



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:06 AM UTC

PDB ID : 5FGZ / pdb_00005fgz
Title : E. coli PBP1b in complex with FPI-1465
Authors : King, D.T.; Strynadka, N.C.J.
Deposited on : 2015-12-21
Resolution : 2.85 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

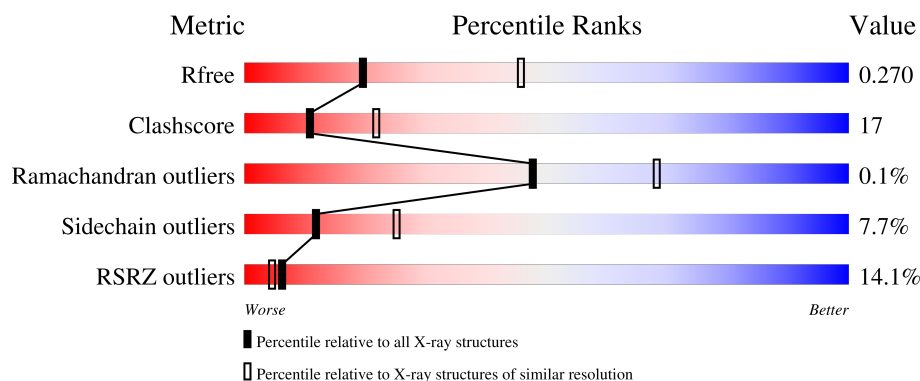
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5VW	A	902	-	-	X	-

2 Entry composition [i](#)

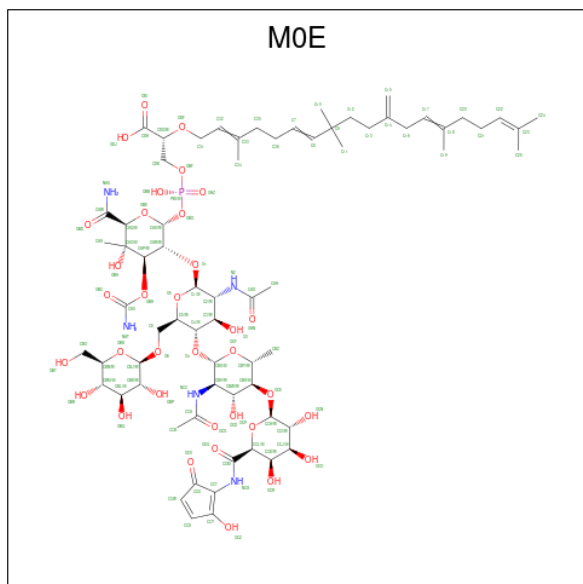
There are 4 unique types of molecules in this entry. The entry contains 5633 atoms, of which 18 are hydrogens and 0 are deuteriums.

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.

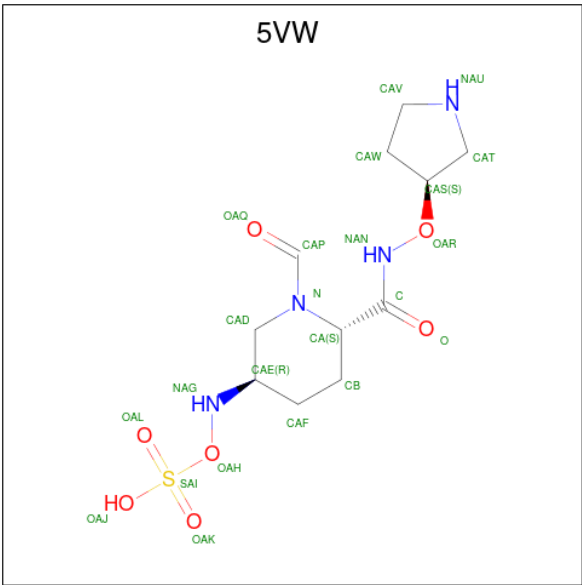
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	5456	3456	960	1014	26	0	0	0

- Molecule 2 is MOENOMYCIN (CCD ID: M0E) (formula: C₆₉H₁₀₆N₅O₃₄P).



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

- Molecule 3 is [[(3 {R},6 {S})-1-methanoyl-6-[[[(3 {S})-pyrrolidin-3-yl]oxycarbamoyl]piperidin-3-yl]amino] hydrogen sulfate (CCD ID: 5VW) (formula: C₁₁H₂₀N₄O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	S	0	0
			41	11	18	4	7	1		

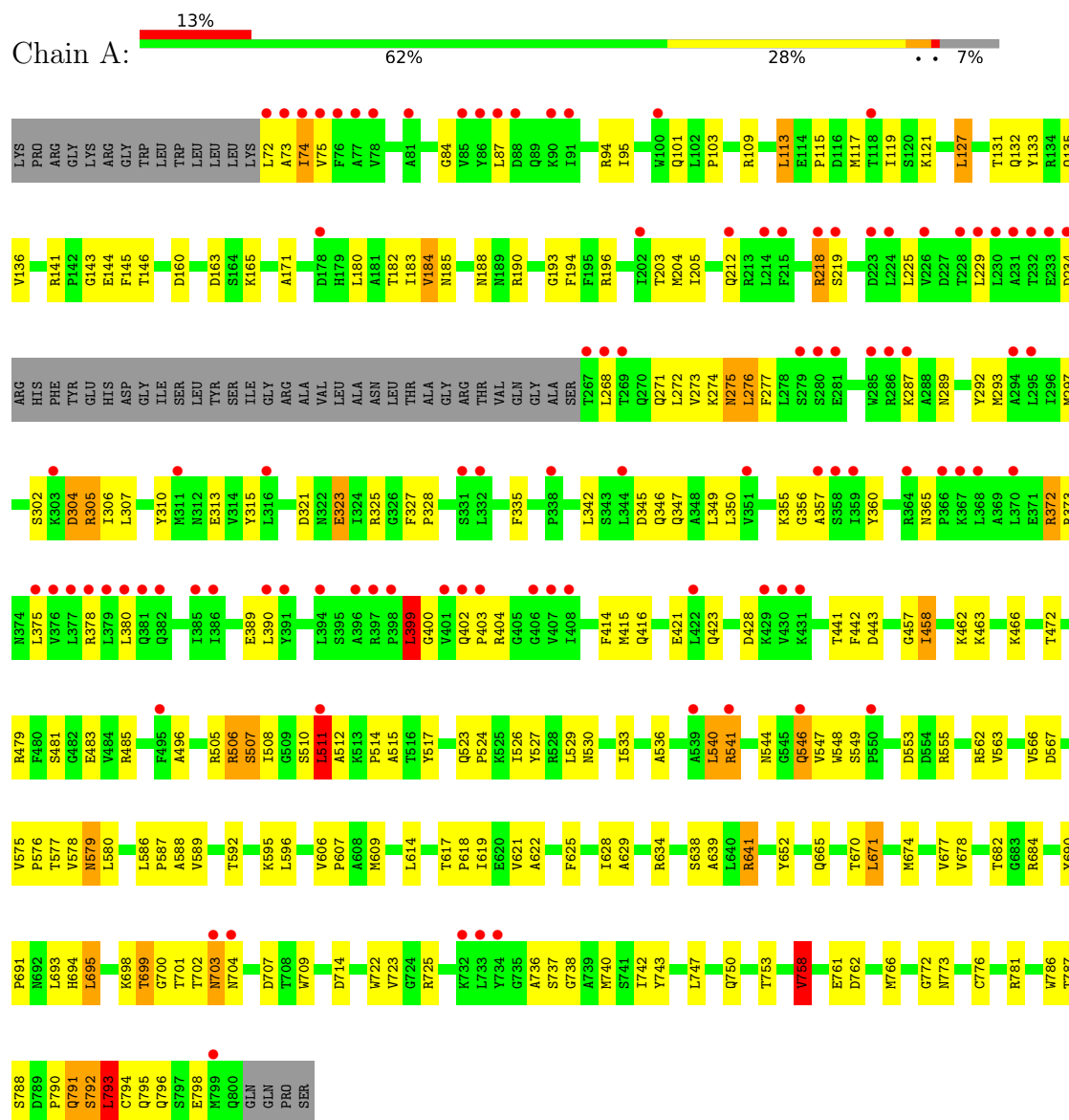
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		

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: 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	62.48Å 63.22Å 293.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.22 – 2.85 63.22 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.9 (63.22-2.85) 93.9 (63.22-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.238 , 0.292 (Not available) , 0.270	Depositor DCC
R_{free} test set	1389 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.085 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5633	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, 5VW

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	0.87	1/5564 (0.0%)	1.07	17/7552 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	762	ASP	CA-C	-5.01	1.46	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	ARG	N-CA-C	7.32	118.26	108.38
1	A	579	ASN	N-CA-C	-7.13	102.56	111.11
1	A	399	LEU	N-CA-C	6.02	118.62	111.33
1	A	540	LEU	N-CA-C	5.88	119.54	107.37
1	A	788	SER	N-CA-C	-5.74	105.00	112.23
1	A	758	VAL	N-CA-C	-5.69	101.92	107.55
1	A	184	VAL	N-CA-C	5.63	115.99	108.11
1	A	549	SER	CA-C-N	5.62	125.80	119.90
1	A	549	SER	C-N-CA	5.62	125.80	119.90
1	A	536	ALA	CA-C-N	5.54	126.76	119.84
1	A	536	ALA	C-N-CA	5.54	126.76	119.84
1	A	74	ILE	N-CA-C	-5.47	107.04	111.91
1	A	496	ALA	N-CA-C	5.46	117.14	108.79
1	A	546	GLN	N-CA-C	5.23	117.07	110.33
1	A	113	LEU	N-CA-C	-5.13	101.91	110.17
1	A	793	LEU	N-CA-C	5.07	116.62	111.14
1	A	677	VAL	N-CA-C	-5.01	105.51	110.62

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	5456	0	5505	178	0
2	A	77	0	59	12	0
3	A	23	18	18	10	0
4	A	59	0	0	0	0
All	All	5615	18	5582	185	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 17.

All (185) 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:902:5VW:NAN	3:A:902:5VW:OAR	1.74	1.21
1:A:506:ARG:NH1	1:A:707:ASP:OD1	1.94	1.00
1:A:313:GLU:OE1	1:A:325:ARG:NH2	1.96	0.99
1:A:510:SER:HB2	1:A:700:GLY:HA2	1.48	0.94
1:A:117:MET:HE3	1:A:119:ILE:HG21	1.57	0.86
1:A:776:CYS:SG	1:A:793:LEU:HD13	2.18	0.84
1:A:315:TYR:CE2	1:A:323:GLU:HB3	2.14	0.83
1:A:506:ARG:NH2	1:A:725:ARG:O	2.13	0.82
1:A:510:SER:O	1:A:512:ALA:N	2.14	0.81
1:A:510:SER:C	1:A:512:ALA:H	1.88	0.80
1:A:315:TYR:HE2	1:A:323:GLU:HB3	1.51	0.76
1:A:127:LEU:O	1:A:131:THR:HG22	1.85	0.76
1:A:355:LYS:O	2:A:901:M0E:H3	1.88	0.74
1:A:402:GLN:HB3	1:A:404:ARG:HB3	1.69	0.74
1:A:703:ASN:N	3:A:902:5VW:H15	2.03	0.74
1:A:349:LEU:HB2	1:A:399:LEU:HD23	1.71	0.73
1:A:693:LEU:HB3	1:A:695:LEU:HD13	1.70	0.73
1:A:766:MET:HE2	1:A:793:LEU:HD23	1.71	0.73
1:A:703:ASN:H	3:A:902:5VW:H15	1.54	0.72
1:A:481:SER:OG	1:A:483:GLU:HG3	1.90	0.71
1:A:355:LYS:O	2:A:901:M0E:O5	2.08	0.69
1:A:462:LYS:O	1:A:466:LYS:N	2.24	0.69
1:A:790:PRO:O	1:A:791:GLN:OE1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HG3	1:A:399:LEU:HG	1.75	0.68
1:A:271:GLN:NE2	2:A:901:M0E:HAT2	1.91	0.66
1:A:117:MET:HE3	1:A:119:ILE:CG2	2.25	0.65
1:A:508:ILE:HB	1:A:511:LEU:HB3	1.79	0.64
1:A:273:VAL:O	1:A:277:PHE:HB2	1.96	0.64
1:A:629:ALA:HA	1:A:671:LEU:HD21	1.78	0.64
1:A:511:LEU:HD22	1:A:709:TRP:CD2	2.33	0.64
1:A:117:MET:CE	1:A:119:ILE:HG21	2.27	0.63
1:A:592:THR:O	1:A:596:LEU:HG	1.98	0.63
1:A:790:PRO:C	1:A:791:GLN:OE1	2.41	0.63
1:A:113:LEU:HD22	1:A:117:MET:HE1	1.80	0.62
1:A:136:VAL:HG23	1:A:146:THR:HG22	1.83	0.61
1:A:567:ASP:OD2	1:A:781:ARG:NH2	2.27	0.61
1:A:188:ASN:O	1:A:190:ARG:HG3	2.02	0.60
1:A:72:LEU:HD13	1:A:74:ILE:HB	1.83	0.59
1:A:670:THR:HG22	1:A:674:MET:CE	2.33	0.59
3:A:902:5VW:NAN	3:A:902:5VW:CAS	2.66	0.59
1:A:335:PHE:CE1	1:A:346:GLN:HG2	2.39	0.58
1:A:511:LEU:HD22	1:A:709:TRP:CG	2.38	0.58
1:A:563:VAL:O	1:A:563:VAL:HG23	2.03	0.58
1:A:510:SER:C	1:A:512:ALA:N	2.52	0.57
2:A:901:M0E:O6	2:A:901:M0E:HBO2	2.04	0.57
1:A:355:LYS:O	2:A:901:M0E:C5	2.53	0.57
1:A:335:PHE:CE2	1:A:346:GLN:HB3	2.40	0.57
1:A:523:GLN:HB3	1:A:526:ILE:HG12	1.87	0.56
1:A:575:VAL:HB	1:A:576:PRO:HD3	1.87	0.56
1:A:313:GLU:CD	1:A:325:ARG:HH21	2.10	0.55
1:A:479:ARG:HG3	1:A:629:ALA:HB1	1.88	0.55
1:A:703:ASN:HB2	3:A:902:5VW:H16	1.89	0.55
1:A:403:PRO:N	1:A:404:ARG:HA	2.21	0.55
1:A:690:TYR:HB3	1:A:693:LEU:HD12	1.89	0.55
1:A:483:GLU:OE2	1:A:641:ARG:NH1	2.40	0.55
1:A:84:GLY:HA3	1:A:292:TYR:OH	2.07	0.54
1:A:271:GLN:CD	2:A:901:M0E:HAT2	2.15	0.54
1:A:360:TYR:CZ	1:A:372:ARG:HG2	2.42	0.54
1:A:682:THR:HG21	3:A:902:5VW:OAK	2.07	0.54
1:A:315:TYR:CD1	1:A:357:ALA:HB1	2.43	0.54
1:A:665:GLN:HG2	1:A:786:TRP:CD1	2.42	0.53
1:A:315:TYR:CD2	1:A:323:GLU:HB3	2.42	0.53
1:A:737:SER:HA	1:A:740:MET:HB2	1.90	0.53
1:A:698:LYS:HG3	1:A:699:THR:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLN:C	1:A:793:LEU:N	2.63	0.52
1:A:94:ARG:NH1	1:A:276:LEU:O	2.43	0.52
1:A:180:LEU:HD21	1:A:183:ILE:HG12	1.92	0.52
1:A:389:GLU:HG3	1:A:390:LEU:HD12	1.92	0.52
1:A:628:ILE:HD13	1:A:674:MET:HE1	1.91	0.52
1:A:670:THR:HG22	1:A:674:MET:HE2	1.91	0.52
1:A:113:LEU:CD2	1:A:117:MET:HE1	2.40	0.52
1:A:533:ILE:HD11	1:A:580:LEU:HD13	1.91	0.52
1:A:355:LYS:O	2:A:901:M0E:C3	2.56	0.51
1:A:365:ASN:O	1:A:365:ASN:OD1	2.28	0.51
1:A:652:TYR:CD2	1:A:652:TYR:C	2.89	0.51
1:A:703:ASN:H	3:A:902:5VW:CAW	2.23	0.50
1:A:540:LEU:N	1:A:548:TRP:O	2.45	0.50
1:A:163:ASP:HB2	1:A:196:ARG:HH12	1.76	0.50
2:A:901:M0E:HDG	2:A:901:M0E:HAQ	1.93	0.50
1:A:508:ILE:HB	1:A:511:LEU:CB	2.42	0.50
1:A:690:TYR:CB	1:A:693:LEU:HD12	2.42	0.50
1:A:360:TYR:CD2	1:A:372:ARG:HG3	2.47	0.50
1:A:702:THR:CA	3:A:902:5VW:H15	2.42	0.49
1:A:271:GLN:O	1:A:275:ASN:OD1	2.30	0.49
1:A:272:LEU:CD2	1:A:276:LEU:HD22	2.41	0.49
1:A:87:LEU:HD22	1:A:293:MET:HE3	1.94	0.49
1:A:349:LEU:HD22	1:A:399:LEU:CD2	2.42	0.49
1:A:315:TYR:CD1	1:A:357:ALA:CB	2.96	0.48
1:A:315:TYR:HD1	1:A:357:ALA:CB	2.26	0.48
1:A:399:LEU:HD22	1:A:400:GLY:N	2.28	0.48
1:A:185:ASN:HB3	1:A:188:ASN:OD1	2.14	0.48
1:A:218:ARG:HD3	1:A:304:ASP:CG	2.39	0.48
1:A:506:ARG:O	1:A:507:SER:C	2.56	0.48
1:A:737:SER:HA	1:A:740:MET:HE3	1.95	0.48
1:A:791:GLN:O	1:A:792:SER:C	2.53	0.48
1:A:355:LYS:HG3	1:A:356:GLY:N	2.28	0.48
1:A:714:ASP:HB2	1:A:753:THR:O	2.14	0.48
1:A:758:VAL:HG12	1:A:758:VAL:O	2.12	0.48
1:A:701:THR:N	3:A:902:5VW:OAQ	2.41	0.47
1:A:287:LYS:HE2	1:A:287:LYS:C	2.39	0.47
1:A:315:TYR:CE1	1:A:357:ALA:HB1	2.49	0.47
1:A:702:THR:HA	3:A:902:5VW:H15	1.96	0.47
1:A:737:SER:O	1:A:738:GLY:C	2.57	0.47
1:A:443:ASP:C	1:A:443:ASP:OD2	2.56	0.47
1:A:73:ALA:HB1	1:A:75:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:CD2	1:A:276:LEU:CD2	2.92	0.47
1:A:275:ASN:HD21	2:A:901:M0E:HAH1	1.78	0.47
1:A:421:GLU:OE2	1:A:638:SER:HB2	2.15	0.47
1:A:218:ARG:NH1	1:A:307:LEU:HD21	2.30	0.47
1:A:511:LEU:CD2	1:A:621:VAL:HG11	2.44	0.47
1:A:791:GLN:OE1	1:A:791:GLN:N	2.47	0.47
2:A:901:M0E:OBC	2:A:901:M0E:HAH3	2.15	0.47
1:A:373:ARG:HD2	1:A:373:ARG:C	2.40	0.47
1:A:665:GLN:HG2	1:A:786:TRP:NE1	2.30	0.47
1:A:218:ARG:HG3	1:A:219:SER:N	2.29	0.46
1:A:327:PHE:N	1:A:328:PRO:CD	2.78	0.46
1:A:141:ARG:NH2	1:A:342:LEU:O	2.49	0.46
1:A:271:GLN:O	1:A:272:LEU:C	2.59	0.46
1:A:606:VAL:O	1:A:607:PRO:C	2.59	0.46
1:A:795:GLN:O	1:A:798:GLU:HG2	2.16	0.46
1:A:103:PRO:HB2	1:A:205:ILE:O	2.16	0.46
1:A:625:PHE:HA	1:A:628:ILE:HG22	1.98	0.46
1:A:305:ARG:O	1:A:305:ARG:HG3	2.15	0.45
1:A:133:TYR:HA	1:A:143:GLY:O	2.16	0.45
1:A:441:THR:N	1:A:639:ALA:O	2.49	0.45
1:A:619:ILE:O	1:A:622:ALA:HB3	2.16	0.45
1:A:423:GLN:NE2	1:A:428:ASP:OD1	2.48	0.45
1:A:182:THR:C	1:A:183:ILE:HG13	2.40	0.45
1:A:458:ILE:HD11	1:A:472:THR:HB	1.98	0.45
1:A:72:LEU:HB3	1:A:74:ILE:N	2.32	0.45
1:A:773:ASN:HB3	1:A:796:GLN:CG	2.47	0.45
1:A:481:SER:OG	1:A:483:GLU:CG	2.60	0.45
1:A:678:VAL:O	1:A:684:ARG:HA	2.17	0.45
1:A:540:LEU:O	1:A:541:ARG:C	2.60	0.45
1:A:302:SER:O	1:A:306:ILE:HG12	2.16	0.45
1:A:457:GLY:HA3	1:A:742:ILE:CD1	2.47	0.45
1:A:135:GLN:HA	1:A:145:PHE:O	2.16	0.44
1:A:375:LEU:O	1:A:378:ARG:HG3	2.18	0.44
2:A:901:M0E:H61	2:A:901:M0E:O1	2.16	0.44
1:A:345:ASP:OD2	1:A:346:GLN:HG3	2.18	0.44
1:A:225:LEU:HD13	1:A:347:GLN:CG	2.48	0.44
1:A:203:THR:OG1	1:A:204:MET:N	2.50	0.43
1:A:578:VAL:O	1:A:579:ASN:C	2.61	0.43
1:A:514:PRO:O	1:A:515:ALA:C	2.60	0.43
1:A:415:MET:O	1:A:416:GLN:C	2.60	0.43
1:A:529:LEU:HB3	1:A:566:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:TRP:CZ3	1:A:722:TRP:HB2	2.54	0.43
1:A:743:TYR:CE2	1:A:747:LEU:HD11	2.54	0.43
1:A:327:PHE:CD1	1:A:350:LEU:HD23	2.53	0.43
1:A:508:ILE:HA	1:A:709:TRP:NE1	2.34	0.43
1:A:194:PHE:CD1	1:A:194:PHE:C	2.97	0.43
1:A:586:LEU:N	1:A:587:PRO:CD	2.82	0.43
1:A:315:TYR:HE2	1:A:323:GLU:CB	2.27	0.43
1:A:524:PRO:HG3	1:A:786:TRP:CE3	2.54	0.42
1:A:160:ASP:OD1	1:A:165:LYS:HG3	2.19	0.42
1:A:588:ALA:O	1:A:589:VAL:C	2.60	0.42
1:A:360:TYR:CE2	1:A:372:ARG:CG	3.02	0.42
1:A:690:TYR:O	1:A:691:PRO:C	2.62	0.42
1:A:791:GLN:HG3	1:A:794:CYS:SG	2.59	0.42
2:A:901:M0E:OCN	2:A:901:M0E:HBZ1	2.19	0.42
1:A:595:LYS:O	1:A:634:ARG:HD3	2.20	0.42
1:A:132:GLN:OE1	1:A:132:GLN:N	2.53	0.41
1:A:526:ILE:HG13	1:A:527:TYR:CD2	2.55	0.41
1:A:628:ILE:HD11	1:A:670:THR:CG2	2.50	0.41
1:A:229:LEU:HD11	1:A:310:TYR:CE2	2.55	0.41
1:A:115:PRO:HD2	1:A:193:GLY:O	2.20	0.41
1:A:699:THR:HB	1:A:736:ALA:CB	2.50	0.41
1:A:776:CYS:SG	1:A:793:LEU:CD1	3.02	0.41
1:A:414:PHE:CE1	1:A:442:PHE:HB2	2.55	0.41
1:A:472:THR:OG1	1:A:723:VAL:HG22	2.20	0.41
1:A:141:ARG:HG2	1:A:144:GLU:CD	2.46	0.41
1:A:530:ASN:ND2	1:A:772:GLY:O	2.49	0.41
1:A:234:ASP:HB2	1:A:268:LEU:HG	2.03	0.41
1:A:517:TYR:HH	1:A:577:THR:HG1	1.60	0.41
1:A:315:TYR:HB2	1:A:325:ARG:HD2	2.02	0.41
1:A:109:ARG:HG2	1:A:442:PHE:O	2.21	0.40
1:A:171:ALA:HA	1:A:184:VAL:O	2.21	0.40
1:A:510:SER:HB3	1:A:699:THR:O	2.20	0.40
1:A:511:LEU:HD23	1:A:621:VAL:HG11	2.03	0.40
1:A:743:TYR:CZ	1:A:747:LEU:HD21	2.57	0.40
1:A:702:THR:CG2	1:A:707:ASP:HB2	2.52	0.40
1:A:218:ARG:HD2	1:A:304:ASP:O	2.22	0.40
1:A:95:ILE:HD11	1:A:297:MET:HE1	2.03	0.40
1:A:617:THR:O	1:A:618:PRO:C	2.64	0.40
1:A:690:TYR:HB3	1:A:693:LEU:CD1	2.52	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	693/747 (93%)	635 (92%)	57 (8%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	LEU

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	587/627 (94%)	542 (92%)	45 (8%)	12	25

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	121	LYS
1	A	127	LEU
1	A	212	GLN
1	A	218	ARG
1	A	274	LYS
1	A	275	ASN
1	A	276	LEU
1	A	289	ASN
1	A	304	ASP

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Mol	Chain	Res	Type
1	A	305	ARG
1	A	321	ASP
1	A	323	GLU
1	A	372	ARG
1	A	380	LEU
1	A	399	LEU
1	A	458	ILE
1	A	463	LYS
1	A	485	ARG
1	A	505	ARG
1	A	506	ARG
1	A	507	SER
1	A	511	LEU
1	A	541	ARG
1	A	544	ASN
1	A	546	GLN
1	A	547	VAL
1	A	553	ASP
1	A	555	ARG
1	A	609	MET
1	A	614	LEU
1	A	641	ARG
1	A	671	LEU
1	A	694	HIS
1	A	695	LEU
1	A	699	THR
1	A	703	ASN
1	A	704	ASN
1	A	750	GLN
1	A	758	VAL
1	A	761	GLU
1	A	787	THR
1	A	791	GLN
1	A	792	SER
1	A	793	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	365	ASN
1	A	464	GLN

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Mol	Chain	Res	Type
1	A	552	ASN
1	A	665	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 oligosaccharides 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	A	901	-	79,81,114	0.99	4 (5%)	112,122,166	1.27	12 (10%)
3	5VW	A	902	1	20,24,24	5.90	4 (20%)	20,33,33	3.37	8 (40%)

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	A	901	-	-	13/52/158/206	0/5/5/6
3	5VW	A	902	1	-	0/9/37/37	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	5VW	OAR-NAN	24.53	1.74	1.40
3	A	902	5VW	CAD-CAE	-6.84	1.40	1.52
2	A	901	M0E	OBH-CAV	5.50	1.46	1.35
3	A	902	5VW	CAW-CAV	-5.07	1.45	1.53
2	A	901	M0E	O6-CBJ	2.79	1.44	1.40
2	A	901	M0E	CCK-CCL	2.47	1.57	1.53
2	A	901	M0E	PBI-OBF	2.14	1.67	1.59
3	A	902	5VW	CAW-CAS	-2.02	1.41	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	5VW	CB-CAF-CAE	7.30	119.50	111.49
3	A	902	5VW	OAQ-CAP-N	-7.11	107.95	125.34
3	A	902	5VW	C-CA-N	6.78	127.67	111.21
2	A	901	M0E	OBH-CAV-NAT	5.43	119.34	110.92
3	A	902	5VW	OAR-NAN-C	5.20	126.82	117.87
2	A	901	M0E	OCP-CCL-CCK	4.14	117.66	109.48
3	A	902	5VW	CB-CA-C	-3.72	105.17	112.17
2	A	901	M0E	OBG-CAX-CAR	3.58	114.94	108.38
2	A	901	M0E	OBH-CAV-OBC	-3.08	118.35	123.06
3	A	902	5VW	CAV-CAW-CAS	3.00	108.45	104.15
3	A	902	5VW	CAF-CAE-CAD	2.74	113.27	109.71
2	A	901	M0E	ODJ-CDH-CDG	2.71	118.48	112.74
3	A	902	5VW	O-C-CA	2.64	127.04	120.69
2	A	901	M0E	CBU-O4-C4	-2.58	111.87	117.98
2	A	901	M0E	CAQ-CAW-NAU	2.46	118.78	117.34
2	A	901	M0E	CCH-OCE-CBX	-2.30	112.53	117.98
2	A	901	M0E	O1-CAR-CAX	-2.20	102.91	108.47
2	A	901	M0E	OBC-CAV-NAT	-2.07	122.31	125.58
2	A	901	M0E	O5-C5-C6	2.05	110.76	106.69
2	A	901	M0E	ODI-CDH-CDG	-2.05	118.51	122.60

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	M0E	CDG-CDK-OBF-PBI
2	A	901	M0E	OBC-CAV-OBH-CAP
2	A	901	M0E	NAT-CAV-OBH-CAP
2	A	901	M0E	CAH-CAG-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	901	M0E	OAN-CAG-N2-C2
2	A	901	M0E	OBS-CBJ-O6-C6
2	A	901	M0E	OCG-CCA-NCC-CBV
2	A	901	M0E	CCB-CCA-NCC-CBV
2	A	901	M0E	OBS-CBN-CBO-OBT
2	A	901	M0E	CBK-CBJ-O6-C6
2	A	901	M0E	CAP-CAR-O1-C1
2	A	901	M0E	C4-C5-C6-O6
2	A	901	M0E	CAX-CAR-O1-C1

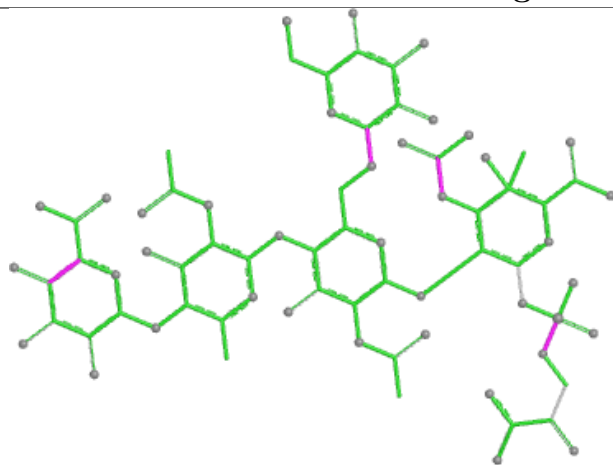
There are no ring outliers.

2 monomers are involved in 22 short contacts:

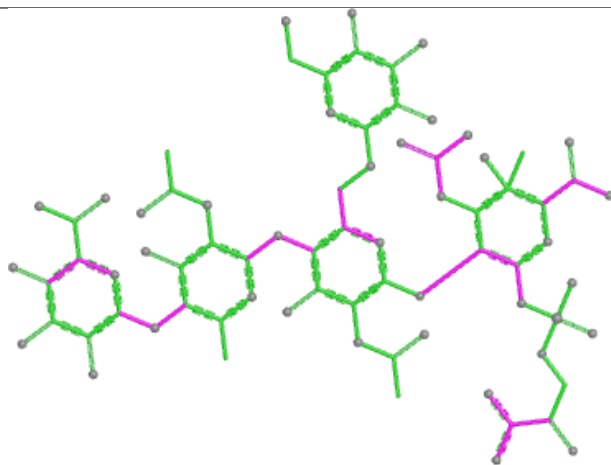
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	M0E	12	0
3	A	902	5VW	10	0

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.

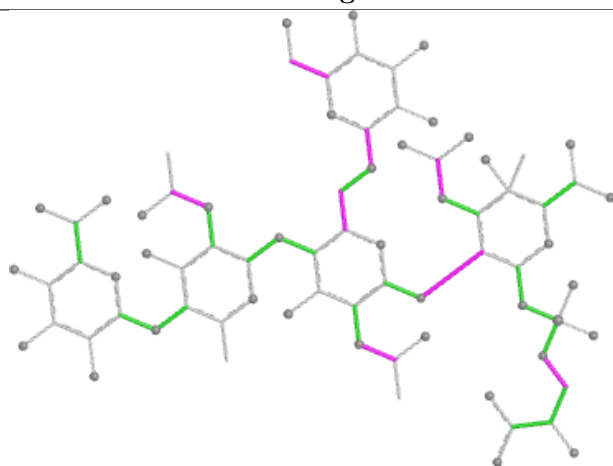
Ligand M0E A 901



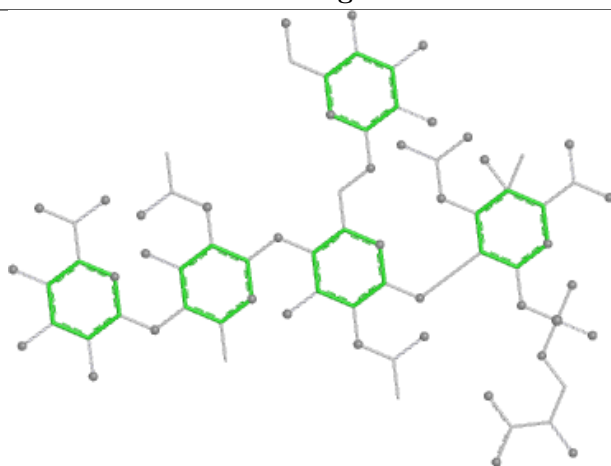
Bond lengths



Bond angles

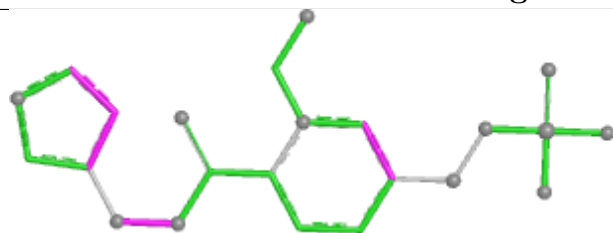


Torsions

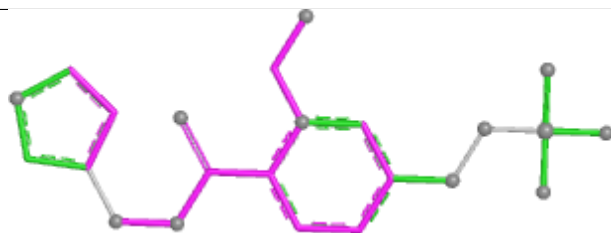


Rings

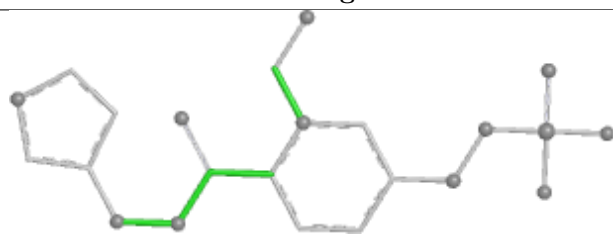
Ligand 5VW A 902



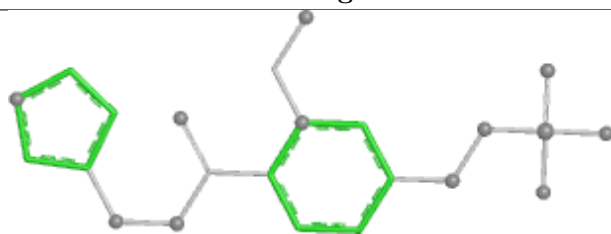
Bond lengths



Bond angles



Torsions



Rings

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%)	0.73	98 (14%) 6 4	17, 51, 131, 193	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	5.9
1	A	86	TYR	5.6
1	A	407	VAL	5.4
1	A	734	TYR	4.8
1	A	401	VAL	4.6
1	A	495	PHE	4.5
1	A	408	ILE	4.5
1	A	378	ARG	4.1
1	A	232	THR	4.0
1	A	357	ALA	3.8
1	A	280	SER	3.7
1	A	385	ILE	3.6
1	A	77	ALA	3.6
1	A	511	LEU	3.6
1	A	381	GLN	3.5
1	A	704	ASN	3.5
1	A	267	THR	3.5
1	A	359	ILE	3.4
1	A	344	LEU	3.3
1	A	367	LYS	3.3
1	A	286	ARG	3.3
1	A	396	ALA	3.3
1	A	358	SER	3.3
1	A	269	THR	3.2
1	A	224	LEU	3.1
1	A	229	LEU	3.1
1	A	73	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	406	GLY	3.1
1	A	368	LEU	3.1
1	A	76	PHE	3.0
1	A	87	LEU	3.0
1	A	178	ASP	3.0
1	A	295	LEU	2.9
1	A	386	ILE	2.9
1	A	338	PRO	2.9
1	A	379	LEU	2.9
1	A	85	VAL	2.9
1	A	215	PHE	2.8
1	A	303	LYS	2.8
1	A	268	LEU	2.8
1	A	223	ASP	2.8
1	A	390	LEU	2.7
1	A	81	ALA	2.7
1	A	118	THR	2.7
1	A	546	GLN	2.7
1	A	422	LEU	2.7
1	A	541	ARG	2.7
1	A	78	VAL	2.6
1	A	316	LEU	2.6
1	A	75	VAL	2.6
1	A	430	VAL	2.6
1	A	375	LEU	2.6
1	A	218	ARG	2.5
1	A	370	LEU	2.5
1	A	234	ASP	2.5
1	A	72	LEU	2.5
1	A	403	PRO	2.5
1	A	285	TRP	2.5
1	A	376	VAL	2.5
1	A	331	SER	2.5
1	A	279	SER	2.4
1	A	382	GLN	2.4
1	A	366	PRO	2.4
1	A	90	LYS	2.4
1	A	402	GLN	2.4
1	A	391	TYR	2.4
1	A	377	LEU	2.4
1	A	398	PRO	2.4
1	A	332	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	TRP	2.3
1	A	397	ARG	2.3
1	A	311	MET	2.2
1	A	294	ALA	2.2
1	A	214	LEU	2.2
1	A	226	VAL	2.2
1	A	732	LYS	2.2
1	A	733	LEU	2.2
1	A	212	GLN	2.2
1	A	219	SER	2.2
1	A	230	LEU	2.2
1	A	380	LEU	2.2
1	A	394	LEU	2.1
1	A	281	GLU	2.1
1	A	703	ASN	2.1
1	A	799	MET	2.1
1	A	287	LYS	2.1
1	A	364	ARG	2.1
1	A	539	ALA	2.1
1	A	233	GLU	2.1
1	A	431	LYS	2.1
1	A	550	PRO	2.1
1	A	91	ILE	2.1
1	A	202	ILE	2.1
1	A	88	ASP	2.1
1	A	228	THR	2.1
1	A	429	LYS	2.0
1	A	74	ILE	2.0
1	A	351	VAL	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 ⓘ

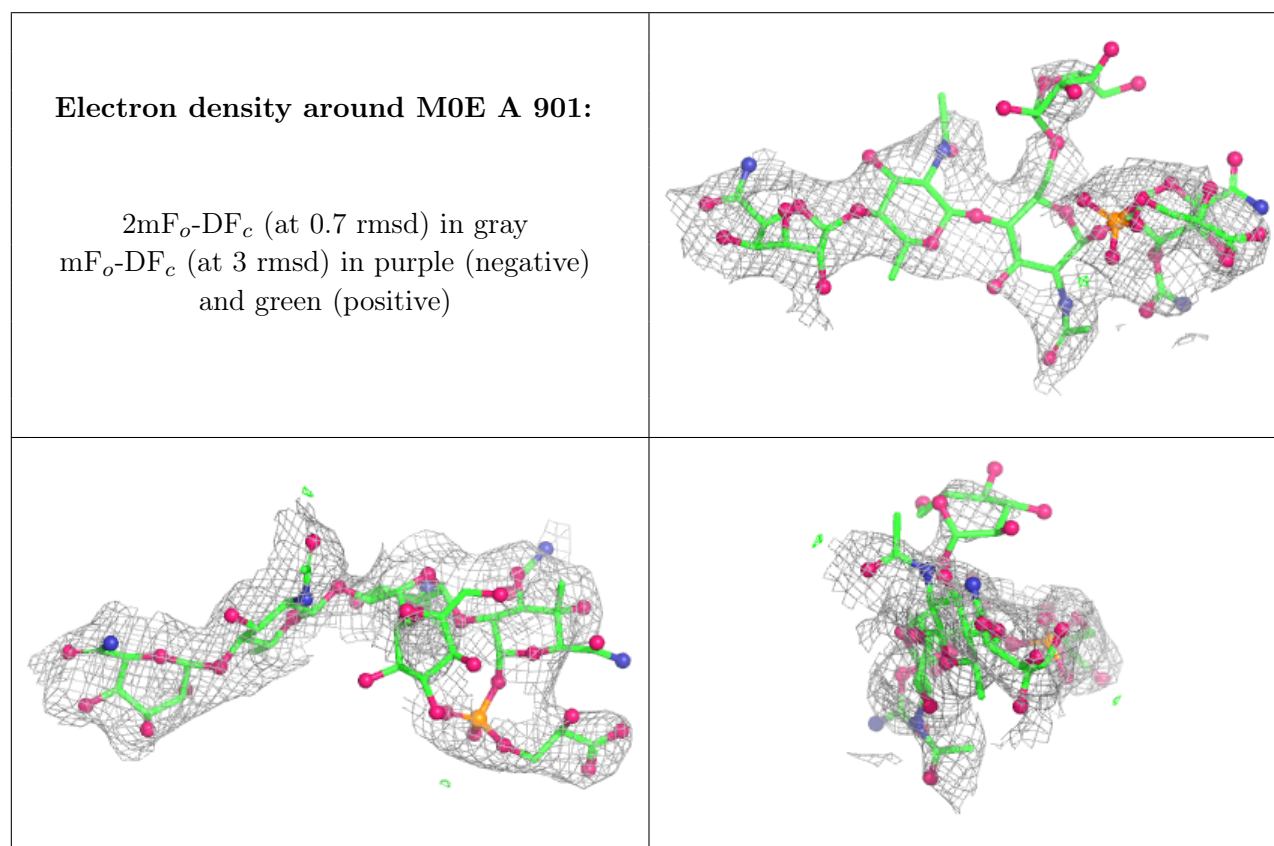
There are no oligosaccharides in this entry.

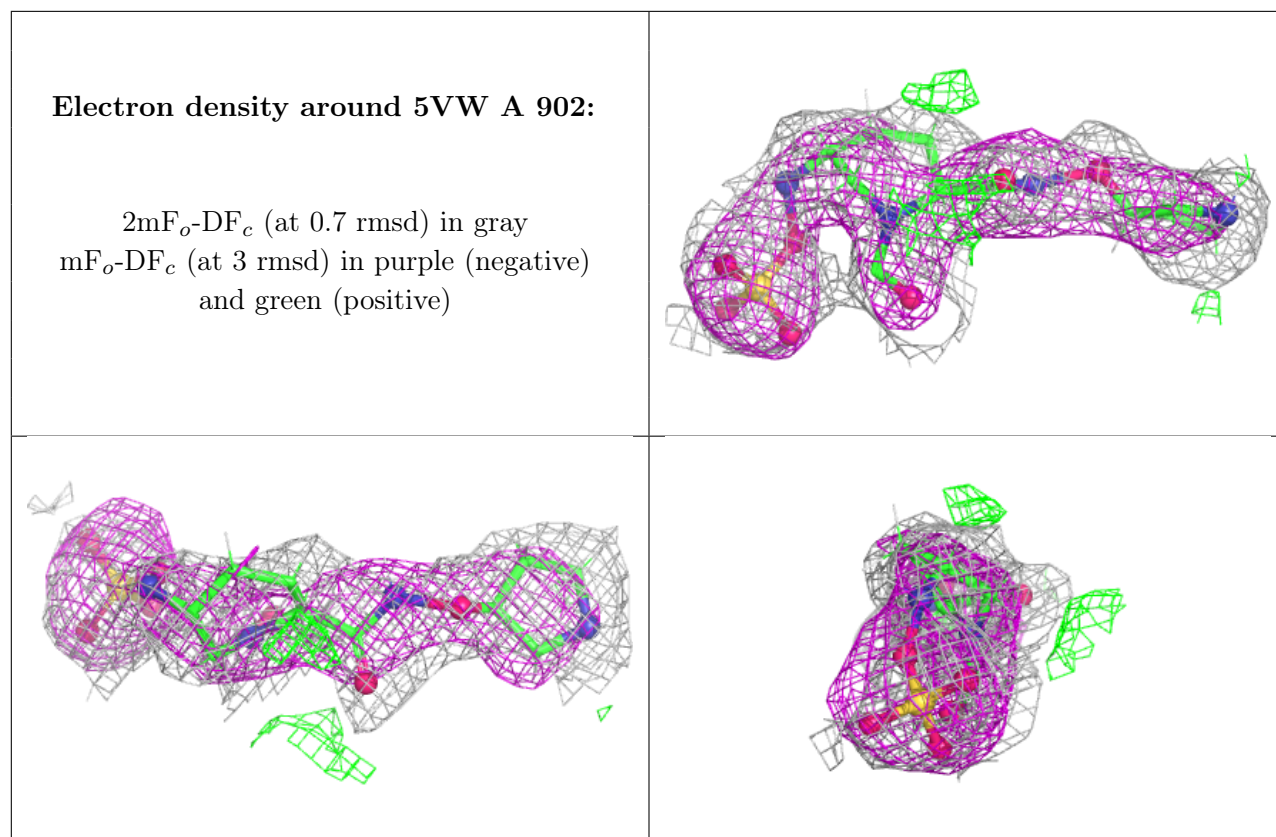
6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	M0E	A	901	77/109	0.68	0.17	74,110,134,144	0
3	5VW	A	902	23/23	0.80	0.16	20,20,20,20	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.