYS
1	B	250	LYS
1	B	266	LYS
1	B	279	ASN
1	B	304	ASN
1	B	318	ASP
1	B	335	MSE
1	B	337	LYS
1	B	368	LYS
1	B	375	ILE

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Mol	Chain	Res	Type
1	B	379	ARG
1	B	380	ASP
1	B	387	ARG
1	B	413	MSE
1	B	425	SER
1	B	428	GLN
1	B	472	ASN
1	B	487	GLU
1	B	501	SER
1	B	520	THR
1	B	521	TYR
1	B	537	THR
1	B	541	ASP
1	B	550	ASP
1	B	559	MSE
1	B	569	SER
1	B	639	SER
1	B	677	ASN
1	B	685	ASN
1	B	687	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
1	A	598	ASN
1	A	629	GLN
1	A	692	HIS
1	B	92	GLN
1	B	151	GLN
1	B	279	ASN
1	B	282	ASN

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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	M0E	B	901	-	85,89,114	1.53	6 (7%)	118,134,166	1.72	26 (22%)
2	M0E	A	901	-	85,89,114	1.56	7 (8%)	118,134,166	1.64	24 (20%)

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	M0E	B	901	-	-	22/56/175/206	0/6/6/6
2	M0E	A	901	-	-	22/56/175/206	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	M0E	CCX-CCW	8.49	1.54	1.35
2	A	901	M0E	CCX-CCW	8.39	1.53	1.35
2	A	901	M0E	OCQ-CCM	6.75	1.36	1.23
2	B	901	M0E	OCQ-CCM	6.56	1.36	1.23
2	B	901	M0E	CCT-NCS	-3.48	1.33	1.41
2	B	901	M0E	CCT-CCU	-3.34	1.39	1.49
2	A	901	M0E	CCX-CCY	3.09	1.53	1.43
2	A	901	M0E	CCT-CCU	-3.08	1.40	1.49
2	B	901	M0E	CCX-CCY	2.94	1.53	1.43
2	A	901	M0E	CCT-NCS	-2.78	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	M0E	O6-CBJ	2.70	1.44	1.40
2	A	901	M0E	O6-CBJ	2.56	1.44	1.40
2	A	901	M0E	O4-CBU	2.01	1.47	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	M0E	CCW-CCX-CCY	-5.85	103.45	108.28
2	A	901	M0E	CCW-CCX-CCY	-5.40	103.82	108.28
2	B	901	M0E	OBH-CAV-NAT	4.99	118.34	110.58
2	A	901	M0E	OBH-CAV-OBC	-4.96	118.67	123.69
2	B	901	M0E	OBH-CAV-OBC	-4.77	118.87	123.69
2	B	901	M0E	OCP-CCH-CCI	-4.68	100.44	110.35
2	A	901	M0E	OBH-CAV-NAT	4.63	117.78	110.58
2	A	901	M0E	OBH-CAP-CAO	4.47	114.50	108.12
2	A	901	M0E	C6-O6-CBJ	-4.32	105.29	113.74
2	A	901	M0E	CCL-CCM-NCS	3.94	120.20	114.25
2	B	901	M0E	OBH-CAP-CAO	3.82	113.56	108.12
2	B	901	M0E	CBJ-OBS-CBN	-3.68	106.46	113.69
2	A	901	M0E	C3-C4-C5	-3.61	102.65	110.93
2	B	901	M0E	C1-O1-CAR	-3.59	109.09	117.96
2	A	901	M0E	CBU-OCF-CBY	-3.59	107.50	113.67
2	B	901	M0E	OBG-CAX-CAR	-3.42	102.11	108.38
2	B	901	M0E	O6-CBJ-CBK	3.27	113.40	108.30
2	B	901	M0E	OCE-CCH-CCI	3.21	116.42	108.10
2	B	901	M0E	CCL-CCM-NCS	3.12	118.97	114.25
2	A	901	M0E	OCP-CCH-CCI	-3.06	103.88	110.35
2	B	901	M0E	O6-C6-C5	2.92	114.45	109.05
2	A	901	M0E	CCW-CCU-CCT	2.84	110.97	106.65
2	A	901	M0E	OCF-CBY-CBZ	2.79	112.73	106.70
2	B	901	M0E	OBH-CAP-CAR	-2.70	102.31	108.00
2	B	901	M0E	CBU-O4-C4	-2.69	111.31	117.96
2	A	901	M0E	OCF-CBY-CBX	-2.64	104.22	109.13
2	A	901	M0E	O4-C4-C3	2.62	114.26	107.28
2	A	901	M0E	C6-C5-C4	-2.57	106.97	113.33
2	A	901	M0E	OCE-CBX-CBW	2.55	114.07	107.28
2	B	901	M0E	CBU-OCF-CBY	-2.52	109.33	113.67
2	B	901	M0E	O5-C5-C6	2.45	111.61	106.67
2	B	901	M0E	CCW-CCU-CCT	2.45	110.37	106.65
2	A	901	M0E	O6-CBJ-CBK	2.40	112.05	108.30
2	A	901	M0E	OCE-CCH-CCI	2.36	114.20	108.10
2	B	901	M0E	C6-O6-CBJ	-2.29	109.26	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	M0E	OBS-CBN-CBO	2.26	112.05	106.44
2	A	901	M0E	CCH-OCE-CBX	-2.24	112.42	117.96
2	B	901	M0E	ODJ-CDH-CDG	2.24	117.64	112.72
2	A	901	M0E	OBE-CAX-CAR	2.23	113.93	109.51
2	A	901	M0E	CBW-CBX-CBY	-2.23	107.02	110.30
2	B	901	M0E	OCE-CBX-CBW	2.21	113.17	107.28
2	B	901	M0E	OBE-CAX-OBG	2.18	114.21	111.36
2	B	901	M0E	CBU-CBV-NCC	-2.15	107.30	111.00
2	B	901	M0E	OBF-CDK-CDG	2.12	114.07	107.94
2	A	901	M0E	ODI-CDH-CDG	-2.12	118.40	122.54
2	B	901	M0E	C3-C4-C5	-2.10	106.10	110.93
2	A	901	M0E	CCK-CCL-CCM	2.03	114.98	111.33
2	A	901	M0E	ODJ-CDH-CDG	2.01	117.14	112.72
2	B	901	M0E	C3-C2-N2	-2.00	106.83	110.62
2	A	901	M0E	CBZ-CBY-CBX	2.00	116.46	113.41

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	M0E	ODF-CDG-CDK-OBF
2	A	901	M0E	CDH-CDG-CDK-OBF
2	A	901	M0E	OBE-CAQ-CAW-NAU
2	A	901	M0E	OBC-CAV-OBH-CAP
2	A	901	M0E	NAT-CAV-OBH-CAP
2	A	901	M0E	OCP-CCL-CCM-OCQ
2	A	901	M0E	OCP-CCL-CCM-NCS
2	A	901	M0E	CCK-CCL-CCM-OCQ
2	A	901	M0E	CCK-CCL-CCM-NCS
2	A	901	M0E	CCU-CCT-NCS-CCM
2	B	901	M0E	ODF-CDG-CDK-OBF
2	B	901	M0E	CAR-CAP-OBH-CAV
2	B	901	M0E	OBC-CAV-OBH-CAP
2	B	901	M0E	NAT-CAV-OBH-CAP
2	B	901	M0E	OCP-CCL-CCM-OCQ
2	B	901	M0E	CCK-CCL-CCM-OCQ
2	B	901	M0E	CCK-CCL-CCM-NCS
2	B	901	M0E	CCU-CCT-NCS-CCM
2	B	901	M0E	CAX-OBG-PBI-OBF
2	B	901	M0E	CDK-OBF-PBI-OBG
2	B	901	M0E	CBK-CBJ-O6-C6
2	B	901	M0E	OBS-CBJ-O6-C6

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Mol	Chain	Res	Type	Atoms
2	B	901	M0E	CAO-CAP-OBH-CAV
2	A	901	M0E	CDK-OBF-PBI-OBG
2	A	901	M0E	C5-C6-O6-CBJ
2	A	901	M0E	CDK-OBF-PBI-OBB
2	A	901	M0E	CDK-OBF-PBI-OAZ
2	B	901	M0E	CDK-OBF-PBI-OBB
2	B	901	M0E	CDK-OBF-PBI-OAZ
2	B	901	M0E	OCP-CCL-CCM-NCS
2	A	901	M0E	CCY-CCT-NCS-CCM
2	B	901	M0E	CCY-CCT-NCS-CCM
2	A	901	M0E	CDG-CDK-OBF-PBI
2	A	901	M0E	CAX-OBG-PBI-OBB
2	A	901	M0E	OBE-CAQ-CAW-OBD
2	B	901	M0E	CAX-OBG-PBI-OBB
2	B	901	M0E	CBY-CBX-OCE-CCH
2	B	901	M0E	CBW-CBX-OCE-CCH
2	A	901	M0E	CAX-OBG-PBI-OBF
2	A	901	M0E	CDK-CDG-CDH-ODI
2	A	901	M0E	CAR-CAP-OBH-CAV
2	A	901	M0E	CAO-CAP-OBH-CAV
2	B	901	M0E	CCI-CCH-OCE-CBX
2	B	901	M0E	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	M0E	5	0
2	A	901	M0E	6	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 M0E B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand M0E A 901

Bond lengths

Bond angles

Torsions

Rings
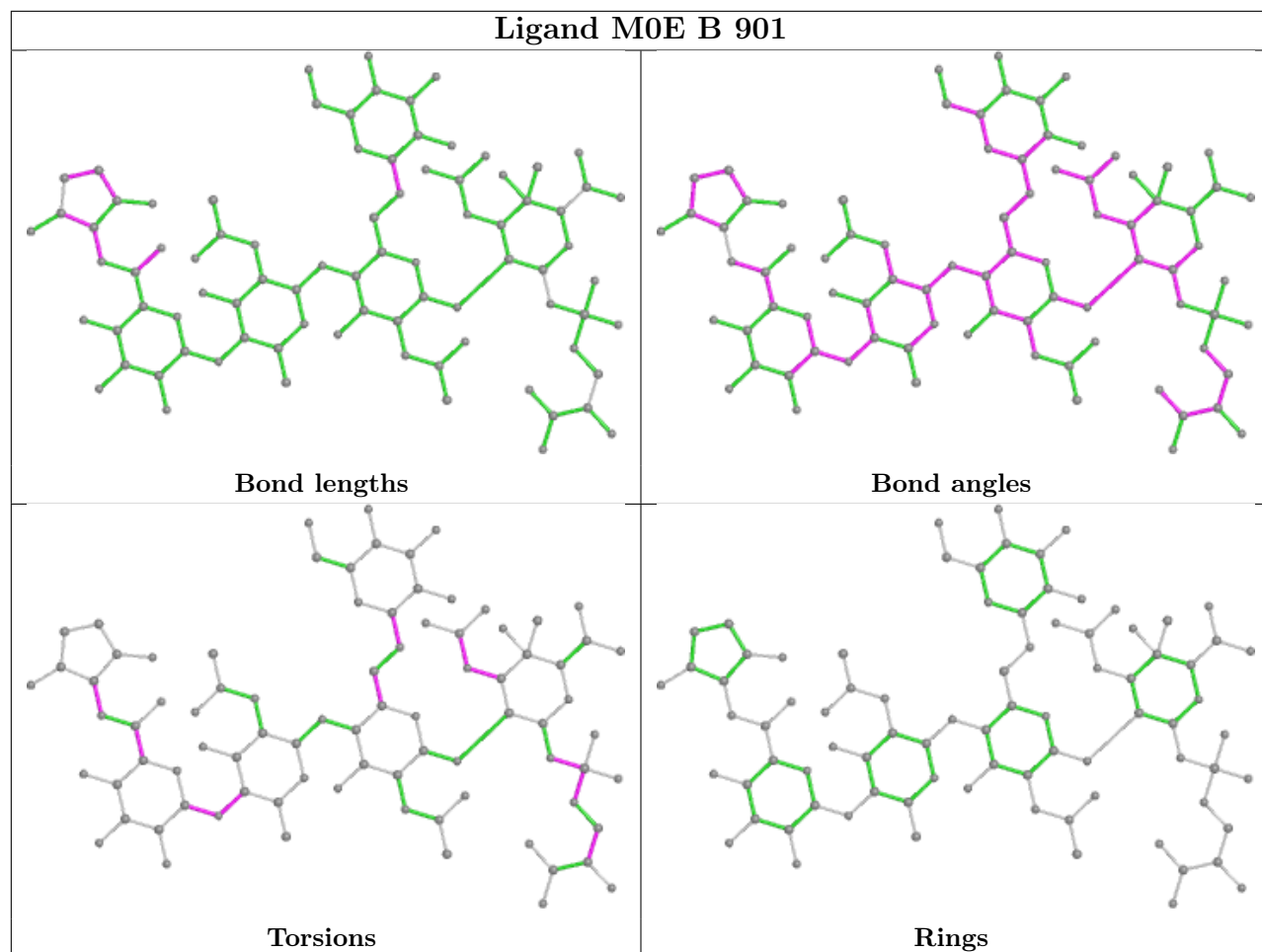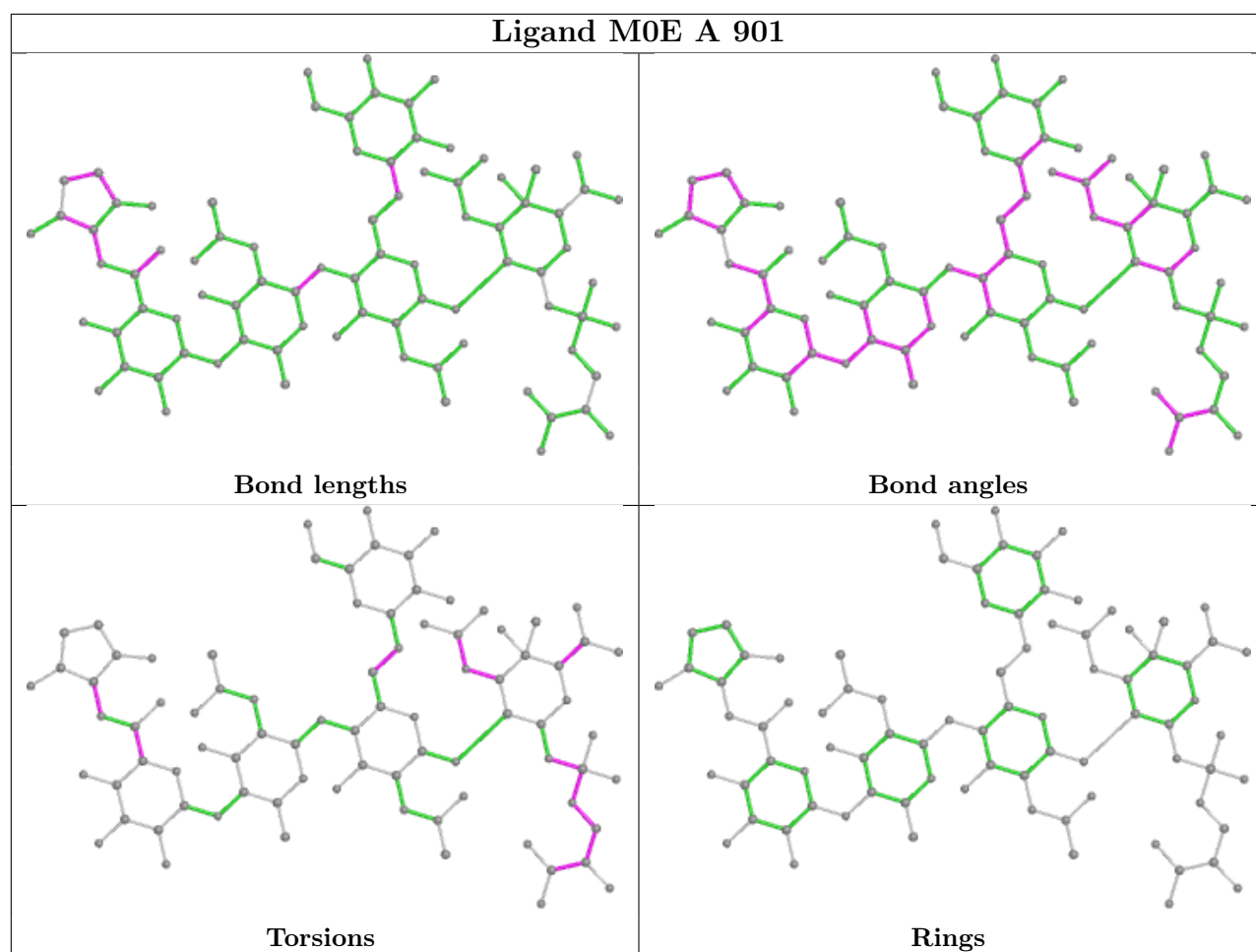
5.7 Other polymers ⓘ

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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	605/669 (90%)	1.28	122 (20%)	1	0	31, 71, 107, 127	0
1	B	606/669 (90%)	1.14	102 (16%)	1	1	33, 72, 108, 127	0
All	All	1211/1338 (90%)	1.21	224 (18%)	1	1	31, 72, 108, 127	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	TYR	13.8
1	B	164	SER	12.7
1	A	162	HIS	11.7
1	A	164	SER	9.9
1	A	124	LEU	9.8
1	B	692	HIS	9.5
1	A	325	LEU	9.0
1	A	165	ILE	7.6
1	B	198	SER	7.6
1	A	133	ILE	7.4
1	A	160	SER	7.1
1	A	159	LEU	7.1
1	B	437	TYR	6.8
1	B	161	GLN	6.8
1	B	684	ASN	6.7
1	A	132	ALA	6.6
1	A	692	HIS	6.5
1	A	161	GLN	6.3
1	B	134	GLY	6.1
1	A	128	ARG	6.1
1	B	162	HIS	5.9
1	B	691	THR	5.8
1	B	406	TYR	5.8
1	A	460	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	131	GLY	5.8
1	A	444	THR	5.7
1	A	129	LEU	5.6
1	A	125	ASP	5.6
1	B	130	PHE	5.6
1	A	114	GLU	5.6
1	B	132	ALA	5.4
1	B	145	GLY	5.4
1	B	160	SER	5.4
1	A	691	THR	5.3
1	B	156	ASP	5.3
1	B	424	GLU	5.1
1	A	130	PHE	5.0
1	B	146	ALA	5.0
1	A	145	GLY	5.0
1	B	265	ASP	4.8
1	A	664	LYS	4.7
1	A	438	ASP	4.6
1	A	437	TYR	4.6
1	B	685	ASN	4.5
1	B	195	ILE	4.4
1	A	200	GLY	4.4
1	A	436	ASN	4.4
1	A	264	THR	4.3
1	A	269	GLU	4.3
1	A	470	ALA	4.3
1	A	173	TYR	4.3
1	B	165	ILE	4.2
1	B	173	TYR	4.2
1	B	135	LYS	4.2
1	A	123	ALA	4.1
1	B	124	LEU	4.1
1	B	158	PHE	4.1
1	A	604	ALA	4.1
1	A	166	GLY	4.0
1	A	291	ILE	4.0
1	A	442	HIS	3.9
1	A	91	GLY	3.9
1	A	405	ALA	3.8
1	A	67	ALA	3.8
1	A	156	ASP	3.7
1	A	226	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	265	ASP	3.7
1	A	252	THR	3.7
1	A	500	ALA	3.7
1	A	317	LYS	3.7
1	B	136	ASN	3.6
1	B	196	TYR	3.6
1	B	163	LYS	3.5
1	A	181	GLU	3.5
1	A	638	HIS	3.5
1	B	183	SER	3.4
1	A	183	SER	3.4
1	A	158	PHE	3.4
1	A	235	ASN	3.4
1	A	240	TYR	3.3
1	B	664	LYS	3.3
1	A	457	ILE	3.3
1	B	67	ALA	3.3
1	B	415	TRP	3.2
1	B	127	LYS	3.2
1	A	217	LYS	3.2
1	B	326	GLN	3.2
1	B	291	ILE	3.2
1	A	246	ALA	3.2
1	A	157	ALA	3.1
1	B	200	GLY	3.1
1	B	425	SER	3.1
1	A	473	ASP	3.1
1	B	423	ASP	3.1
1	B	279	ASN	3.1
1	A	290	ASN	3.1
1	B	180	GLN	3.1
1	A	383	ASP	3.1
1	A	196	TYR	3.1
1	A	439	THR	3.0
1	A	684	ASN	3.0
1	B	459	ALA	3.0
1	A	326	GLN	3.0
1	B	182	TYR	3.0
1	B	181	GLU	3.0
1	B	272	LYS	3.0
1	B	439	THR	3.0
1	B	315	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	133	ILE	2.9
1	B	421	ILE	2.9
1	A	414	LYS	2.9
1	B	290	ASN	2.9
1	A	163	LYS	2.9
1	A	172	ALA	2.9
1	A	425	SER	2.9
1	B	128	ARG	2.9
1	A	146	ALA	2.9
1	A	94	HIS	2.8
1	A	318	ASP	2.8
1	A	668	SER	2.8
1	B	314	LYS	2.8
1	A	263	ILE	2.8
1	A	92	GLN	2.8
1	B	93	ARG	2.8
1	B	398	SER	2.8
1	B	581	GLY	2.7
1	A	182	TYR	2.7
1	A	535	GLY	2.7
1	B	456	ASN	2.7
1	A	191	TYR	2.7
1	B	384	VAL	2.7
1	B	466	VAL	2.7
1	A	688	ASN	2.7
1	B	168	LYS	2.7
1	B	233	VAL	2.7
1	A	180	GLN	2.6
1	A	199	ASP	2.6
1	A	666	PRO	2.6
1	B	455	PHE	2.6
1	A	496	LEU	2.6
1	B	159	LEU	2.6
1	B	385	VAL	2.6
1	A	178	LEU	2.5
1	A	244	LYS	2.5
1	A	406	TYR	2.5
1	A	428	GLN	2.5
1	A	279	ASN	2.5
1	B	563	THR	2.5
1	A	255	TYR	2.5
1	B	297	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	238	ASN	2.5
1	A	238	ASN	2.4
1	A	148	THR	2.4
1	A	429	VAL	2.4
1	A	600	PRO	2.4
1	B	125	ASP	2.4
1	A	186	ASP	2.4
1	B	91	GLY	2.4
1	B	432	SER	2.4
1	A	572	GLY	2.4
1	A	619	SER	2.4
1	B	261	LYS	2.4
1	B	457	ILE	2.4
1	A	245	ALA	2.3
1	A	582	ALA	2.3
1	B	449	ASP	2.3
1	B	237	TYR	2.3
1	A	461	LYS	2.3
1	A	169	ALA	2.3
1	B	166	GLY	2.3
1	A	581	GLY	2.3
1	B	690	SER	2.3
1	A	73	ILE	2.3
1	B	226	TYR	2.3
1	B	574	GLY	2.3
1	A	401	LYS	2.3
1	A	592	GLU	2.2
1	A	574	GLY	2.2
1	B	473	ASP	2.2
1	A	286	GLU	2.2
1	A	447	ILE	2.2
1	B	73	ILE	2.2
1	A	433	THR	2.2
1	A	556	LEU	2.2
1	B	172	ALA	2.2
1	B	663	PHE	2.2
1	A	571	TYR	2.2
1	B	176	TYR	2.2
1	A	152	GLN	2.2
1	B	126	TYR	2.2
1	B	688	ASN	2.2
1	B	557	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	239	ILE	2.2
1	A	296	ASP	2.1
1	A	560	LEU	2.1
1	B	438	ASP	2.1
1	A	68	LYS	2.1
1	A	95	GLU	2.1
1	A	198	SER	2.1
1	B	585	GLY	2.1
1	A	213	ASN	2.1
1	B	575	VAL	2.1
1	B	686	THR	2.1
1	B	211	TYR	2.1
1	B	436	ASN	2.1
1	B	148	THR	2.1
1	B	422	GLN	2.1
1	B	463	TRP	2.1
1	B	149	LEU	2.1
1	B	556	LEU	2.1
1	A	422	GLN	2.1
1	A	93	ARG	2.1
1	B	267	GLN	2.1
1	A	563	THR	2.1
1	A	153	VAL	2.1
1	A	316	PHE	2.1
1	A	421	ILE	2.0
1	B	567	TYR	2.0
1	A	477	LYS	2.0
1	A	680	GLY	2.0
1	B	321	LEU	2.0
1	B	68	LYS	2.0
1	A	484	LEU	2.0
1	B	448	TYR	2.0

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

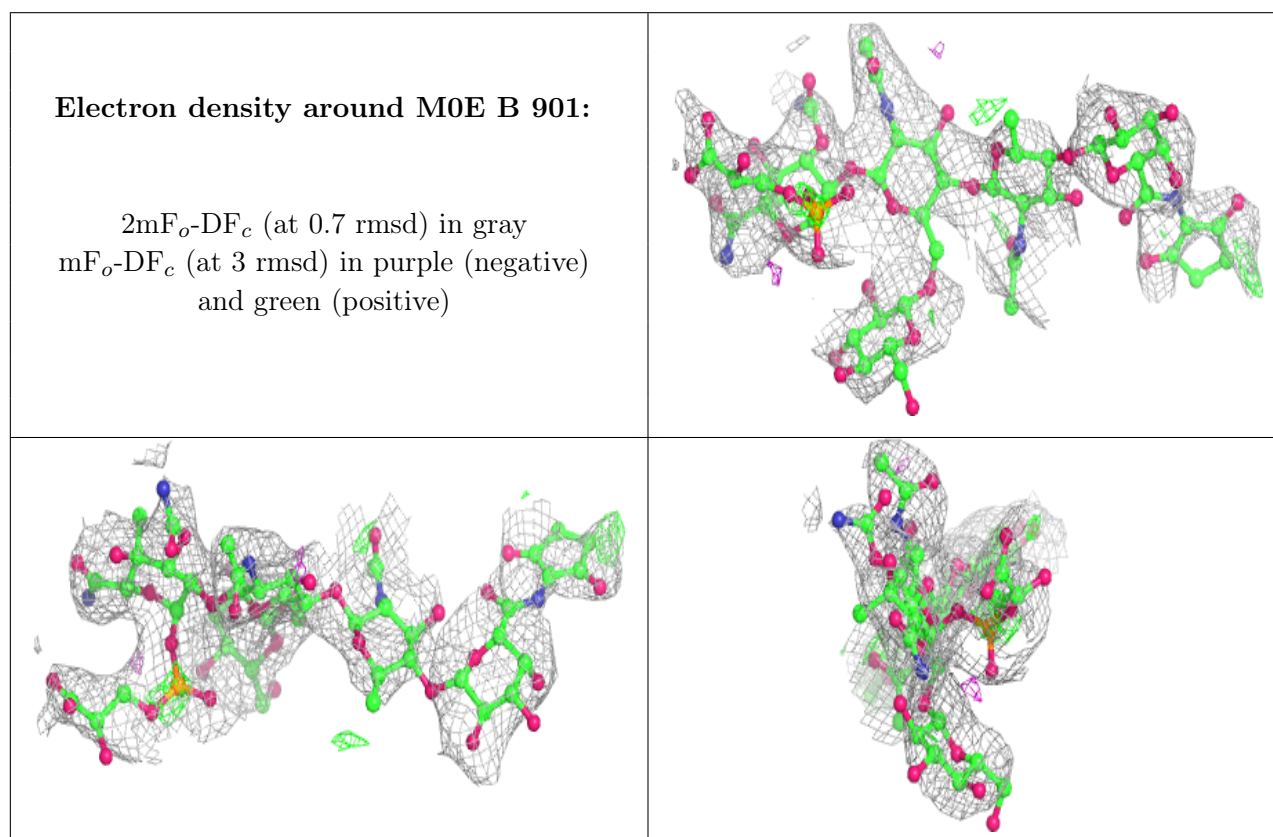There are no non-standard protein/DNA/RNA residues in this entry.

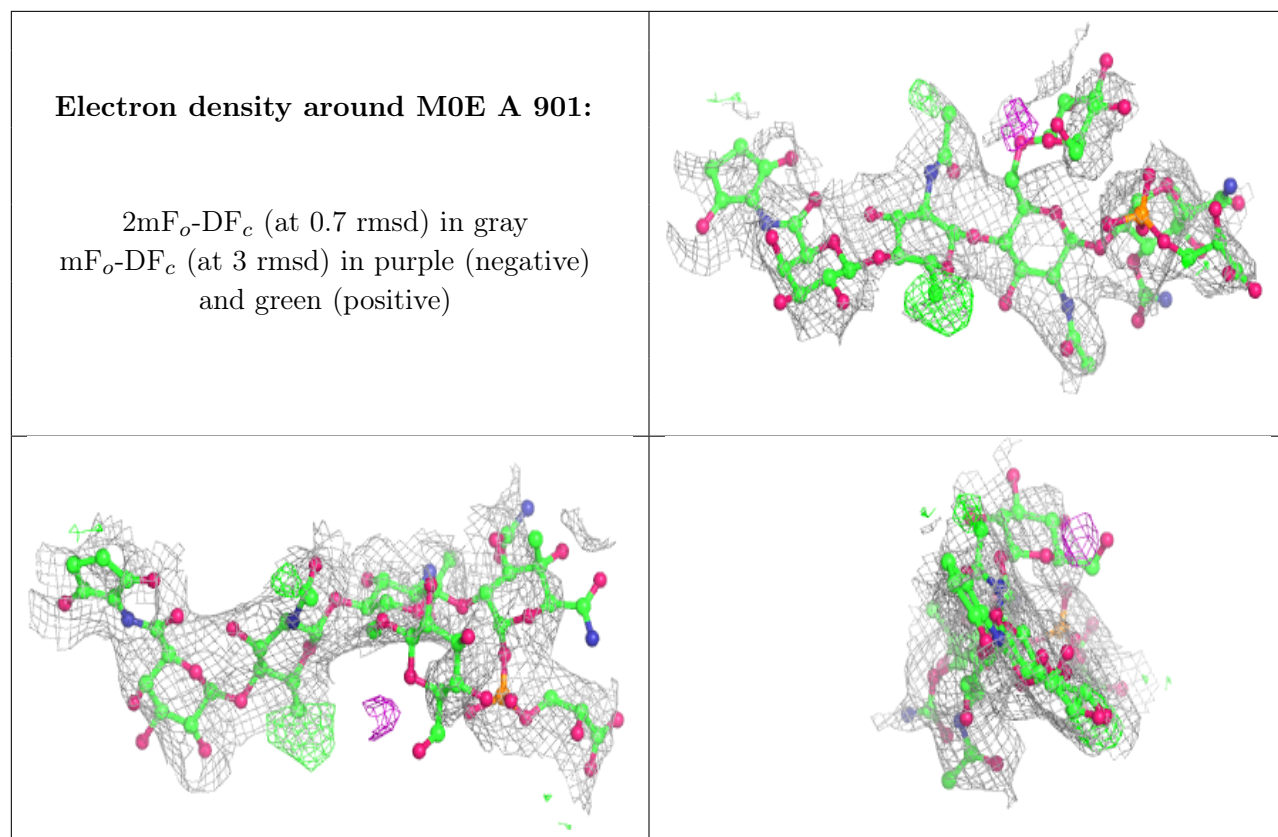## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	M0E	B	901	84/109	0.64	0.34	113,116,124,124	0
2	M0E	A	901	84/109	0.66	0.31	113,116,124,125	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 M0E B 901:

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

Electron density around M0E A 901:

$2mF_o$-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 ⓘ

There are no such residues in this entry.