



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 5FBT / pdb_00005fbt
Title : Crystal structure of rifampin phosphotransferase RPH-Lm from *Listeria monocytogenes* in complex with rifampin
Authors : Stogios, P.J.; Wawrzak, Z.; Skarina, T.; Yim, V.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2015-12-14
Resolution : 2.70 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

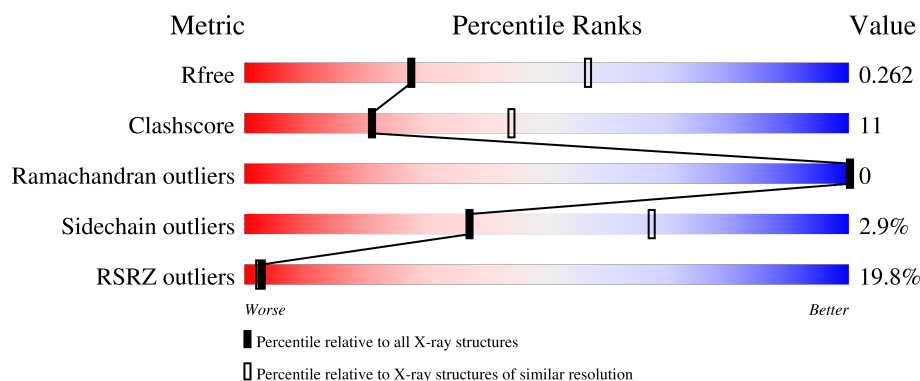
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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.

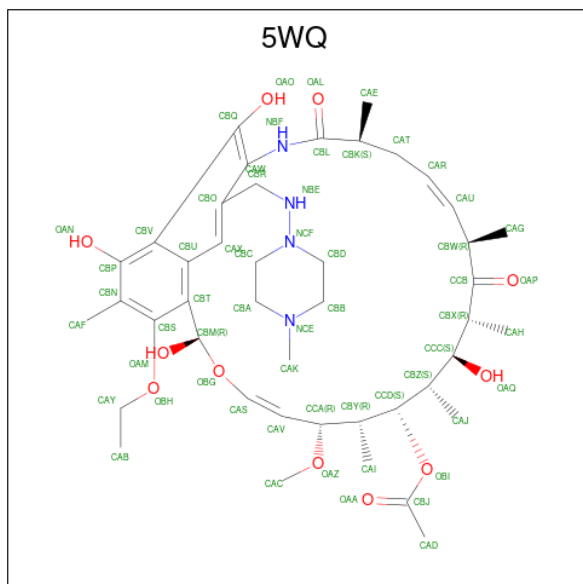
Mol	Chain	Length	Quality of chain
1	A	867	17% 70% 16% • 11%

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 Phosphoenolpyruvate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	769	Total	C	N	O	S	Se	0	2	0
			5801	3682	970	1122	4	23			

- Molecule 2 is Rifampin (CCD ID: 5WQ) (formula: $C_{43}H_{64}N_4O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			58	43	4	11		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

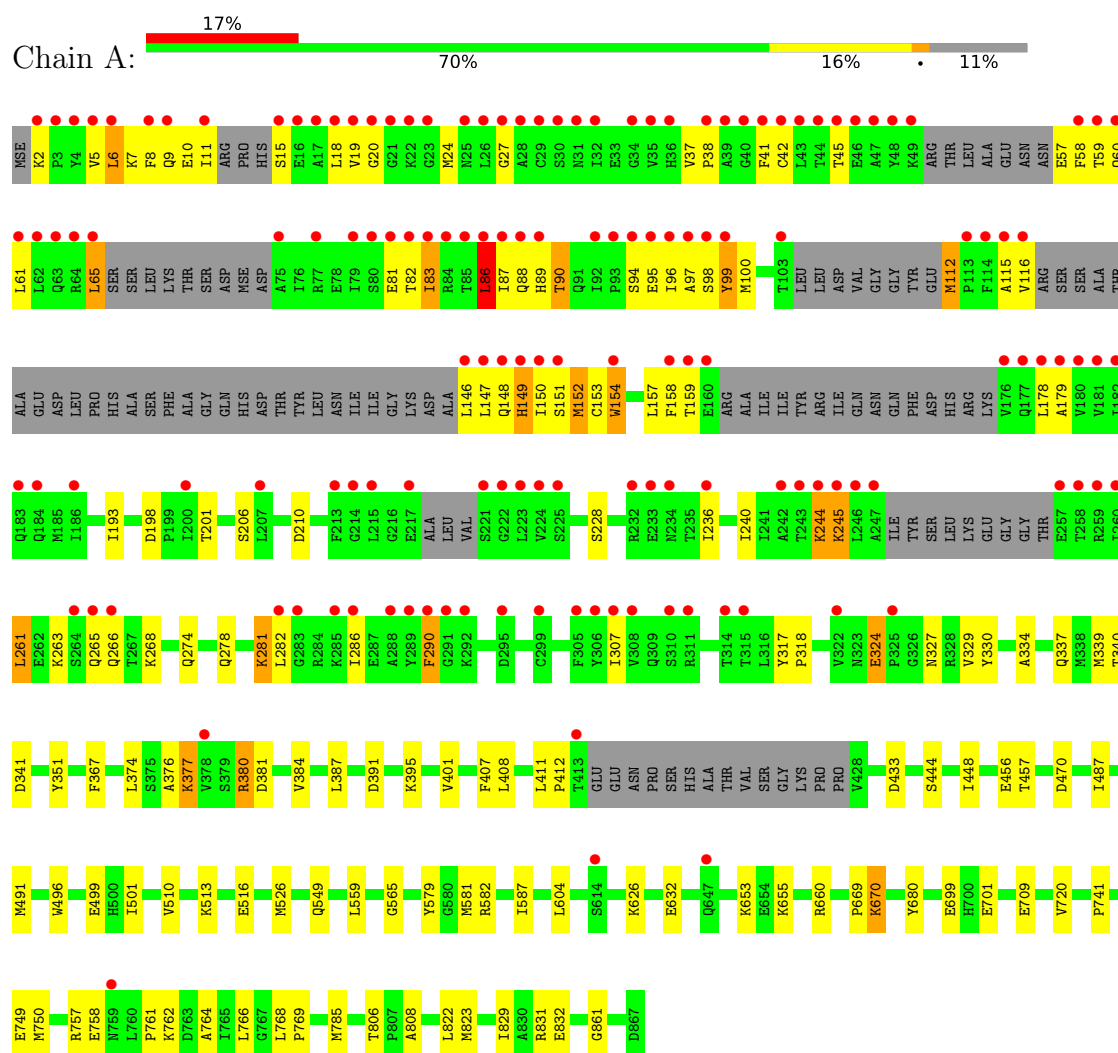
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total 177	O 177	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: Phosphoenolpyruvate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.28Å 149.28Å 193.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.98 – 2.70 24.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.98-2.70) 92.8 (24.98-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.260 0.227 , 0.262	Depositor DCC
R_{free} test set	1741 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: CL, 5WQ

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	0.47	0/5879	0.95	38/7933 (0.5%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LEU	N-CA-C	11.26	123.12	111.07
1	A	149	HIS	N-CA-C	9.98	122.23	111.36
1	A	263	LYS	N-CA-C	9.08	121.18	111.28
1	A	99	TYR	N-CA-C	-9.02	100.86	112.23
1	A	90	THR	N-CA-C	-8.61	99.05	110.24
1	A	261	LEU	N-CA-C	7.75	120.94	109.24
1	A	245	LYS	N-CA-C	7.34	122.52	112.90
1	A	83	ILE	CA-C-N	-7.21	109.33	122.38
1	A	83	ILE	C-N-CA	-7.21	109.33	122.38
1	A	148	GLN	N-CA-C	-7.09	103.48	111.07
1	A	158	PHE	N-CA-C	7.03	122.22	112.45
1	A	266	GLN	N-CA-C	6.35	118.20	111.28
1	A	38	PRO	O-C-N	6.09	130.01	123.01
1	A	236	ILE	N-CA-C	-5.97	98.02	107.15
1	A	152	MSE	CA-C-N	5.96	128.55	120.44
1	A	152	MSE	C-N-CA	5.96	128.55	120.44
1	A	82	THR	N-CA-C	-5.85	105.24	112.38
1	A	2	LYS	CA-C-N	-5.84	114.73	120.98
1	A	2	LYS	C-N-CA	-5.84	114.73	120.98
1	A	154	TRP	N-CA-C	-5.81	104.95	111.28
1	A	88	GLN	O-C-N	5.61	128.06	122.12
1	A	324	GLU	CA-C-N	-5.55	114.24	119.90
1	A	324	GLU	C-N-CA	-5.55	114.24	119.90
1	A	37	VAL	CA-C-N	-5.53	113.86	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	VAL	C-N-CA	-5.53	113.86	119.83
1	A	148	GLN	CA-C-N	5.51	128.12	120.29
1	A	148	GLN	C-N-CA	5.51	128.12	120.29
1	A	159	THR	N-CA-C	-5.40	105.39	111.28
1	A	391	ASP	CA-C-N	5.38	125.05	119.56
1	A	391	ASP	C-N-CA	5.38	125.05	119.56
1	A	9	GLN	N-CA-C	-5.37	106.57	113.01
1	A	61	LEU	N-CA-C	-5.35	105.45	111.28
1	A	281	LYS	N-CA-C	-5.33	105.48	111.28
1	A	265	GLN	CA-C-N	5.30	127.38	120.28
1	A	265	GLN	C-N-CA	5.30	127.38	120.28
1	A	307	ILE	N-CA-C	5.22	116.22	108.23
1	A	154	TRP	O-C-N	5.06	127.48	122.12
1	A	151	SER	N-CA-C	5.03	116.85	111.36

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	5801	0	5596	119	0
2	A	58	0	64	11	0
3	A	1	0	0	0	0
4	A	177	0	0	2	0
All	All	6037	0	5660	127	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 11.

All (127) 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:154:TRP:O	1:A:157:LEU:HD12	1.59	0.99
1:A:87:ILE:HA	1:A:90:THR:HG22	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:CG2	1:A:24:MSE:HE3	1.99	0.91
1:A:94:SER:HA	1:A:97:ALA:HB3	1.54	0.90
1:A:87:ILE:HA	1:A:90:THR:CG2	2.01	0.89
1:A:87:ILE:CA	1:A:90:THR:HG22	2.05	0.85
1:A:19:VAL:CG2	1:A:24:MSE:CE	2.60	0.79
1:A:57:GLU:HG2	1:A:58:PHE:H	1.47	0.79
1:A:154:TRP:CD1	1:A:178:LEU:HD22	2.21	0.75
1:A:19:VAL:HG22	1:A:24:MSE:HE3	1.68	0.74
1:A:6:LEU:O	1:A:42:CYS:N	2.22	0.73
1:A:86:LEU:HD12	1:A:86:LEU:O	1.90	0.72
1:A:387:LEU:HD21	2:A:901:5WQ:H63	1.72	0.72
2:A:901:5WQ:H16	2:A:901:5WQ:H1	1.70	0.72
1:A:178:LEU:C	1:A:178:LEU:HD23	2.16	0.71
1:A:89:HIS:O	1:A:90:THR:C	2.34	0.70
1:A:57:GLU:HG2	1:A:58:PHE:N	2.06	0.69
1:A:57:GLU:CG	1:A:58:PHE:H	2.06	0.69
1:A:757:ARG:HB2	1:A:766:LEU:HD11	1.75	0.68
1:A:324:GLU:N	1:A:324:GLU:OE2	2.27	0.68
1:A:374:LEU:HA	1:A:380:ARG:HB2	1.77	0.67
1:A:154:TRP:HD1	1:A:178:LEU:HD22	1.60	0.67
1:A:97:ALA:HA	1:A:100:MSE:HE3	1.78	0.66
1:A:244:LYS:NZ	1:A:268:LYS:O	2.29	0.65
1:A:286:ILE:HD12	1:A:286:ILE:H	1.60	0.64
1:A:87:ILE:C	1:A:90:THR:HG22	2.23	0.64
1:A:19:VAL:HG23	1:A:24:MSE:HE3	1.79	0.64
1:A:149:HIS:HA	1:A:152:MSE:HG2	1.80	0.63
1:A:178:LEU:HD23	1:A:179:ALA:N	2.14	0.62
1:A:94:SER:O	1:A:98:SER:N	2.32	0.62
1:A:154:TRP:HA	1:A:178:LEU:HD13	1.81	0.62
1:A:15:SER:HB2	1:A:18:LEU:HB3	1.81	0.61
1:A:822:LEU:O	1:A:831:ARG:NH2	2.30	0.60
1:A:81:GLU:HA	1:A:83:ILE:HG22	1.84	0.60
1:A:491:MSE:HG2	1:A:823:MSE:HE2	1.83	0.59
1:A:761:PRO:HB2	1:A:764:ALA:HB2	1.85	0.59
1:A:8:PHE:HE1	1:A:42:CYS:HB2	1.68	0.58
1:A:86:LEU:HD12	1:A:90:THR:HB	1.86	0.58
1:A:87:ILE:O	1:A:90:THR:HG22	2.04	0.58
1:A:95:GLU:O	1:A:99:TYR:N	2.38	0.56
1:A:86:LEU:HD12	1:A:86:LEU:C	2.32	0.55
1:A:96:ILE:HA	1:A:99:TYR:HB3	1.88	0.55
1:A:86:LEU:O	1:A:90:THR:N	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:MSE:SE	1:A:582:ARG:HD2	2.57	0.54
1:A:330:TYR:HB3	1:A:367:PHE:HB3	1.90	0.54
1:A:768:LEU:HD12	1:A:769:PRO:HD2	1.90	0.54
1:A:157:LEU:HD11	1:A:178:LEU:HB2	1.91	0.53
1:A:18:LEU:HD12	1:A:45:THR:HG22	1.90	0.53
1:A:487:ILE:HD11	1:A:669:PRO:HG2	1.91	0.53
1:A:604:LEU:HG	1:A:785:MSE:HE2	1.89	0.53
1:A:193:ILE:HG22	1:A:210:ASP:HB2	1.90	0.53
1:A:6:LEU:HA	1:A:10:GLU:OE2	2.10	0.52
1:A:87:ILE:HA	1:A:90:THR:HG21	1.89	0.52
1:A:626:LYS:NZ	4:A:1008:HOH:O	2.42	0.52
1:A:785:MSE:HE3	1:A:808:ALA:HB2	1.91	0.52
1:A:245:LYS:O	1:A:261:LEU:CB	2.58	0.51
2:A:901:5WQ:CAU	2:A:901:5WQ:H55	2.24	0.51
1:A:157:LEU:HD12	1:A:157:LEU:H	1.75	0.51
1:A:65:LEU:O	1:A:65:LEU:HD12	2.11	0.51
1:A:7:LYS:O	1:A:11:ILE:HG13	2.10	0.50
1:A:115:ALA:C	1:A:116:VAL:CG1	2.85	0.50
1:A:154:TRP:O	1:A:157:LEU:CD1	2.47	0.50
1:A:20:GLY:O	1:A:24:MSE:HG2	2.12	0.49
1:A:15:SER:HB2	1:A:18:LEU:CB	2.42	0.49
1:A:89:HIS:C	1:A:90:THR:O	2.52	0.49
1:A:24:MSE:O	1:A:27:GLY:N	2.46	0.49
1:A:337:GLN:HG2	1:A:587:ILE:HD13	1.95	0.49
1:A:327:ASN:HD22	1:A:407:PHE:HA	1.77	0.49
1:A:579:TYR:C	1:A:581:MSE:H	2.21	0.48
2:A:901:5WQ:H31	2:A:901:5WQ:H23	1.95	0.48
1:A:516:GLU:HA	1:A:832:GLU:HA	1.96	0.48
1:A:769:PRO:HD3	1:A:861:GLY:HA3	1.96	0.48
1:A:741:PRO:HB3	1:A:750:MSE:HB3	1.96	0.48
1:A:501:ILE:HG13	1:A:510:VAL:HG11	1.96	0.48
1:A:178:LEU:C	1:A:178:LEU:CD2	2.85	0.47
1:A:198:ASP:HB2	1:A:206:SER:HB3	1.96	0.47
1:A:244:LYS:HZ1	1:A:268:LYS:C	2.23	0.47
1:A:278:GLN:O	1:A:282:LEU:N	2.44	0.47
1:A:470:ASP:OD2	1:A:680:TYR:OH	2.30	0.47
1:A:115:ALA:C	1:A:116:VAL:HG13	2.39	0.47
1:A:150:ILE:O	1:A:153:CYS:HB3	2.15	0.47
1:A:516:GLU:O	1:A:660:ARG:NH2	2.48	0.47
1:A:81:GLU:C	1:A:83:ILE:N	2.71	0.46
1:A:281:LYS:O	1:A:282:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HB	1:A:749:GLU:HG3	1.97	0.46
1:A:444:SER:O	1:A:448:ILE:HG12	2.16	0.46
1:A:806:THR:HG23	1:A:829:ILE:HG21	1.97	0.46
1:A:7:LYS:HA	1:A:41:PHE:HA	1.98	0.45
2:A:901:5WQ:H37	2:A:901:5WQ:H43	1.52	0.45
1:A:146:LEU:HB3	1:A:147:LEU:H	1.46	0.45
1:A:327:ASN:HB3	1:A:407:PHE:CE1	2.52	0.45
1:A:337:GLN:OE1	1:A:670:LYS:NZ	2.33	0.45
1:A:59:THR:HG23	1:A:60:GLN:N	2.32	0.45
1:A:387:LEU:HD11	2:A:901:5WQ:H63	1.99	0.44
1:A:377:LYS:HB2	1:A:411:LEU:HD13	1.99	0.44
2:A:901:5WQ:H47	4:A:1040:HOH:O	2.17	0.44
1:A:11:ILE:HG21	1:A:24:MSE:HE2	2.00	0.44
1:A:377:LYS:HE3	1:A:381:ASP:OD2	2.18	0.44
1:A:699:GLU:OE1	1:A:701:GLU:N	2.35	0.43
1:A:433:ASP:OD1	1:A:433:ASP:N	2.50	0.43
1:A:228:SER:HB3	1:A:240:ILE:HB	2.00	0.43
2:A:901:5WQ:H42	2:A:901:5WQ:OBI	2.19	0.43
1:A:327:ASN:ND2	1:A:407:PHE:HA	2.33	0.43
1:A:496:TRP:CE3	1:A:655:LYS:HG3	2.53	0.43
1:A:112:MSE:HE3	1:A:112:MSE:HB2	1.75	0.42
1:A:513:LYS:HE2	1:A:513:LYS:HB2	1.88	0.42
1:A:339:MSE:SE	1:A:341:ASP:HB2	2.70	0.42
1:A:456:GLU:HG2	1:A:457:THR:HG23	2.00	0.42
1:A:559:LEU:O	1:A:565:GLY:HA3	2.19	0.42
1:A:11:ILE:CG2	1:A:24:MSE:HE1	2.50	0.41
2:A:901:5WQ:H20	2:A:901:5WQ:H28	1.81	0.41
1:A:334:ALA:HB1	1:A:340:THR:HA	2.02	0.41
1:A:86:LEU:O	1:A:90:THR:HB	2.20	0.41
1:A:351:TYR:CZ	2:A:901:5WQ:H54	2.56	0.41
1:A:290:PHE:HD1	1:A:290:PHE:HA	1.71	0.41
1:A:317:TYR:HA	1:A:318:PRO:HD3	1.89	0.41
1:A:324:GLU:N	1:A:324:GLU:CD	2.78	0.41
1:A:709:GLU:H	1:A:709:GLU:CD	2.28	0.41
2:A:901:5WQ:H23	2:A:901:5WQ:H25	1.71	0.41
1:A:329:VAL:HG21	1:A:401:VAL:HG11	2.02	0.40
1:A:374:LEU:HA	1:A:380:ARG:CB	2.48	0.40
1:A:632:GLU:OE2	1:A:653:LYS:NZ	2.48	0.40
1:A:376:ALA:O	1:A:380:ARG:HB3	2.21	0.40
1:A:374:LEU:HD23	1:A:380:ARG:HB2	2.03	0.40
1:A:384:VAL:HG13	1:A:395:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD23	1:A:179:ALA:C	2.47	0.40
1:A:411:LEU:HA	1:A:412:PRO:HD3	1.92	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	751/867 (87%)	703 (94%)	48 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	591/721 (82%)	574 (97%)	17 (3%)	37	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	LEU
1	A	65	LEU
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	112	MSE
1	A	244	LYS
1	A	274	GLN
1	A	290	PHE
1	A	377	LYS
1	A	380	ARG
1	A	408	LEU
1	A	499	GLU
1	A	549	GLN
1	A	670	LYS
1	A	720	VAL
1	A	758	GLU
1	A	762	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	450	HIS
1	A	557	ASN
1	A	700	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	5WQ	A	901	-	61,61,61	2.67	19 (31%)	83,87,87	1.47	13 (15%)

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	5WQ	A	901	-	-	31/63/76/76	0/3/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	5WQ	CAK-NCE	-8.26	1.26	1.46
2	A	901	5WQ	NBE-NCF	-7.31	1.26	1.43
2	A	901	5WQ	CBS-CBT	5.83	1.43	1.37
2	A	901	5WQ	CBD-NCF	-5.79	1.36	1.46
2	A	901	5WQ	CBL-NBF	5.23	1.47	1.35
2	A	901	5WQ	CBC-NCF	-5.13	1.37	1.46
2	A	901	5WQ	CBA-NCE	-4.43	1.35	1.46
2	A	901	5WQ	CBB-NCE	-3.90	1.37	1.46
2	A	901	5WQ	OBG-CAS	3.86	1.46	1.37
2	A	901	5WQ	OBG-CBM	3.85	1.45	1.41
2	A	901	5WQ	OBI-CBJ	3.80	1.43	1.35
2	A	901	5WQ	CAW-CBO	3.36	1.61	1.51
2	A	901	5WQ	CAX-CBO	3.22	1.42	1.37
2	A	901	5WQ	CAW-NBE	-3.09	1.44	1.47
2	A	901	5WQ	CAX-CBU	2.99	1.48	1.42
2	A	901	5WQ	CAG-CBW	-2.50	1.50	1.54
2	A	901	5WQ	CAH-CBX	-2.44	1.48	1.53
2	A	901	5WQ	CBR-NBF	2.29	1.47	1.43
2	A	901	5WQ	CBR-CBO	2.13	1.43	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	5WQ	OBI-CBJ-CAD	4.91	119.85	111.09
2	A	901	5WQ	CBB-CBD-NCF	4.28	114.17	109.50
2	A	901	5WQ	CBA-CBC-NCF	4.20	114.09	109.50
2	A	901	5WQ	CBT-CBS-CBN	-3.39	119.70	123.78
2	A	901	5WQ	CBZ-CCD-CBY	-2.88	108.86	114.68
2	A	901	5WQ	CCC-CBZ-CCD	2.64	115.62	110.58
2	A	901	5WQ	CBD-NCF-CBC	2.61	115.02	110.35
2	A	901	5WQ	CAW-CBO-CAX	-2.56	119.59	121.92
2	A	901	5WQ	CBX-CCB-CBW	2.53	120.89	117.09
2	A	901	5WQ	CBY-CCA-CAV	-2.46	106.79	112.11
2	A	901	5WQ	CAW-NBE-NCF	-2.40	108.89	111.71
2	A	901	5WQ	CBK-CBL-NBF	2.15	120.72	114.96
2	A	901	5WQ	OAL-CBL-NBF	-2.11	119.47	123.92

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	5WQ	OAM-CBM-CBT-CBU
2	A	901	5WQ	OAM-CBM-OBG-CAS
2	A	901	5WQ	CAV-CAS-OBG-CBM
2	A	901	5WQ	CAS-CAV-CCA-OAZ
2	A	901	5WQ	CAS-CAV-CCA-CBY
2	A	901	5WQ	CBY-CCA-OAZ-CAC
2	A	901	5WQ	CBY-CCD-OBI-CBJ
2	A	901	5WQ	CAJ-CBZ-CCD-CBY
2	A	901	5WQ	CCC-CBZ-CCD-CBY
2	A	901	5WQ	CAJ-CBZ-CCD-OBI
2	A	901	5WQ	CCC-CBZ-CCD-OBI
2	A	901	5WQ	CAD-CBJ-OBI-CCD
2	A	901	5WQ	CAH-CBX-CCC-CBZ
2	A	901	5WQ	CCB-CBX-CCC-CBZ
2	A	901	5WQ	CCB-CBX-CCC-OAQ
2	A	901	5WQ	CCC-CBX-CCB-OAP
2	A	901	5WQ	CCC-CBX-CCB-CBW
2	A	901	5WQ	CAR-CAU-CBW-CCB
2	A	901	5WQ	OAA-CBJ-OBI-CCD
2	A	901	5WQ	CBZ-CCD-OBI-CBJ
2	A	901	5WQ	OBG-CAS-CAV-CCA
2	A	901	5WQ	CAH-CBX-CCC-OAQ
2	A	901	5WQ	CAR-CAU-CBW-CAG
2	A	901	5WQ	OAM-CBM-CBT-CBS
2	A	901	5WQ	CBO-CAW-NBE-NCF

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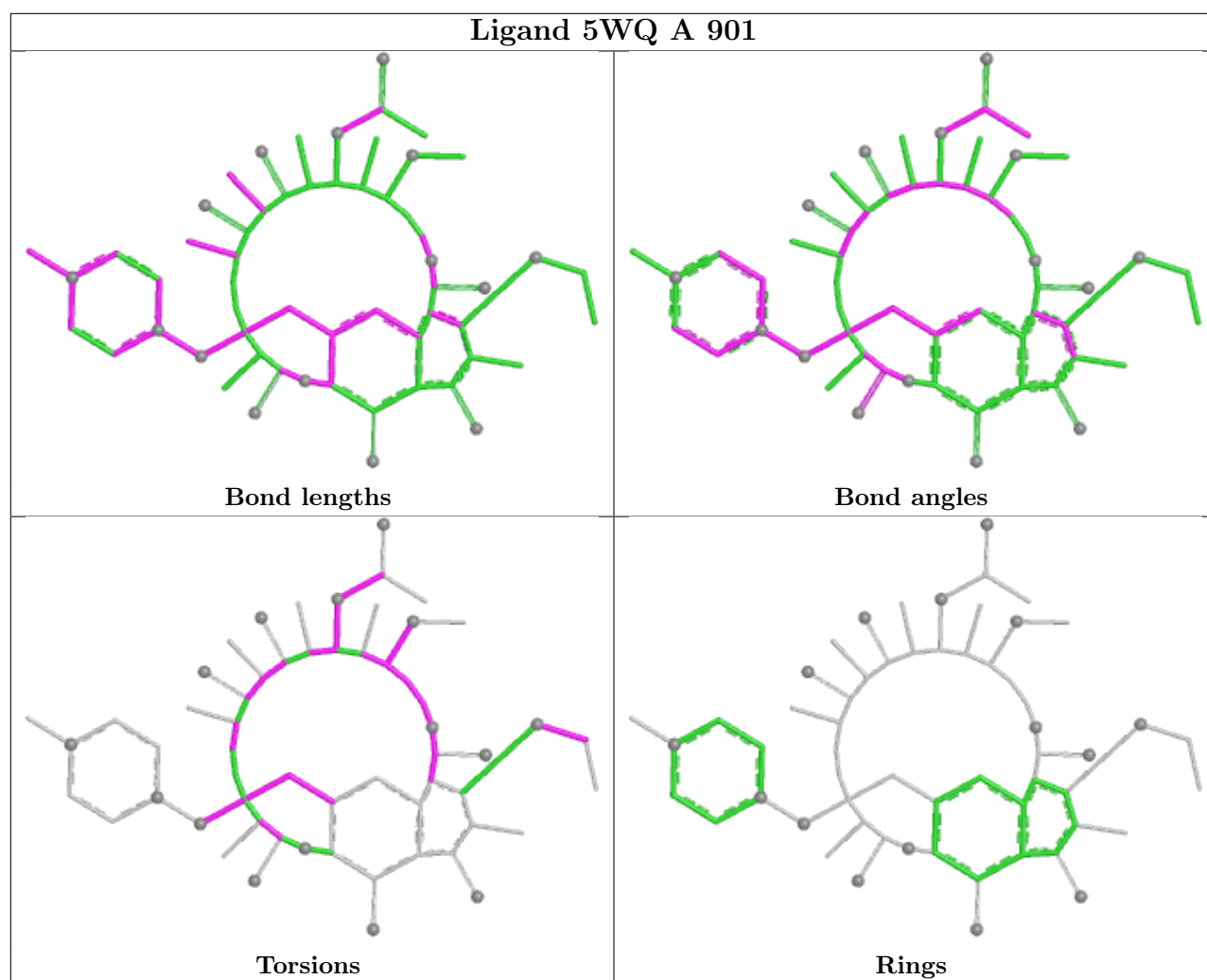
Mol	Chain	Res	Type	Atoms
2	A	901	5WQ	CAT-CBK-CBL-OAL
2	A	901	5WQ	CAT-CBK-CBL-NBF
2	A	901	5WQ	OBG-CBM-CBT-CBS
2	A	901	5WQ	CAI-CBY-CCA-CAV
2	A	901	5WQ	CAB-CAY-OBH-CBS
2	A	901	5WQ	NBE-CAW-CBO-CBR

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	5WQ	11	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	746/867 (86%)	0.76	148 (19%) 3 2	22, 55, 153, 230	2 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	LEU	11.7
1	A	179	ALA	10.6
1	A	4	TYR	7.1
1	A	184	GLN	6.9
1	A	181	VAL	6.3
1	A	97	ALA	6.3
1	A	23	GLY	6.2
1	A	22	LYS	6.2
1	A	289	TYR	6.1
1	A	40	GLY	5.9
1	A	283	GLY	5.8
1	A	26	LEU	5.8
1	A	81	GLU	5.6
1	A	180	VAL	5.6
1	A	30	SER	5.4
1	A	58	PHE	5.3
1	A	146	LEU	5.3
1	A	247	ALA	5.2
1	A	176	VAL	5.1
1	A	34	GLY	5.0
1	A	48	TYR	5.0
1	A	215	LEU	5.0
1	A	306	TYR	5.0
1	A	27	GLY	4.9
1	A	65	LEU	4.9
1	A	95	GLU	4.9
1	A	38	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	96	ILE	4.8
1	A	15	SER	4.8
1	A	87	ILE	4.6
1	A	8	PHE	4.5
1	A	29	CYS	4.5
1	A	47	ALA	4.4
1	A	84	ARG	4.4
1	A	243	THR	4.4
1	A	94	SER	4.3
1	A	154	TRP	4.3
1	A	89	HIS	4.3
1	A	258	THR	4.2
1	A	36	HIS	4.2
1	A	2	LYS	4.1
1	A	160	GLU	4.1
1	A	35	VAL	4.1
1	A	49	LYS	4.0
1	A	80	SER	4.0
1	A	11	ILE	4.0
1	A	225	SER	4.0
1	A	183	GLN	4.0
1	A	5	VAL	4.0
1	A	75	ALA	3.9
1	A	99	TYR	3.9
1	A	246	LEU	3.9
1	A	6	LEU	3.9
1	A	41	PHE	3.8
1	A	305	PHE	3.8
1	A	158	PHE	3.8
1	A	82	THR	3.8
1	A	245	LYS	3.8
1	A	9	GLN	3.7
1	A	44	THR	3.7
1	A	221	SER	3.7
1	A	177	GLN	3.7
1	A	236	ILE	3.6
1	A	232	ARG	3.6
1	A	18	LEU	3.6
1	A	88	GLN	3.6
1	A	116	VAL	3.6
1	A	86	LEU	3.6
1	A	222	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	290	PHE	3.5
1	A	147	LEU	3.4
1	A	178	LEU	3.4
1	A	3	PRO	3.4
1	A	16	GLU	3.3
1	A	19	VAL	3.3
1	A	182	ILE	3.3
1	A	103	THR	3.3
1	A	159	THR	3.3
1	A	115	ALA	3.3
1	A	322	VAL	3.3
1	A	378	VAL	3.3
1	A	233	GLU	3.2
1	A	260	ILE	3.2
1	A	93	PRO	3.2
1	A	259	ARG	3.2
1	A	63	GLN	3.2
1	A	314	THR	3.2
1	A	150	ILE	3.2
1	A	234	ASN	3.1
1	A	217	GLU	3.1
1	A	266	GLN	3.1
1	A	28	ALA	3.1
1	A	17	ALA	3.1
1	A	265	GLN	3.0
1	A	282	LEU	3.0
1	A	286	ILE	2.9
1	A	291	GLY	2.9
1	A	264	SER	2.9
1	A	186	ILE	2.9
1	A	42	CYS	2.9
1	A	299	CYS	2.9
1	A	214	GLY	2.9
1	A	98	SER	2.9
1	A	79	ILE	2.9
1	A	325	PRO	2.8
1	A	113	PRO	2.8
1	A	39	ALA	2.8
1	A	288	ALA	2.7
1	A	213	PHE	2.7
1	A	31	ASN	2.7
1	A	32	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	151	SER	2.7
1	A	285	LYS	2.7
1	A	83	ILE	2.7
1	A	114	PHE	2.7
1	A	308	VAL	2.7
1	A	61	LEU	2.6
1	A	25	ASN	2.6
1	A	759	ASN	2.6
1	A	92	ILE	2.6
1	A	46	GLU	2.6
1	A	413	THR	2.5
1	A	223	LEU	2.4
1	A	148	GLN	2.4
1	A	64	ARG	2.4
1	A	242	ALA	2.4
1	A	45	THR	2.4
1	A	311	ARG	2.4
1	A	85	THR	2.4
1	A	149	HIS	2.3
1	A	292	LYS	2.3
1	A	244	LYS	2.3
1	A	315	THR	2.3
1	A	295	ASP	2.3
1	A	310	SER	2.3
1	A	20	GLY	2.3
1	A	62	LEU	2.2
1	A	60	GLN	2.1
1	A	307	ILE	2.1
1	A	224	VAL	2.1
1	A	614	SER	2.1
1	A	200	ILE	2.1
1	A	257	GLU	2.1
1	A	207	LEU	2.1
1	A	21	GLY	2.1
1	A	77	ARG	2.0
1	A	59	THR	2.0
1	A	647	GLN	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 oligosaccharides in this entry.

6.4 Ligands

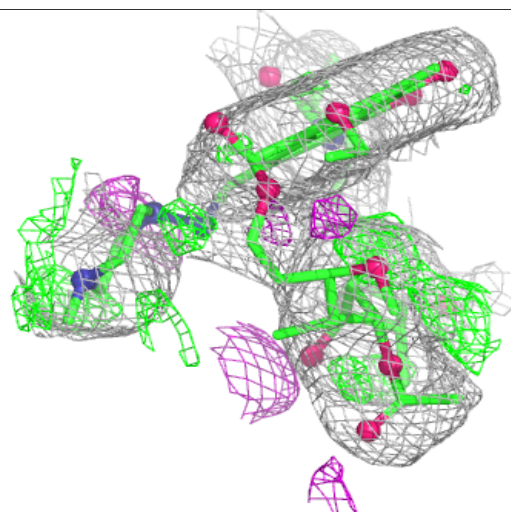
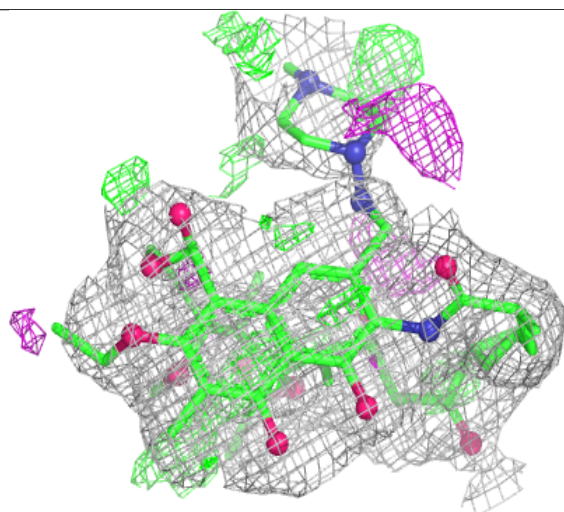
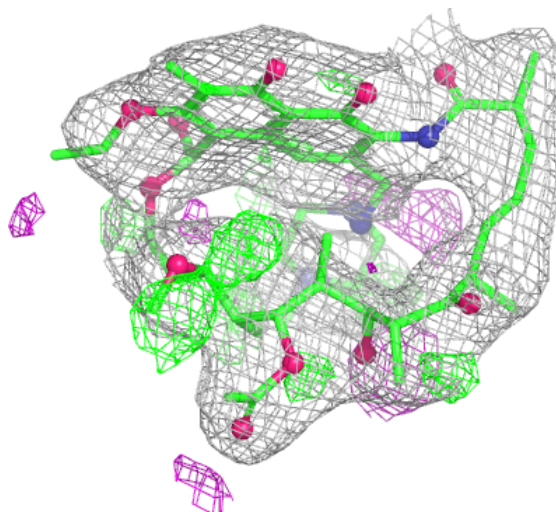
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5WQ	A	901	58/58	0.86	0.19	28,63,133,136	0
3	CL	A	902	1/1	0.99	0.04	46,46,46,46	1

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 5WQ 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.