



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:46 PM UTC

PDB ID : 5HLD / pdb_00005hld
Title : E. coli PBP1b in complex with acyl-CENTA and moenomycin
Authors : King, D.T.; Strynadka, N.C.J.
Deposited on : 2016-01-14
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

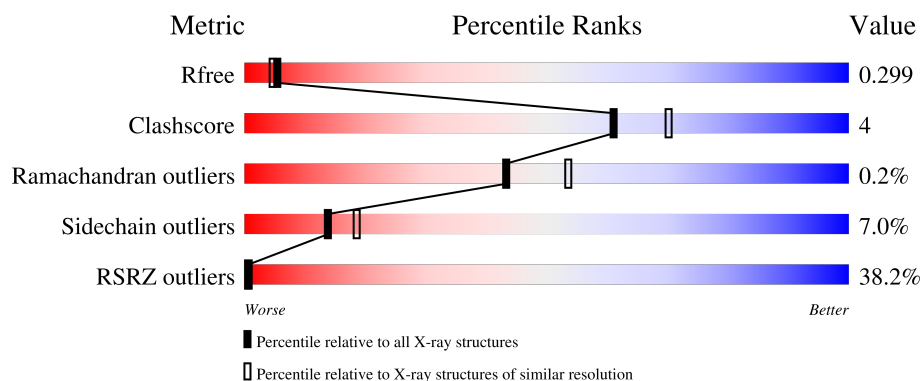
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	33% 75% 11% 13%

2 Entry composition [i](#)

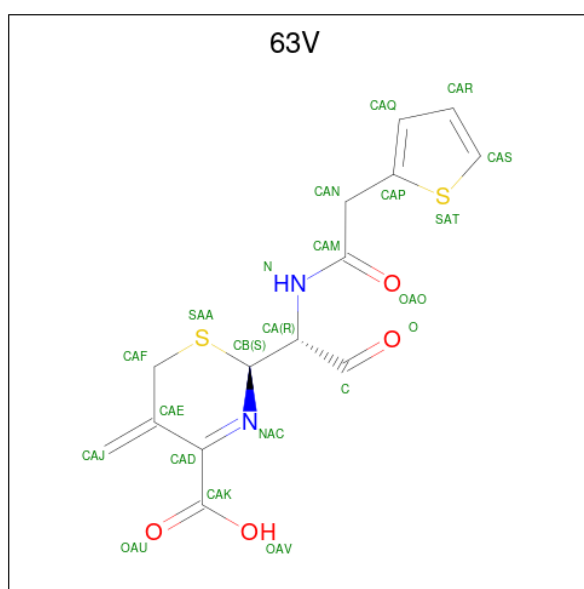
There are 4 unique types of molecules in this entry. The entry contains 5349 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

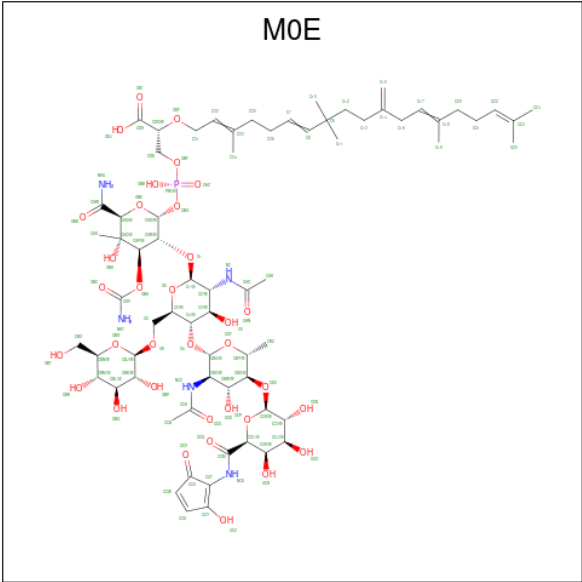
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	649	5063	3209	887	942	25	0	0	0

- Molecule 2 is (2S)-5-methylidene-2-[(1R)-2-oxo-1-[(thiophen-2-ylacetyl)amino]ethyl]-5,6-dihydro-2H-1,3-thiazine-4-carboxylic acid (CCD ID: 63V) (formula: $C_{14}H_{14}N_2O_4S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	22	14	2	4	2	0	0

- Molecule 3 is MOENOMYCIN (CCD ID: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	77	39	5	32	1	0	0

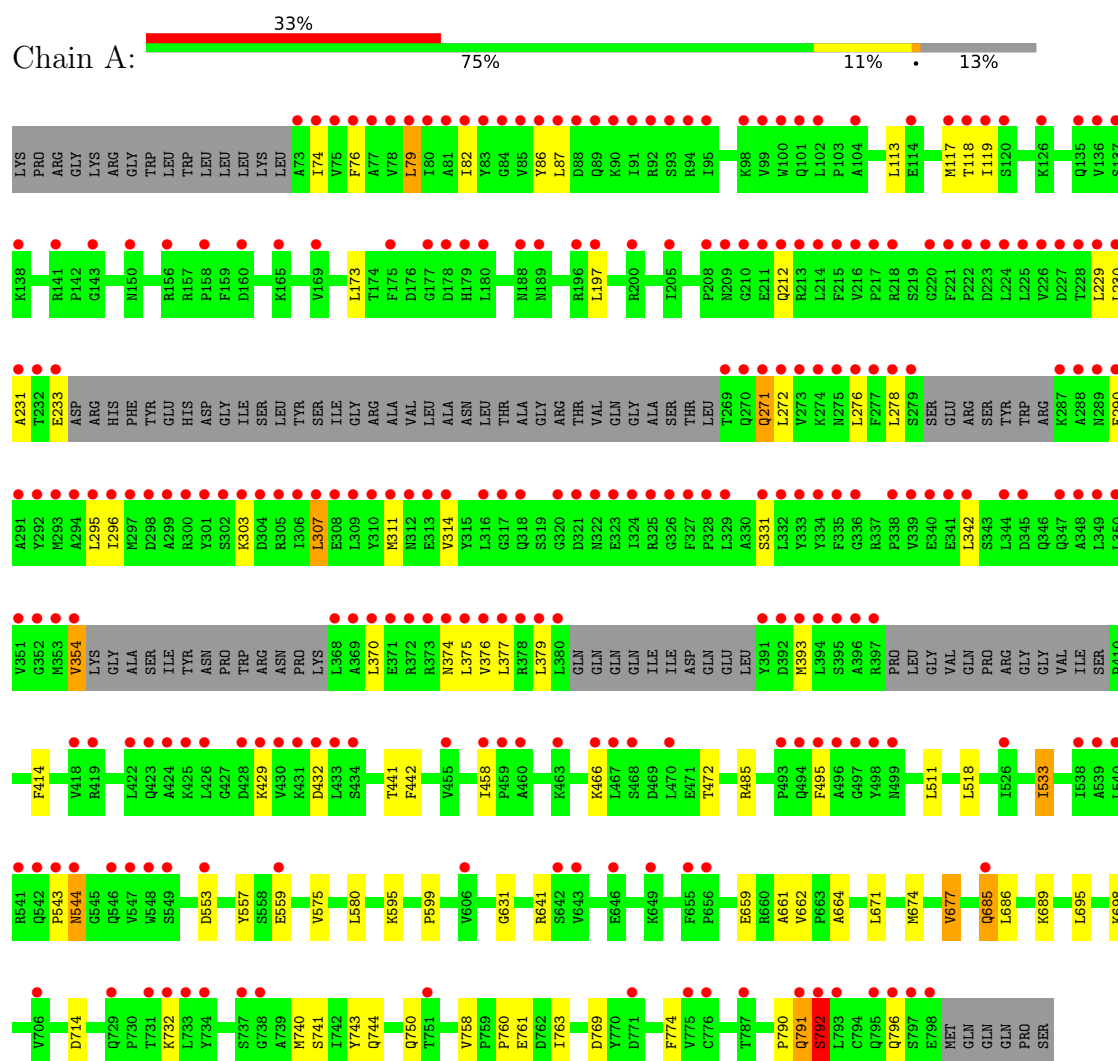
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		

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 1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.34Å 63.94Å 294.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.82 – 2.31 33.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	91.2 (33.82-2.31) 91.2 (33.82-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.253 , 0.279 0.272 , 0.299	Depositor DCC
R_{free} test set	2384 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5349	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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

5.1 Standard geometry

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

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	0.78	0/5157	1.33	18/6992 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	792	SER	N-CA-C	-8.12	102.00	112.23
1	A	231	ALA	CA-C-N	6.49	133.38	121.70
1	A	231	ALA	C-N-CA	6.49	133.38	121.70
1	A	87	LEU	N-CA-C	-6.24	105.32	113.12
1	A	769	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	714	ASP	CA-CB-CG	5.88	118.47	112.60
1	A	792	SER	CA-C-N	5.85	128.12	120.28
1	A	792	SER	C-N-CA	5.85	128.12	120.28
1	A	758	VAL	N-CA-C	-5.83	101.87	107.76
1	A	314	VAL	N-CA-C	5.76	116.84	109.30
1	A	441	THR	CA-C-N	5.58	129.03	121.05
1	A	441	THR	C-N-CA	5.58	129.03	121.05
1	A	791	GLN	CA-C-N	5.47	129.98	120.68
1	A	791	GLN	C-N-CA	5.47	129.98	120.68
1	A	599	PRO	CA-C-N	5.30	127.39	120.28
1	A	599	PRO	C-N-CA	5.30	127.39	120.28
1	A	296	ILE	CA-C-N	5.16	127.46	120.65
1	A	296	ILE	C-N-CA	5.16	127.46	120.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5063	0	5111	30	0
2	A	22	0	0	1	0
3	A	77	0	58	16	0
4	A	187	0	0	0	0
All	All	5349	0	5169	43	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 4.

All (43) 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	1.44
3:A:902:M0E:CAX	3:A:902:M0E:OBG	1.67	1.42
3:A:902:M0E:O1	3:A:902:M0E:CAR	1.65	1.41
3:A:902:M0E:CAR	3:A:902:M0E:C1	2.27	1.12
3:A:902:M0E:CAV	3:A:902:M0E:CAP	2.54	0.85
1:A:278:LEU:HD11	1:A:290:GLU:HB3	1.65	0.77
1:A:741:SER:O	1:A:744:GLN:HG2	1.90	0.71
3:A:902:M0E:O1	3:A:902:M0E:CAP	2.37	0.70
1:A:233:GLU:OE2	1:A:271:GLN:NE2	2.34	0.61
1:A:595:LYS:HB3	1:A:661:ALA:HB1	1.86	0.58
3:A:902:M0E:HAS2	3:A:902:M0E:OBD	2.04	0.56
3:A:902:M0E:HCB2	3:A:902:M0E:HBH	1.87	0.56
3:A:902:M0E:CAX	3:A:902:M0E:PBI	2.93	0.55
3:A:902:M0E:CAR	3:A:902:M0E:H1	2.32	0.55
3:A:902:M0E:OCP	3:A:902:M0E:OCD	2.18	0.54
1:A:761:GLU:H	1:A:761:GLU:CD	2.17	0.53
1:A:117:MET:HE3	1:A:119:ILE:HG21	1.92	0.51
1:A:271:GLN:HG3	3:A:902:M0E:HAT2	1.76	0.50
1:A:790:PRO:C	1:A:792:SER:H	2.20	0.49
1:A:79:LEU:HA	1:A:82:ILE:HG12	1.94	0.49
1:A:760:PRO:HD2	1:A:763:ILE:HG13	1.94	0.49
1:A:674:MET:HA	1:A:677:VAL:HG13	1.94	0.48
1:A:271:GLN:CG	3:A:902:M0E:HAT2	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:LEU:HD11	1:A:743:TYR:HD2	1.79	0.47
1:A:553:ASP:HB3	2:A:901:63V:SAA	2.56	0.46
1:A:374:ASN:HA	1:A:377:LEU:HD12	1.98	0.46
1:A:113:LEU:HD13	1:A:173:LEU:HD21	1.98	0.46
3:A:902:M0E:CAX	3:A:902:M0E:O1	2.56	0.44
1:A:376:VAL:HA	1:A:379:LEU:HD12	1.99	0.44
1:A:533:ILE:HD12	1:A:580:LEU:HD13	1.99	0.44
1:A:458:ILE:HD11	1:A:472:THR:HB	1.99	0.44
1:A:543:PRO:HA	1:A:544:ASN:HA	1.71	0.44
1:A:774:PHE:N	1:A:796:GLN:HG2	2.32	0.44
1:A:685:GLN:HG3	1:A:740:MET:CE	2.48	0.43
1:A:331:SER:HB3	1:A:342:LEU:HD11	2.00	0.43
1:A:518:LEU:HD21	1:A:662:VAL:HG21	2.02	0.42
3:A:902:M0E:OBG	3:A:902:M0E:CAR	2.55	0.42
1:A:414:PHE:CE1	1:A:442:PHE:HB2	2.55	0.41
1:A:354:VAL:HG22	3:A:902:M0E:HAH3	2.02	0.41
1:A:557:TYR:HE2	1:A:575:VAL:HG21	1.86	0.41
1:A:631:GLY:O	1:A:664:ALA:HA	2.21	0.41
1:A:307:LEU:O	1:A:311:MET:HG3	2.21	0.41
1:A:229:LEU:HD22	1:A:311:MET:HE3	2.03	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	637/747 (85%)	618 (97%)	18 (3%)	1 (0%)	43 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	791	GLN

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	544/627 (87%)	506 (93%)	38 (7%)	14	18

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	76	PHE
1	A	79	LEU
1	A	86	TYR
1	A	118	THR
1	A	197	LEU
1	A	212	GLN
1	A	230	LEU
1	A	271	GLN
1	A	272	LEU
1	A	276	LEU
1	A	295	LEU
1	A	303	LYS
1	A	307	LEU
1	A	354	VAL
1	A	370	LEU
1	A	375	LEU
1	A	393	MET
1	A	429	LYS
1	A	432	ASP
1	A	466	LYS
1	A	485	ARG
1	A	495	PHE
1	A	511	LEU
1	A	533	ILE
1	A	544	ASN
1	A	559	GLU
1	A	641	ARG
1	A	659	GLU
1	A	671	LEU

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Mol	Chain	Res	Type
1	A	677	VAL
1	A	685	GLN
1	A	689	LYS
1	A	695	LEU
1	A	698	LYS
1	A	732	LYS
1	A	750	GLN
1	A	792	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	148	GLN
1	A	185	ASN
1	A	270	GLN
1	A	312	ASN
1	A	615	ASN
1	A	633	ASN
1	A	657	GLN
1	A	796	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	79,81,114	4.22	41 (51%)	112,122,166	3.00	21 (18%)
2	63V	A	901	1	20,23,23	3.87	6 (30%)	20,31,31	2.62	6 (30%)

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	-	-	19/52/158/206	0/5/5/6
2	63V	A	901	1	-	4/11/31/31	0/1/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	M0E	OBH-CAV	14.74	1.63	1.35
3	A	902	M0E	CDG-CDH	11.56	1.68	1.52
3	A	902	M0E	CAW-NAU	11.28	1.59	1.32
2	A	901	63V	CAD-NAC	10.83	1.38	1.28
3	A	902	M0E	O1-C1	-10.55	1.12	1.41
2	A	901	63V	CAJ-CAE	10.19	1.53	1.32
3	A	902	M0E	CCL-CCM	-9.08	1.41	1.52
3	A	902	M0E	ODF-CDG	-9.04	1.23	1.42
3	A	902	M0E	O1-CAR	8.51	1.65	1.43
3	A	902	M0E	CAV-NAT	7.74	1.47	1.33
3	A	902	M0E	OCD-CBW	7.04	1.60	1.43
3	A	902	M0E	CAH-CAG	6.65	1.64	1.50
3	A	902	M0E	OBR-CBM	-6.14	1.27	1.43
3	A	902	M0E	CBV-NCC	5.64	1.54	1.45
3	A	902	M0E	CAR-CAP	-5.54	1.41	1.52
2	A	901	63V	CAM-N	5.50	1.45	1.34
3	A	902	M0E	O6-C6	5.13	1.52	1.43
3	A	902	M0E	CCA-NCC	4.93	1.50	1.34
2	A	901	63V	CAF-CAE	-4.68	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	M0E	OCP-CCL	4.21	1.51	1.43
3	A	902	M0E	OBH-CAP	4.09	1.52	1.45
3	A	902	M0E	PBI-OBG	4.05	1.71	1.59
3	A	902	M0E	CBZ-CBY	4.04	1.61	1.51
3	A	902	M0E	CBK-CBL	-3.89	1.42	1.52
3	A	902	M0E	CCK-CCL	3.71	1.59	1.53
3	A	902	M0E	O6-CBJ	3.51	1.46	1.40
3	A	902	M0E	CAG-N2	3.36	1.45	1.34
3	A	902	M0E	O5-C5	3.30	1.52	1.44
3	A	902	M0E	CAO-CAP	-3.25	1.49	1.54
2	A	901	63V	CAR-CAS	2.93	1.45	1.34
3	A	902	M0E	CCK-CCJ	-2.82	1.45	1.52
3	A	902	M0E	OCE-CBX	2.70	1.50	1.43
3	A	902	M0E	C6-C5	-2.59	1.43	1.51
3	A	902	M0E	CBJ-CBK	2.55	1.60	1.52
3	A	902	M0E	OBD-CAW	2.49	1.28	1.23
3	A	902	M0E	CBW-CBV	-2.44	1.48	1.53
3	A	902	M0E	OCQ-CCM	-2.41	1.19	1.23
3	A	902	M0E	OCO-CCJ	2.41	1.48	1.43
2	A	901	63V	CAN-CAM	2.19	1.54	1.51
3	A	902	M0E	CCH-CCI	2.16	1.58	1.52
3	A	902	M0E	CBX-CBY	2.14	1.56	1.52
3	A	902	M0E	PBI-OBG	-2.11	1.45	1.55
3	A	902	M0E	OCF-CBU	2.11	1.47	1.41
3	A	902	M0E	O4-CBU	-2.07	1.35	1.41
3	A	902	M0E	CBU-CBV	2.06	1.56	1.53
3	A	902	M0E	OBE-CAQ	2.04	1.47	1.44
3	A	902	M0E	PBI-OBF	2.01	1.67	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	M0E	CAS-CAO-CAQ	-19.21	95.28	111.14
3	A	902	M0E	OBH-CAV-NAT	11.74	129.11	110.92
3	A	902	M0E	OBC-CAV-NAT	-11.34	107.69	125.58
3	A	902	M0E	CAS-CAO-CAP	-9.93	99.63	111.23
2	A	901	63V	CAF-CAE-CAJ	-6.86	108.76	121.59
3	A	902	M0E	OBA-CAO-CAP	6.20	123.81	108.32
2	A	901	63V	CAF-SAA-CB	-5.35	84.56	94.36
2	A	901	63V	CB-NAC-CAD	-5.10	111.88	116.33
3	A	902	M0E	CBU-O4-C4	-3.97	108.56	117.98
3	A	902	M0E	C1-O1-CAR	-3.91	108.70	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	63V	C-CA-N	-3.69	103.99	109.80
3	A	902	M0E	OBA-CAO-CAQ	3.68	114.75	107.68
3	A	902	M0E	CCH-OCE-CBX	-3.64	109.34	117.98
3	A	902	M0E	ODJ-CDH-CDG	3.58	120.31	112.74
3	A	902	M0E	OBD-CAW-CAQ	3.23	121.26	118.93
3	A	902	M0E	CCL-CCM-NCS	3.07	120.93	116.64
3	A	902	M0E	CCB-CCA-NCC	3.06	121.19	116.12
3	A	902	M0E	CBV-NCC-CCA	-2.86	116.42	123.11
3	A	902	M0E	CBZ-CBY-CBX	-2.67	109.42	113.39
3	A	902	M0E	O4-CBU-CBV	2.55	112.21	108.07
3	A	902	M0E	OCG-CCA-NCC	-2.53	117.51	121.98
3	A	902	M0E	CBU-OCF-CBY	-2.51	109.36	113.63
3	A	902	M0E	OAN-CAG-CAH	-2.36	117.84	122.05
2	A	901	63V	CAE-CAF-SAA	2.35	116.49	111.65
3	A	902	M0E	O1-C1-O5	-2.21	104.88	110.69
3	A	902	M0E	O1-CAR-CAP	-2.20	101.26	106.82
2	A	901	63V	CAR-CAS-SAT	-2.03	108.06	113.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	M0E	CAX-OBG-PBI-OBF
3	A	902	M0E	CAX-OBG-PBI-OB
3	A	902	M0E	OBC-CAV-OBH-CAP
3	A	902	M0E	NAT-CAV-OBH-CAP
3	A	902	M0E	OCP-CCL-CCM-NCS
3	A	902	M0E	CCK-CCL-CCM-NCS
3	A	902	M0E	OBS-CBN-CBO-OBT
3	A	902	M0E	OBS-CBJ-O6-C6
3	A	902	M0E	CBM-CBN-CBO-OBT
3	A	902	M0E	CBK-CBJ-O6-C6
3	A	902	M0E	O5-C5-C6-O6
2	A	901	63V	CAE-CAD-CAK-OAU
3	A	902	M0E	OCP-CCL-CCM-OCQ
2	A	901	63V	NAC-CAD-CAK-OAV
3	A	902	M0E	CDK-OBF-PBI-OAZ
3	A	902	M0E	CCK-CCL-CCM-OCQ
2	A	901	63V	OAO-CAM-CAN-CAP
3	A	902	M0E	ODF-CDG-CDH-ODI
3	A	902	M0E	ODF-CDG-CDH-ODJ
3	A	902	M0E	CDK-CDG-CDH-ODI

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Mol	Chain	Res	Type	Atoms
3	A	902	M0E	CDK-CDG-CDH-ODJ
2	A	901	63V	N-CAM-CAN-CAP
3	A	902	M0E	OCP-CCH-OCE-CBX

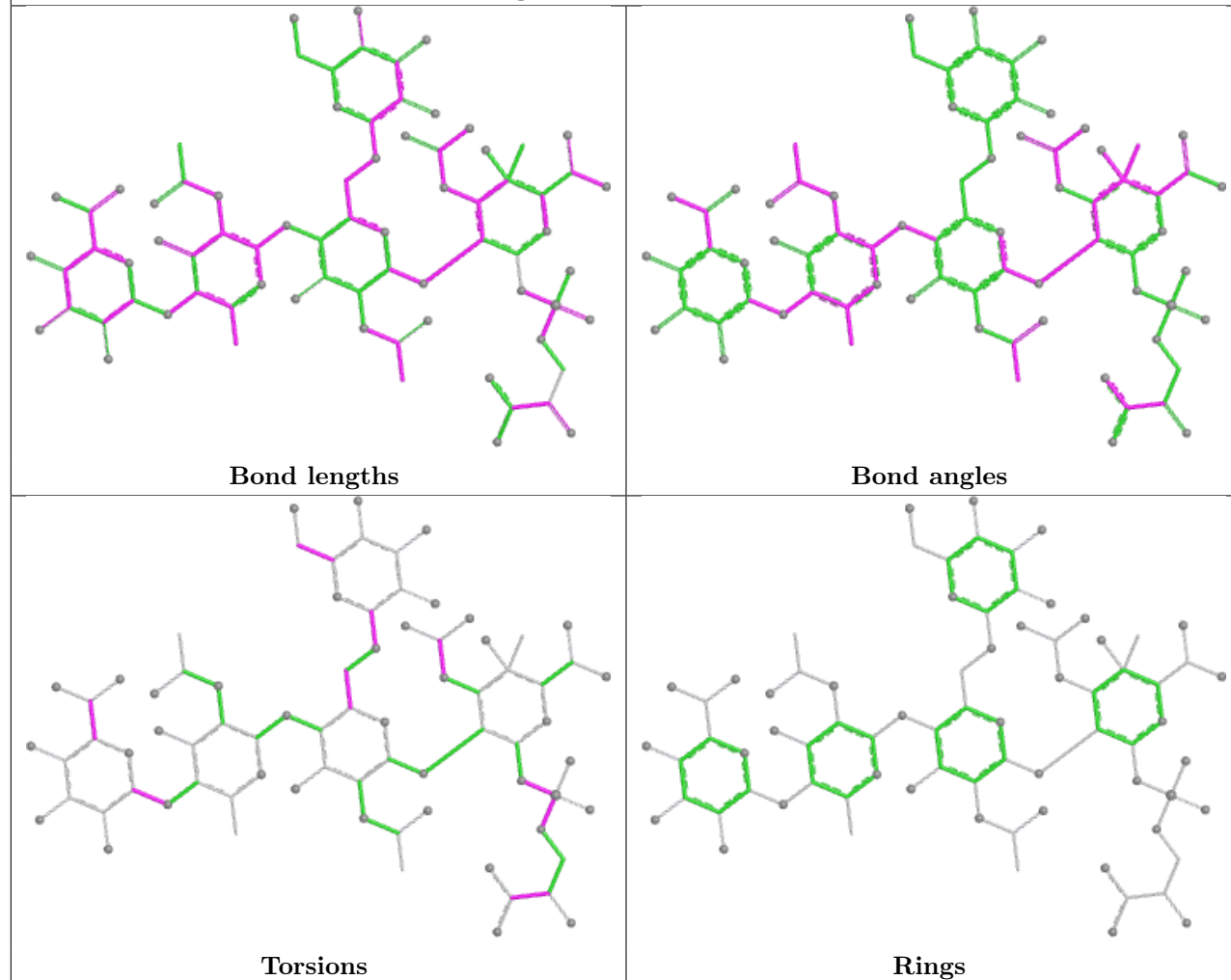
There are no ring outliers.

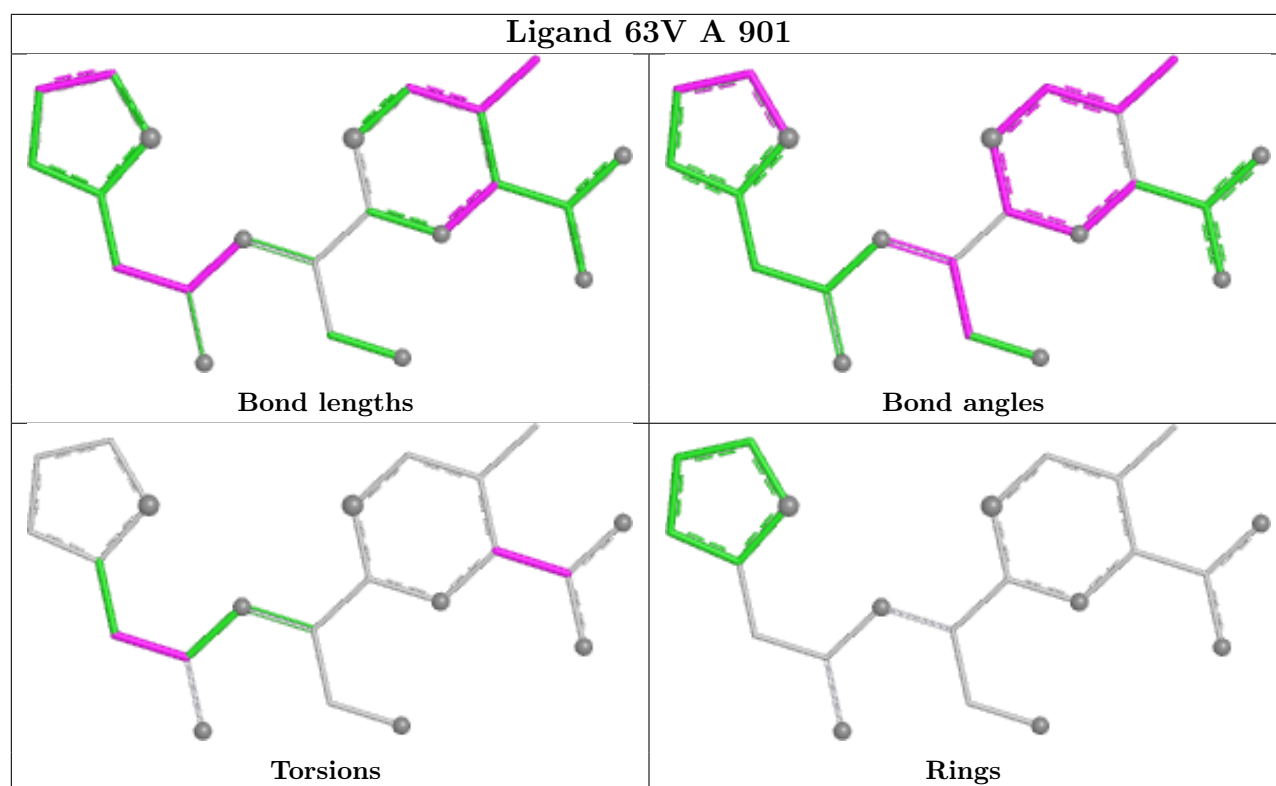
2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	M0E	16	0
2	A	901	63V	1	0

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

Ligand M0E A 902





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	649/747 (86%)	1.86	248 (38%) 1 0	21, 52, 122, 158	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ALA	8.5
1	A	369	ALA	8.0
1	A	75	VAL	7.6
1	A	380	LEU	7.4
1	A	354	VAL	7.1
1	A	368	LEU	6.9
1	A	394	LEU	6.8
1	A	86	TYR	6.7
1	A	74	ILE	6.3
1	A	224	LEU	6.2
1	A	391	TYR	6.1
1	A	377	LEU	6.1
1	A	326	GLY	6.0
1	A	352	GLY	6.0
1	A	273	VAL	6.0
1	A	85	VAL	5.9
1	A	269	THR	5.8
1	A	495	PHE	5.8
1	A	370	LEU	5.7
1	A	375	LEU	5.7
1	A	776	CYS	5.5
1	A	288	ALA	5.4
1	A	275	ASN	5.3
1	A	221	PHE	5.1
1	A	279	SER	5.1
1	A	307	LEU	5.1
1	A	95	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	393	MET	5.0
1	A	334	TYR	5.0
1	A	379	LEU	5.0
1	A	214	LEU	5.0
1	A	77	ALA	4.9
1	A	272	LEU	4.9
1	A	419	ARG	4.9
1	A	372	ARG	4.8
1	A	216	VAL	4.8
1	A	433	LEU	4.8
1	A	296	ILE	4.8
1	A	82	ILE	4.7
1	A	306	ILE	4.7
1	A	76	PHE	4.7
1	A	90	LYS	4.7
1	A	793	LEU	4.6
1	A	89	GLN	4.6
1	A	230	LEU	4.6
1	A	335	PHE	4.6
1	A	278	LEU	4.6
1	A	91	ILE	4.5
1	A	374	ASN	4.5
1	A	342	LEU	4.4
1	A	271	GLN	4.4
1	A	373	ARG	4.3
1	A	226	VAL	4.3
1	A	87	LEU	4.3
1	A	213	ARG	4.2
1	A	229	LEU	4.2
1	A	287	LYS	4.2
1	A	274	LYS	4.1
1	A	291	ALA	4.1
1	A	209	ASN	4.1
1	A	428	ASP	4.1
1	A	371	GLU	4.1
1	A	329	LEU	4.0
1	A	324	ILE	4.0
1	A	302	SER	4.0
1	A	430	VAL	3.9
1	A	233	GLU	3.9
1	A	218	ARG	3.9
1	A	397	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	314	VAL	3.9
1	A	80	ILE	3.9
1	A	301	TYR	3.8
1	A	78	VAL	3.8
1	A	349	LEU	3.8
1	A	396	ALA	3.8
1	A	208	PRO	3.8
1	A	332	LEU	3.8
1	A	270	GLN	3.8
1	A	344	LEU	3.8
1	A	771	ASP	3.8
1	A	303	LYS	3.8
1	A	311	MET	3.7
1	A	79	LEU	3.7
1	A	83	TYR	3.7
1	A	333	TYR	3.7
1	A	88	ASP	3.6
1	A	297	MET	3.6
1	A	350	LEU	3.6
1	A	292	TYR	3.6
1	A	797	SER	3.6
1	A	143	GLY	3.6
1	A	313	GLU	3.5
1	A	339	VAL	3.5
1	A	299	ALA	3.5
1	A	497	GLY	3.5
1	A	309	LEU	3.5
1	A	290	GLU	3.5
1	A	734	TYR	3.5
1	A	316	LEU	3.5
1	A	395	SER	3.4
1	A	547	VAL	3.4
1	A	294	ALA	3.4
1	A	320	GLY	3.4
1	A	431	LYS	3.4
1	A	655	PHE	3.4
1	A	228	THR	3.4
1	A	429	LYS	3.4
1	A	215	PHE	3.4
1	A	300	ARG	3.4
1	A	135	GLN	3.4
1	A	205	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	792	SER	3.3
1	A	220	GLY	3.3
1	A	189	ASN	3.3
1	A	222	PRO	3.3
1	A	277	PHE	3.3
1	A	101	GLN	3.3
1	A	796	GLN	3.3
1	A	304	ASP	3.3
1	A	392	ASP	3.3
1	A	295	LEU	3.3
1	A	289	ASN	3.2
1	A	541	ARG	3.2
1	A	138	LYS	3.2
1	A	493	PRO	3.2
1	A	348	ALA	3.2
1	A	276	LEU	3.2
1	A	787	THR	3.2
1	A	546	GLN	3.2
1	A	196	ARG	3.1
1	A	460	ALA	3.1
1	A	217	PRO	3.1
1	A	225	LEU	3.1
1	A	378	ARG	3.1
1	A	231	ALA	3.1
1	A	312	ASN	3.1
1	A	99	VAL	3.1
1	A	136	VAL	3.1
1	A	376	VAL	3.1
1	A	798	GLU	3.1
1	A	317	GLY	3.1
1	A	336	GLY	3.1
1	A	496	ALA	3.1
1	A	92	ARG	3.1
1	A	98	LYS	3.1
1	A	158	PRO	3.1
1	A	353	MET	3.0
1	A	293	MET	3.0
1	A	169	VAL	3.0
1	A	494	GLN	3.0
1	A	732	LYS	3.0
1	A	126	LYS	2.9
1	A	298	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	466	LYS	2.9
1	A	470	LEU	2.9
1	A	310	TYR	2.8
1	A	656	PRO	2.8
1	A	102	LEU	2.8
1	A	538	ILE	2.8
1	A	210	GLY	2.8
1	A	118	THR	2.7
1	A	544	ASN	2.7
1	A	120	SER	2.7
1	A	212	GLN	2.7
1	A	137	SER	2.7
1	A	328	PRO	2.7
1	A	141	ARG	2.7
1	A	180	LEU	2.7
1	A	791	GLN	2.6
1	A	165	LYS	2.6
1	A	227	ASP	2.6
1	A	643	VAL	2.6
1	A	177	GLY	2.6
1	A	543	PRO	2.6
1	A	341	GLU	2.6
1	A	458	ILE	2.6
1	A	526	ILE	2.6
1	A	424	ALA	2.6
1	A	553	ASP	2.6
1	A	731	THR	2.6
1	A	540	LEU	2.5
1	A	729	GLN	2.5
1	A	422	LEU	2.5
1	A	84	GLY	2.5
1	A	232	THR	2.5
1	A	323	GLU	2.5
1	A	539	ALA	2.5
1	A	179	HIS	2.5
1	A	542	GLN	2.5
1	A	100	TRP	2.5
1	A	351	VAL	2.5
1	A	178	ASP	2.5
1	A	188	ASN	2.5
1	A	321	ASP	2.5
1	A	93	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	432	ASP	2.4
1	A	325	ARG	2.4
1	A	331	SER	2.4
1	A	345	ASP	2.4
1	A	646	GLU	2.4
1	A	327	PHE	2.4
1	A	150	ASN	2.4
1	A	94	ARG	2.4
1	A	305	ARG	2.4
1	A	706	VAL	2.3
1	A	795	GLN	2.3
1	A	347	GLN	2.3
1	A	775	VAL	2.3
1	A	322	ASN	2.3
1	A	104	ALA	2.3
1	A	467	LEU	2.3
1	A	498	TYR	2.3
1	A	559	GLU	2.3
1	A	426	LEU	2.2
1	A	548	TRP	2.2
1	A	200	ARG	2.2
1	A	733	LEU	2.2
1	A	175	PHE	2.2
1	A	423	GLN	2.2
1	A	434	SER	2.2
1	A	223	ASP	2.2
1	A	499	ASN	2.2
1	A	211	GLU	2.2
1	A	463	LYS	2.2
1	A	197	LEU	2.1
1	A	117	MET	2.1
1	A	455	VAL	2.1
1	A	114	GLU	2.1
1	A	751	THR	2.1
1	A	468	SER	2.1
1	A	340	GLU	2.1
1	A	685	GLN	2.1
1	A	338	PRO	2.1
1	A	738	GLY	2.1
1	A	425	LYS	2.1
1	A	308	GLU	2.1
1	A	160	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	459	PRO	2.1
1	A	418	VAL	2.1
1	A	606	VAL	2.1
1	A	549	SER	2.0
1	A	642	SER	2.0
1	A	737	SER	2.0
1	A	81	ALA	2.0
1	A	119	ILE	2.0
1	A	649	LYS	2.0
1	A	318	GLN	2.0
1	A	156	ARG	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

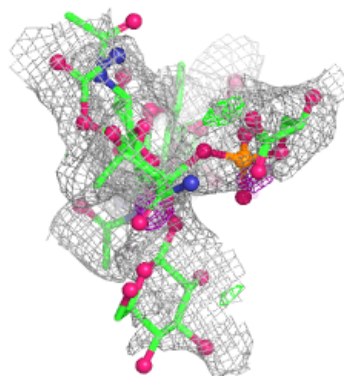
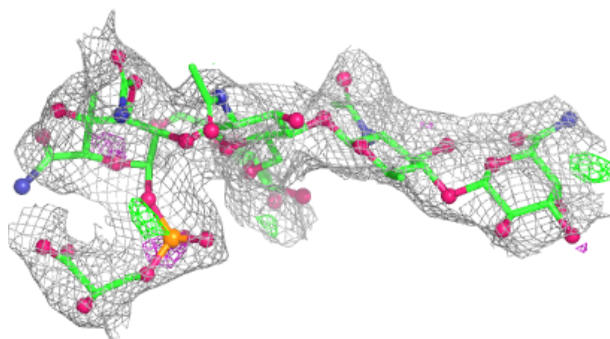
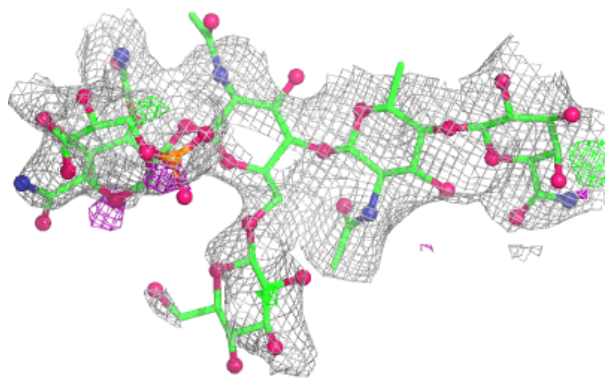
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	M0E	A	902	77/109	0.60	0.19	79,106,125,132	0
2	63V	A	901	22/22	0.93	0.11	28,34,42,44	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.

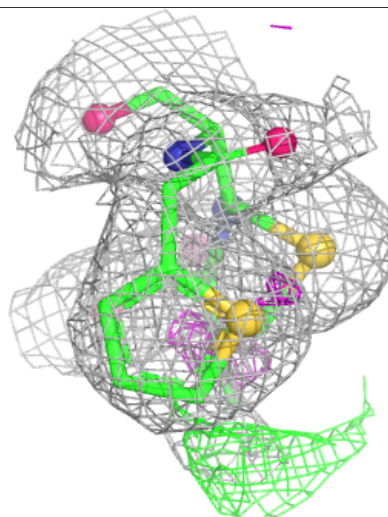
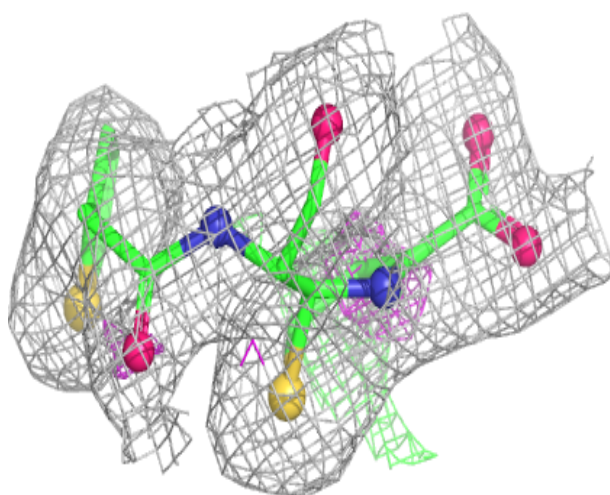
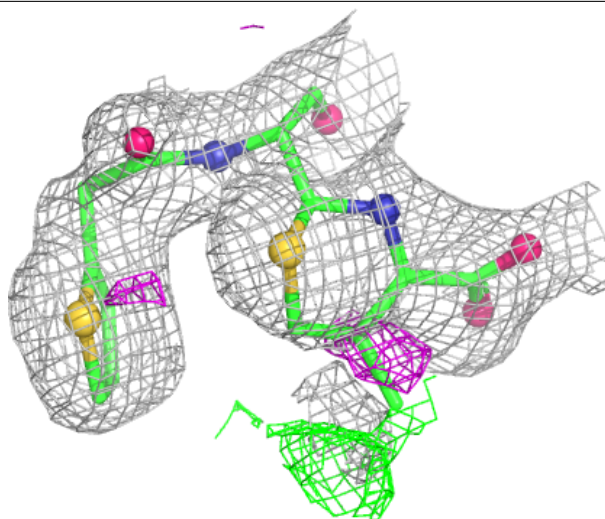
Electron density around M0E A 902:

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



Electron density around 63V 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 [i](#)

There are no such residues in this entry.