



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:48 pm BST

PDB ID : 5HLA
Title : E. coli PBP1b in complex with acyl-cephalexin and moenomycin
Authors : King, D.T.; Strynadka, N.C.J.
Deposited on : 2016-01-14
Resolution : 2.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

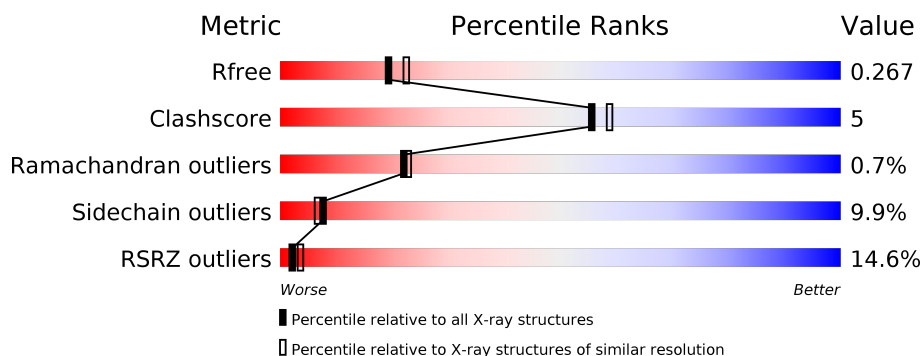
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	747	<div> <div>14%</div> <div>78%</div> <div>13%</div> <div>7%</div> </div>

2 Entry composition [i](#)

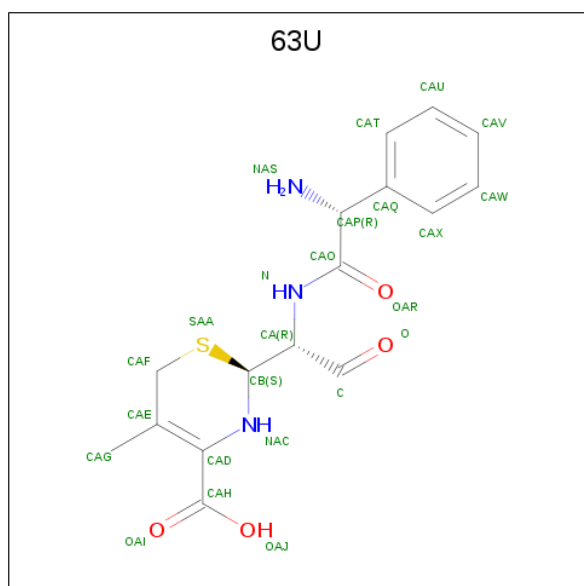
There are 4 unique types of molecules in this entry. The entry contains 5783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1B.

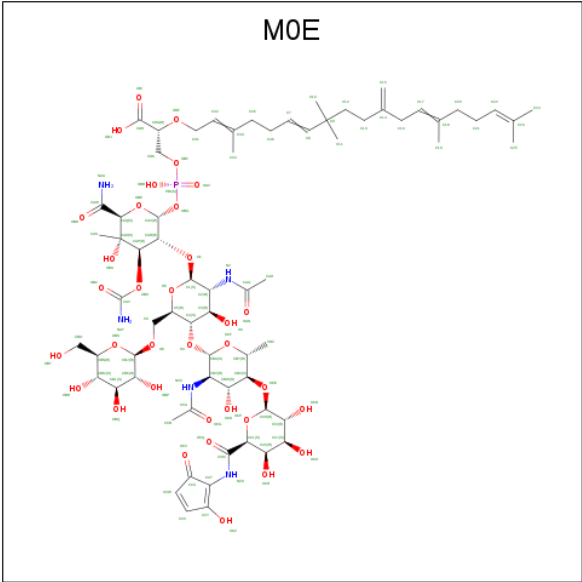
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	5467	3471	959	1011	26	0	0	0

- Molecule 2 is (2S)-2-[(1R)-1-{[(2R)-2-amino-2-phenylacetyl]amino}-2-oxoethyl]-5-methyl-3,6-dihydro-2H-1,3-thiazine-4-carboxylic acid (three-letter code: 63U) (formula: C₁₆H₁₉N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	24	16	3	4	1	0	0

- Molecule 3 is MOENOMYCIN (three-letter code: M0E) (formula: C₆₉H₁₀₆N₅O₃₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	71	36	5	29	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		

- Molecule 1: Penicillin-binding protein 1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.70 Å 63.76 Å 297.62 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.35 – 2.36 62.35 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.1 (62.35-2.36) 93.4 (62.35-2.36)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.37 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.238 , 0.247 0.257 , 0.267	Depositor DCC
R_{free} test set	2448 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.079 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5783	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M0E, 63U

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	0.40	0/5575	0.66	0/7564

There are no bond length outliers.

There are no bond angle outliers.

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	5467	0	5522	42	0
2	A	24	0	0	0	0
3	A	71	0	55	18	0
4	A	221	0	0	0	0
All	All	5783	0	5577	57	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 5.

All (57) 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)
3:A:902:M0E:CAV	3:A:902:M0E:OBH	1.63	1.45
3:A:902:M0E:OBG	3:A:902:M0E:CAX	1.67	1.42
3:A:902:M0E:O1	3:A:902:M0E:CAR	1.65	1.42
3:A:902:M0E:C1	3:A:902:M0E:CAR	2.26	1.13
1:A:239:GLU:HG2	1:A:298:ASP:HB3	1.50	0.93
3:A:902:M0E:CAP	3:A:902:M0E:CAV	2.53	0.87
1:A:544:ASN:HB2	1:A:546:GLN:H	1.51	0.75
1:A:267:THR:O	1:A:271:GLN:OE1	2.09	0.70
3:A:902:M0E:O1	3:A:902:M0E:CAP	2.37	0.70
1:A:544:ASN:H	1:A:545:GLY:HA2	1.59	0.67
3:A:902:M0E:HAS2	3:A:902:M0E:OBD	1.95	0.65
3:A:902:M0E:HCB2	3:A:902:M0E:HBJ	1.82	0.62
1:A:359:ILE:HD12	3:A:902:M0E:HCB1	1.83	0.60
1:A:356:GLY:HA2	3:A:902:M0E:OCG	2.01	0.59
1:A:380:LEU:HD22	1:A:385:ILE:HD11	1.85	0.58
3:A:902:M0E:H1	3:A:902:M0E:CAR	2.31	0.56
3:A:902:M0E:PBI	3:A:902:M0E:CAX	2.93	0.56
1:A:760:PRO:HD2	1:A:763:ILE:HG13	1.88	0.54
1:A:239:GLU:HG2	1:A:298:ASP:CB	2.32	0.52
1:A:398:PRO:O	1:A:399:LEU:HB2	2.10	0.50
1:A:327:PHE:HD1	1:A:350:LEU:HD23	1.77	0.50
1:A:595:LYS:HB3	1:A:661:ALA:HB1	1.94	0.50
1:A:267:THR:HA	1:A:270:GLN:HB2	1.93	0.49
1:A:474:ILE:HG12	1:A:721:THR:HG23	1.94	0.49
1:A:91:ILE:HG23	1:A:95:ILE:HD12	1.95	0.49
1:A:103:PRO:HG3	1:A:212:GLN:HG3	1.95	0.48
1:A:234:ASP:HB2	1:A:268:LEU:HD23	1.94	0.48
1:A:228:THR:HA	1:A:380:LEU:HD21	1.95	0.48
1:A:113:LEU:HD13	1:A:173:LEU:HD21	1.96	0.48
1:A:139:MET:HG3	1:A:146:THR:HG23	1.95	0.48
1:A:378:ARG:HA	1:A:381:GLN:HG2	1.96	0.47
1:A:170:ARG:HG3	1:A:186:MET:HB2	1.95	0.47
1:A:130:ALA:O	1:A:200:ARG:HD3	2.14	0.47
1:A:232:THR:HG23	1:A:233:GLU:HG2	1.96	0.47
1:A:233:GLU:OE2	1:A:271:GLN:NE2	2.45	0.46
1:A:461:LEU:HD22	1:A:733:LEU:HD21	1.95	0.46
1:A:460:ALA:O	1:A:464:GLN:HB2	2.18	0.44
1:A:686:LEU:HD12	1:A:740:MET:HE2	2.00	0.44
1:A:790:PRO:C	1:A:792:SER:H	2.20	0.44
3:A:902:M0E:OCR	3:A:902:M0E:NCS	2.48	0.44
3:A:902:M0E:O1	3:A:902:M0E:CAX	2.56	0.44
1:A:708:THR:HG21	1:A:733:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LEU:HA	1:A:627:THR:HG21	1.99	0.43
3:A:902:M0E:CAG	3:A:902:M0E:NAT	2.81	0.43
1:A:271:GLN:HG2	3:A:902:M0E:HAT2	1.83	0.43
1:A:352:GLY:HA2	1:A:372:ARG:HH11	1.84	0.43
1:A:511:LEU:HD23	1:A:621:VAL:HG11	2.01	0.42
3:A:902:M0E:OCD	3:A:902:M0E:OCP	2.26	0.42
1:A:674:MET:HA	1:A:677:VAL:HG13	2.02	0.42
3:A:902:M0E:OBG	3:A:902:M0E:CAR	2.55	0.41
1:A:232:THR:HG21	1:A:351:VAL:HG13	2.02	0.41
1:A:429:LYS:HA	1:A:430:VAL:C	2.41	0.41
1:A:570:THR:HA	1:A:677:VAL:HG12	2.02	0.41
1:A:736:ALA:O	1:A:740:MET:HB3	2.20	0.41
1:A:303:LYS:H	1:A:303:LYS:HG3	1.52	0.41
1:A:69:LEU:HD22	1:A:69:LEU:HA	1.97	0.40
1:A:476:VAL:HG22	1:A:719:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	689/747 (92%)	650 (94%)	34 (5%)	5 (1%)	22	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	A	237	PHE
1	A	430	VAL
1	A	356	GLY
1	A	790	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
1	A	588/627 (94%)	530 (90%)	58 (10%)	8 7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	74	ILE
1	A	75	VAL
1	A	79	LEU
1	A	89	GLN
1	A	90	LYS
1	A	180	LEU
1	A	197	LEU
1	A	212	GLN
1	A	235	ARG
1	A	238	TYR
1	A	239	GLU
1	A	267	THR
1	A	268	LEU
1	A	272	LEU
1	A	276	LEU
1	A	289	ASN
1	A	295	LEU
1	A	303	LYS
1	A	307	LEU
1	A	321	ASP
1	A	323	GLU
1	A	337	ARG
1	A	344	LEU
1	A	350	LEU
1	A	355	LYS
1	A	359	ILE
1	A	368	LEU
1	A	370	LEU
1	A	372	ARG

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	381	GLN
1	A	387	ASP
1	A	393	MET
1	A	397	ARG
1	A	399	LEU
1	A	402	GLN
1	A	407	VAL
1	A	429	LYS
1	A	431	LYS
1	A	432	ASP
1	A	485	ARG
1	A	495	PHE
1	A	555	ARG
1	A	563	VAL
1	A	600	LYS
1	A	628	ILE
1	A	641	ARG
1	A	659	GLU
1	A	671	LEU
1	A	684	ARG
1	A	686	LEU
1	A	695	LEU
1	A	733	LEU
1	A	750	GLN
1	A	751	THR
1	A	793	LEU
1	A	796	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	236	HIS
1	A	318	GLN

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 carbohydrates 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	$\# Z > 2$
3	M0E	A	902	-	73,75,114	4.01	39 (53%)	106,114,166	2.71	17 (16%)
2	63U	A	901	1	17,25,25	4.03	10 (58%)	19,34,34	3.44	6 (31%)

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
3	M0E	A	902	-	-	13/41/148/206	0/5/5/6
2	63U	A	901	1	-	0/12/35/35	0/1/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	M0E	OBH-CAV	12.33	1.63	1.35
3	A	902	M0E	O1-C1	-10.58	1.12	1.41
3	A	902	M0E	CAW-NAU	10.49	1.59	1.32
3	A	902	M0E	CAV-NAT	9.75	1.51	1.33
2	A	901	63U	CAE-CAD	9.17	1.45	1.34
3	A	902	M0E	O1-CAR	8.27	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	63U	CAX-CAQ	8.21	1.52	1.39
3	A	902	M0E	CCL-CCM	-7.64	1.41	1.52
3	A	902	M0E	OCD-CBW	7.34	1.60	1.43
3	A	902	M0E	CAH-CAG	6.64	1.64	1.50
3	A	902	M0E	OBR-CBM	-6.47	1.27	1.43
3	A	902	M0E	PBI-OBG	6.46	1.71	1.59
2	A	901	63U	CAU-CAT	6.13	1.51	1.38
3	A	902	M0E	CBV-NCC	5.40	1.54	1.45
3	A	902	M0E	CAR-CAP	-5.26	1.41	1.52
3	A	902	M0E	O6-C6	5.07	1.53	1.43
2	A	901	63U	CAW-CAV	4.90	1.51	1.38
3	A	902	M0E	OCP-CCL	4.80	1.51	1.43
3	A	902	M0E	CCA-NCC	4.70	1.50	1.34
3	A	902	M0E	OBH-CAP	4.29	1.52	1.45
2	A	901	63U	CAF-CAE	-4.15	1.46	1.51
3	A	902	M0E	CBZ-CBY	4.05	1.61	1.51
3	A	902	M0E	CBK-CBL	-3.98	1.42	1.52
3	A	902	M0E	OBC-CAV	3.92	1.27	1.21
3	A	902	M0E	CCK-CCL	3.61	1.59	1.53
3	A	902	M0E	O6-CBJ	3.58	1.46	1.40
3	A	902	M0E	O5-C5	3.33	1.52	1.44
3	A	902	M0E	PBI-OBF	3.22	1.67	1.54
2	A	901	63U	CAO-N	3.20	1.41	1.34
3	A	902	M0E	CAG-N2	3.19	1.45	1.34
2	A	901	63U	CA-N	-3.16	1.42	1.46
3	A	902	M0E	CAO-CAP	-3.12	1.49	1.54
3	A	902	M0E	CCK-CCJ	-2.88	1.45	1.52
3	A	902	M0E	OCE-CBX	2.74	1.51	1.43
3	A	902	M0E	CBW-CBV	-2.73	1.48	1.53
2	A	901	63U	CAD-NAC	2.60	1.42	1.33
3	A	902	M0E	CBJ-CBK	2.59	1.60	1.52
3	A	902	M0E	CBX-CBY	2.55	1.57	1.52
3	A	902	M0E	OCO-CCJ	2.50	1.48	1.43
3	A	902	M0E	C6-C5	-2.50	1.43	1.51
3	A	902	M0E	PBI-OBG	-2.42	1.45	1.54
3	A	902	M0E	OBD-CAW	2.39	1.28	1.23
3	A	902	M0E	OCQ-CCM	-2.37	1.19	1.23
3	A	902	M0E	OCF-CBU	2.34	1.47	1.41
2	A	901	63U	CAT-CAQ	-2.31	1.35	1.39
3	A	902	M0E	CCH-CCI	2.26	1.59	1.52
2	A	901	63U	CAH-CAD	-2.08	1.48	1.52
3	A	902	M0E	OCN-CCI	2.06	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	M0E	OAN-CAG	2.02	1.27	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	M0E	CAS-CAO-CAQ	-19.65	95.27	111.11
3	A	902	M0E	CAS-CAO-CAP	-10.38	98.80	111.28
2	A	901	63U	CB-CA-N	-9.35	89.58	109.98
2	A	901	63U	CAG-CAE-CAD	-6.95	114.89	123.53
2	A	901	63U	CB-NAC-CAD	-6.87	102.16	118.32
3	A	902	M0E	OBH-CAV-NAT	6.35	120.45	110.58
3	A	902	M0E	OBA-CAO-CAP	5.86	123.53	108.18
2	A	901	63U	CAF-SAA-CB	-4.68	85.30	94.47
3	A	902	M0E	CAO-CAP-CAR	4.55	121.24	112.06
3	A	902	M0E	C1-O1-CAR	-3.89	108.34	117.96
3	A	902	M0E	CBU-O4-C4	-3.70	108.80	117.96
3	A	902	M0E	OBC-CAV-NAT	-3.68	119.44	125.51
3	A	902	M0E	OBA-CAO-CAQ	3.65	115.00	107.66
3	A	902	M0E	OBH-CAV-OBC	-3.55	120.10	123.69
3	A	902	M0E	CCH-OCE-CBX	-3.47	109.38	117.96
2	A	901	63U	CA-N-CAO	3.09	126.49	123.12
3	A	902	M0E	CBZ-CBY-CBX	-2.55	109.51	113.41
3	A	902	M0E	CCL-CCM-NCS	2.52	120.86	116.73
2	A	901	63U	OAR-CAO-CAP	2.41	124.16	120.99
3	A	902	M0E	CAH-CAG-N2	2.31	120.01	116.10
3	A	902	M0E	CCB-CCA-NCC	2.19	119.80	116.10
3	A	902	M0E	O1-CAR-CAP	-2.15	101.31	106.84
3	A	902	M0E	O1-C1-O5	-2.14	104.69	110.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	M0E	CAX-OBG-PBI-OAZ
3	A	902	M0E	OBE-CAQ-CAW-NAU
3	A	902	M0E	OBC-CAV-OBH-CAP
3	A	902	M0E	NAT-CAV-OBH-CAP
3	A	902	M0E	OBS-CBJ-O6-C6
3	A	902	M0E	CBK-CBJ-O6-C6
3	A	902	M0E	OCP-CCL-CCM-NCS
3	A	902	M0E	CCK-CCL-CCM-OCQ
3	A	902	M0E	OBS-CBN-CBO-OBT

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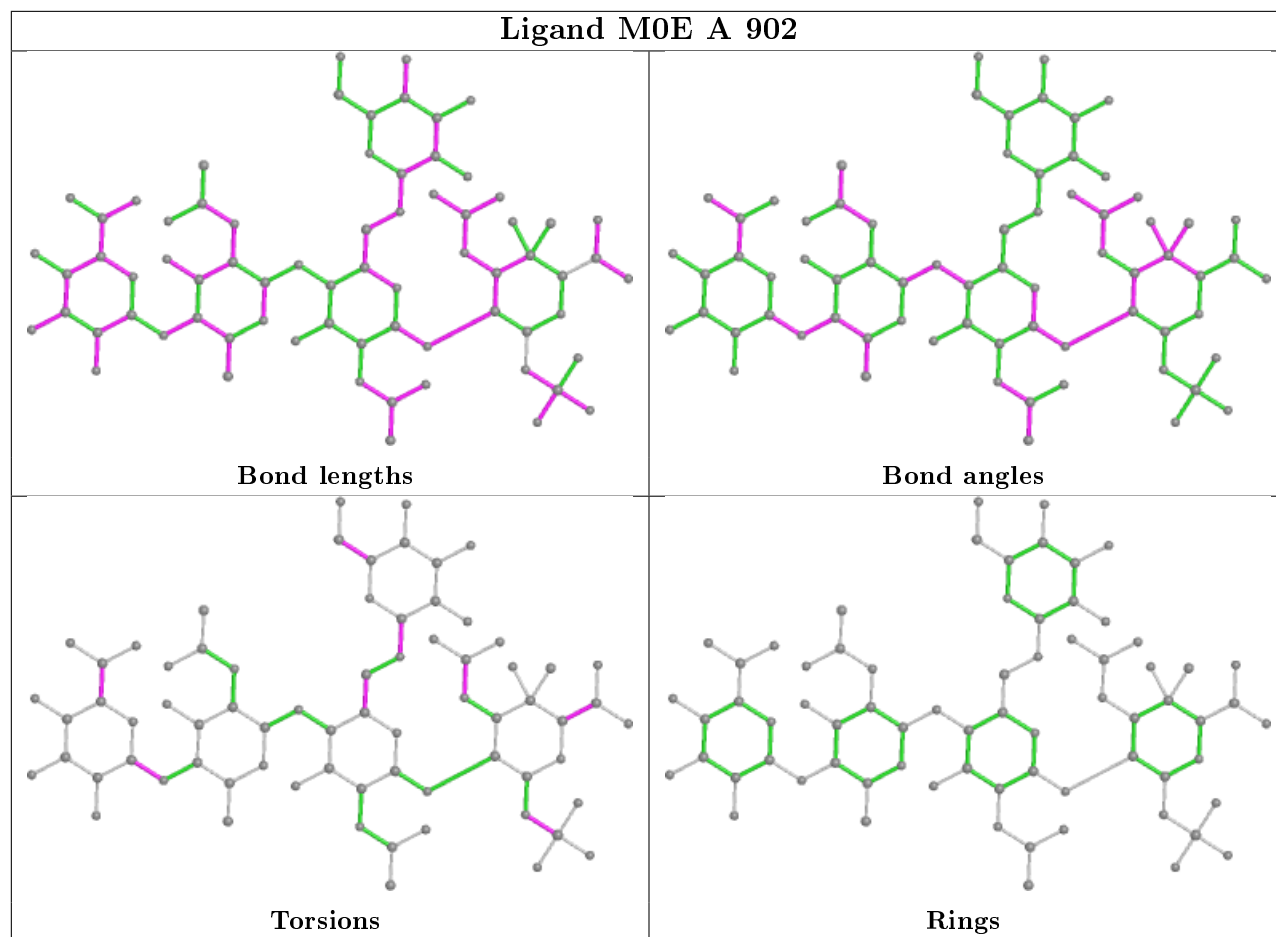
Mol	Chain	Res	Type	Atoms
3	A	902	M0E	CBM-CBN-CBO-OBT
3	A	902	M0E	O5-C5-C6-O6
3	A	902	M0E	CAX-OBG-PBI-OBF
3	A	902	M0E	OCP-CCH-OCE-CBX

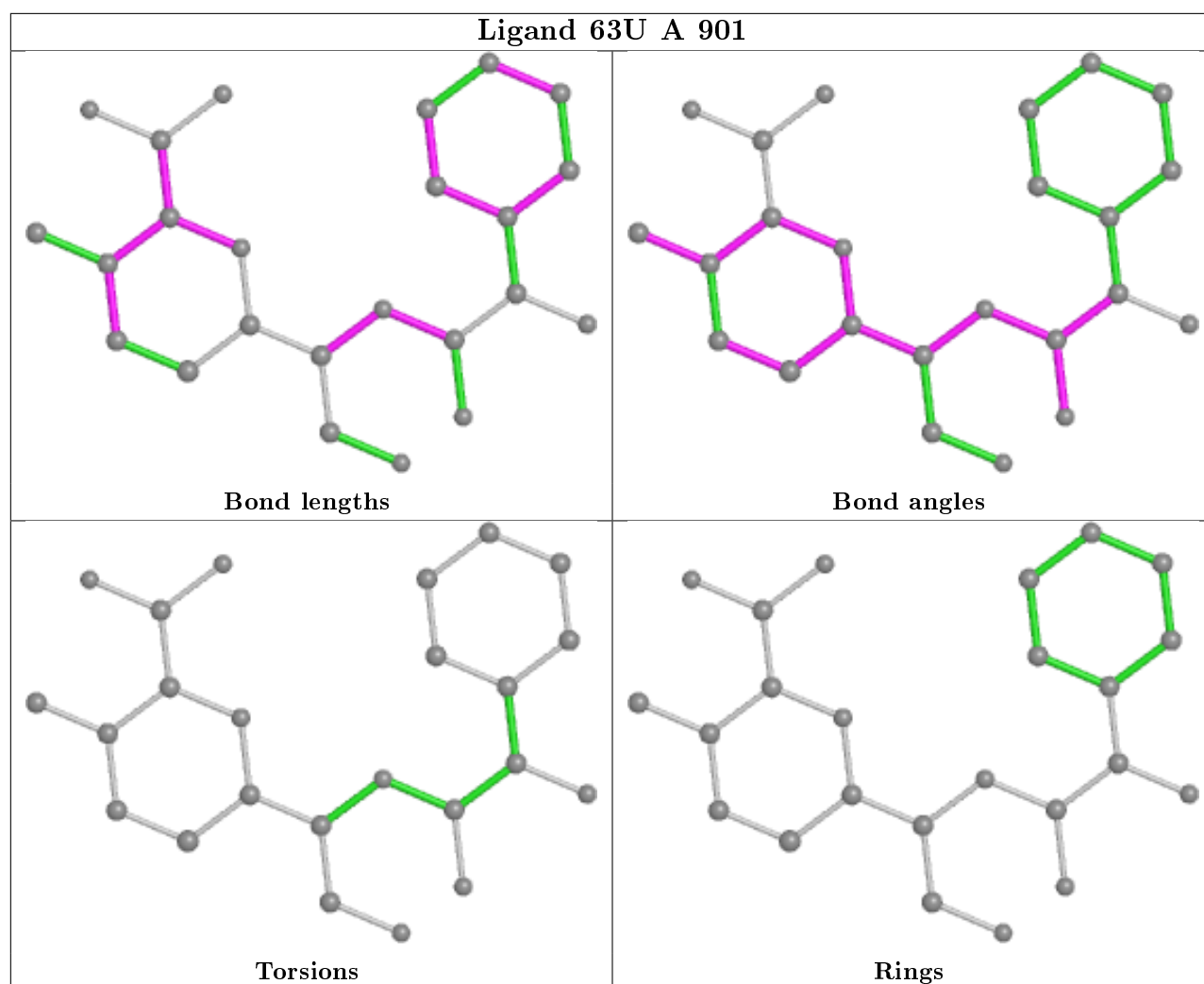
There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	M0E	18	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	697/747 (93%)	0.96	102 (14%) 2 3	19, 50, 120, 139	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	TRP	9.8
1	A	237	PHE	9.0
1	A	76	PHE	8.9
1	A	408	ILE	8.6
1	A	378	ARG	7.4
1	A	390	LEU	6.7
1	A	78	VAL	6.6
1	A	409	SER	6.3
1	A	380	LEU	6.1
1	A	297	MET	6.1
1	A	238	TYR	6.0
1	A	74	ILE	6.0
1	A	75	VAL	6.0
1	A	272	LEU	5.5
1	A	69	LEU	5.4
1	A	268	LEU	5.3
1	A	399	LEU	5.0
1	A	89	GLN	5.0
1	A	342	LEU	4.9
1	A	306	ILE	4.7
1	A	278	LEU	4.7
1	A	406	GLY	4.6
1	A	375	LEU	4.6
1	A	276	LEU	4.5
1	A	335	PHE	4.2
1	A	495	PHE	4.2
1	A	72	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	4.2
1	A	799	MET	4.2
1	A	393	MET	4.1
1	A	386	ILE	4.0
1	A	239	GLU	4.0
1	A	71	LYS	3.9
1	A	381	GLN	3.9
1	A	363	TRP	3.9
1	A	224	LEU	3.9
1	A	407	VAL	3.8
1	A	373	ARG	3.8
1	A	655	PHE	3.7
1	A	85	VAL	3.7
1	A	396	ALA	3.7
1	A	376	VAL	3.7
1	A	432	ASP	3.6
1	A	379	LEU	3.5
1	A	366	PRO	3.5
1	A	267	THR	3.4
1	A	333	TYR	3.4
1	A	368	LEU	3.3
1	A	273	VAL	3.3
1	A	236	HIS	3.3
1	A	301	TYR	3.3
1	A	82	ILE	3.3
1	A	93	SER	3.3
1	A	404	ARG	3.3
1	A	402	GLN	3.2
1	A	295	LEU	3.1
1	A	277	PHE	3.1
1	A	377	LEU	3.1
1	A	428	ASP	3.1
1	A	287	LYS	3.0
1	A	334	TYR	3.0
1	A	359	ILE	3.0
1	A	429	LYS	3.0
1	A	382	GLN	2.9
1	A	230	LEU	2.9
1	A	797	SER	2.8
1	A	302	SER	2.8
1	A	434	SER	2.8
1	A	220	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	205	ILE	2.7
1	A	231	ALA	2.6
1	A	232	THR	2.6
1	A	208	PRO	2.6
1	A	288	ALA	2.6
1	A	319	SER	2.5
1	A	269	THR	2.5
1	A	344	LEU	2.5
1	A	226	VAL	2.5
1	A	332	LEU	2.4
1	A	353	MET	2.4
1	A	497	GLY	2.4
1	A	77	ALA	2.4
1	A	343	SER	2.4
1	A	92	ARG	2.3
1	A	94	ARG	2.3
1	A	349	LEU	2.3
1	A	321	ASP	2.3
1	A	364	ARG	2.3
1	A	385	ILE	2.3
1	A	791	GLN	2.3
1	A	496	ALA	2.3
1	A	79	LEU	2.2
1	A	355	LYS	2.2
1	A	640	LEU	2.2
1	A	370	LEU	2.1
1	A	545	GLY	2.1
1	A	138	LYS	2.1
1	A	734	TYR	2.1
1	A	405	GLY	2.1
1	A	139	MET	2.1
1	A	430	VAL	2.0
1	A	427	GLY	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 ⓘ

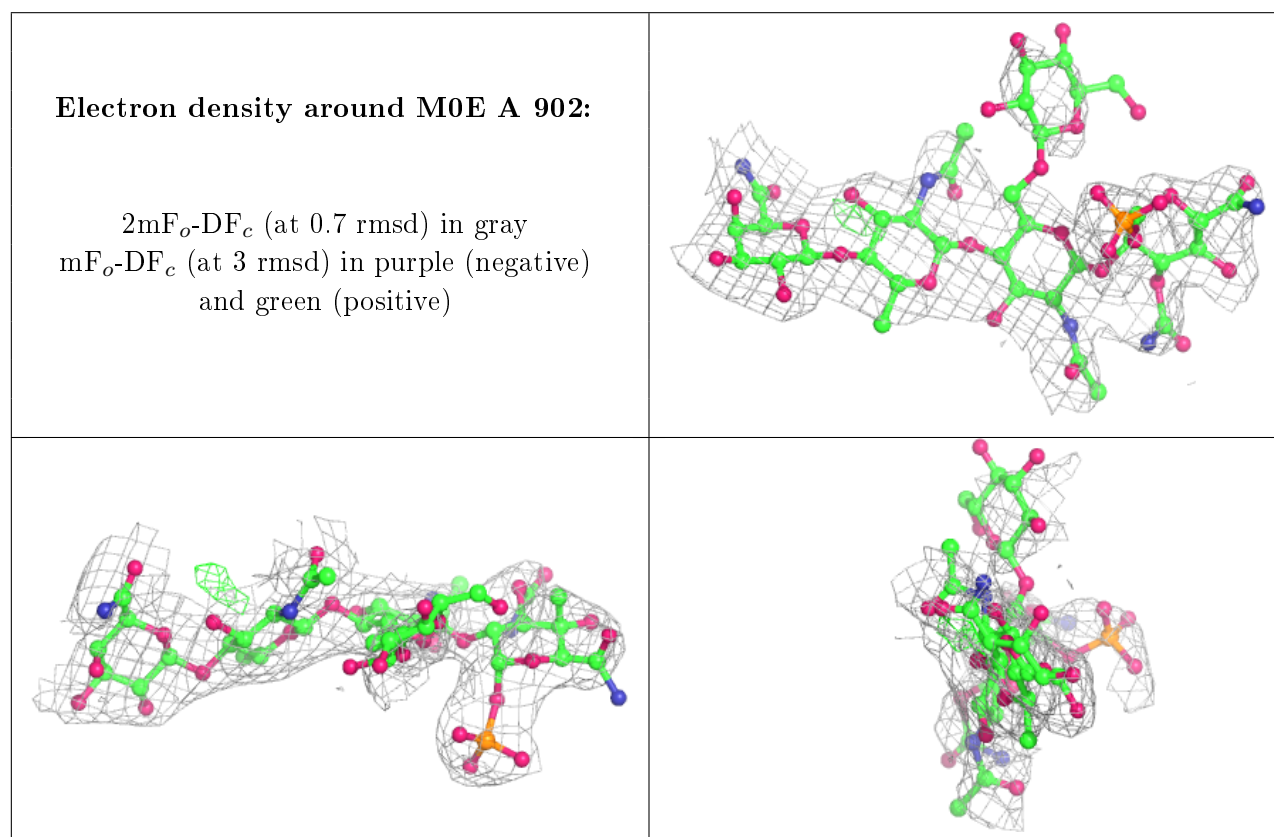
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

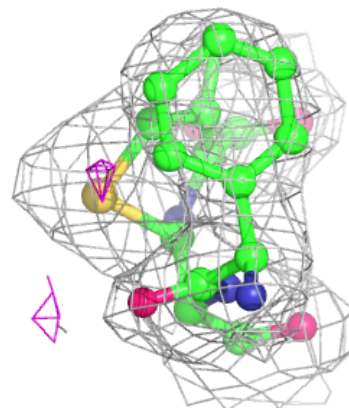
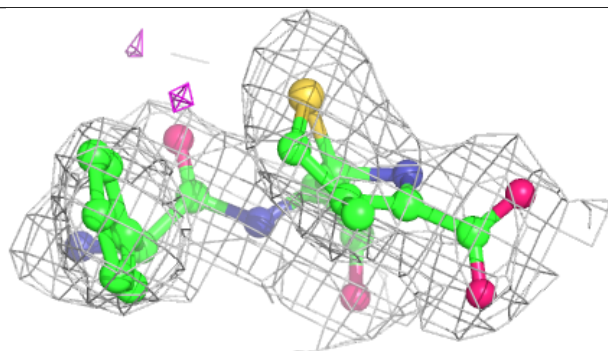
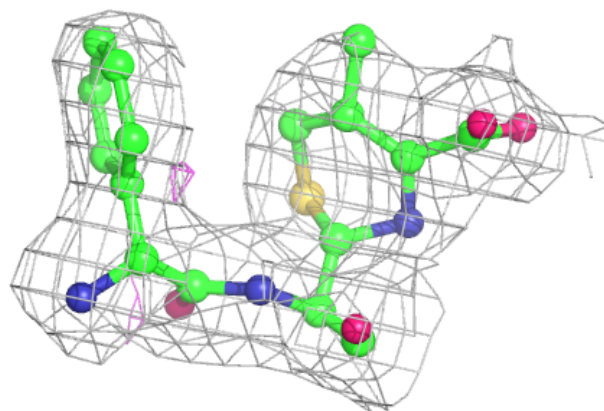
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	M0E	A	902	71/109	0.75	0.23	79,105,125,131	0
2	63U	A	901	24/24	0.91	0.15	43,51,57,61	0

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 63U 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.