Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 05:21 am GMT

PDB ID	:	5OGL
Title	:	Structure of bacterial oligosaccharyltransferase PglB in complex with an acceptor peptide and an lipid-linked oligosaccharide analog
Authors	:	Napiorkowska, M.; Boilevin, J.; Sovdat, T.; Darbre, T.; Reymond, J.-L.; Aebi, M.; Locher, K.P.
Deposited on	:	2017-07-13
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 (i) 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 (i)) were used in the production of this report:

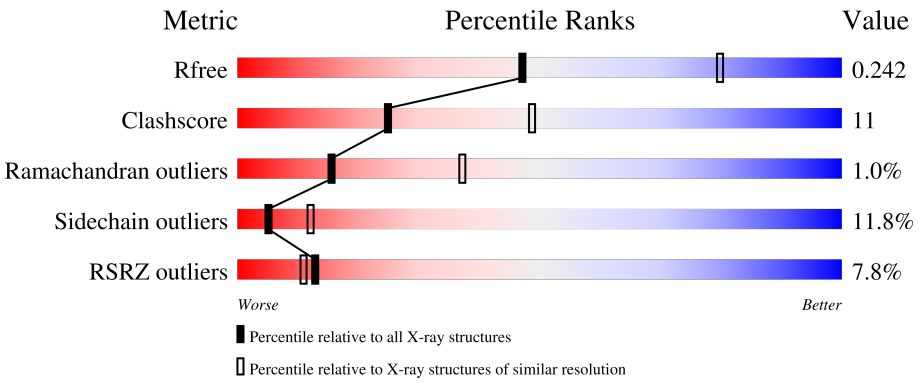
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	713	8%, 70%, 22%, 7% •
2	B	8	62%, 12%, 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5941 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 Undecaprenyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	707	5816	3871	886	1034	25	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP B9KDD4
A	17	ALA	CYS	engineered mutation	UNP B9KDD4
A	30	ALA	CYS	engineered mutation	UNP B9KDD4
A	108	THR	ALA	engineered mutation	UNP B9KDD4
A	350	LEU	CYS	engineered mutation	UNP B9KDD4
A	535	GLN	ASN	engineered mutation	UNP B9KDD4
A	549	PRO	LYS	engineered mutation	UNP B9KDD4
A	550	ASN	ASP	engineered mutation	UNP B9KDD4
A	553	ILE	PHE	engineered mutation	UNP B9KDD4
A	556	PRO	ASN	engineered mutation	UNP B9KDD4
A	600	PRO	ALA	engineered mutation	UNP B9KDD4
A	601	LEU	ILE	engineered mutation	UNP B9KDD4
A	602	ASP	ALA	engineered mutation	UNP B9KDD4
A	606	LYS	THR	engineered mutation	UNP B9KDD4
A	607	GLN	THR	engineered mutation	UNP B9KDD4
A	610	ILE	VAL	engineered mutation	UNP B9KDD4
A	611	THR	MET	engineered mutation	UNP B9KDD4
A	619	SER	ILE	engineered mutation	UNP B9KDD4
A	622	TYR	PHE	engineered mutation	UNP B9KDD4
A	624	SER	ALA	engineered mutation	UNP B9KDD4
A	627	ILE	VAL	engineered mutation	UNP B9KDD4
A	630	ASN	ALA	engineered mutation	UNP B9KDD4
A	663	TYR	PHE	engineered mutation	UNP B9KDD4
A	670	TYR	PHE	engineered mutation	UNP B9KDD4
A	713	GLU	-	expression tag	UNP B9KDD4

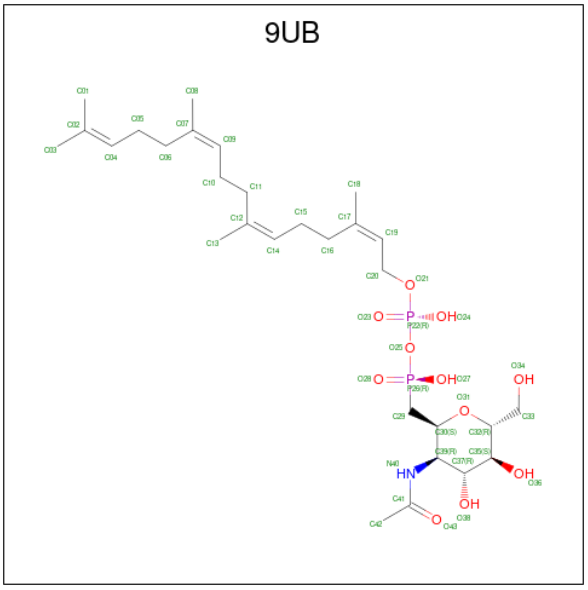
- Molecule 2 is a protein called Substrate mimicking peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	8	59	33	11	15	5	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	2	2	2	0	0

- Molecule 4 is [(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]methyl-[oxidanyl-[(2 {Z},6 {Z},10 {Z})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoxy]phosphoryl]oxy-phosphinic acid (three-letter code: 9UB) (formula: $C_{29}H_{51}NO_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	43	29	1	11	2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0

- Molecule 6 is water.

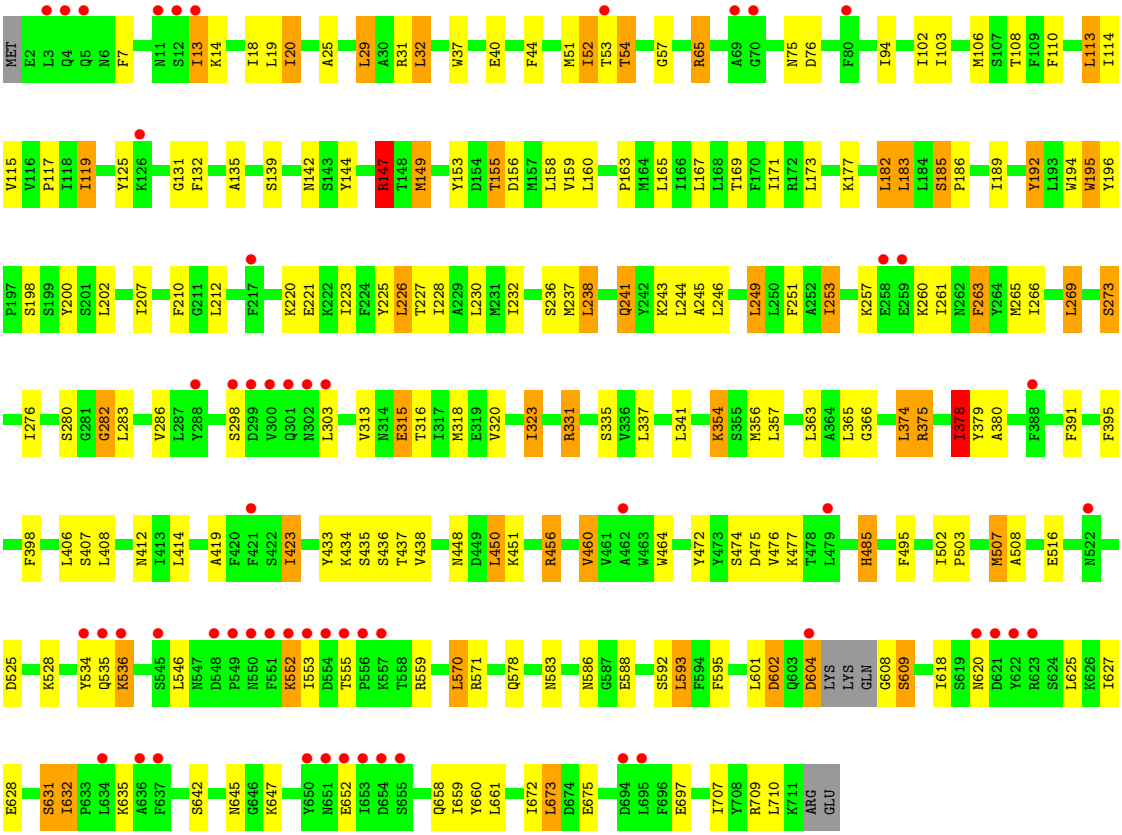
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	19	19	19	0	0
			Total	O		
6	B	1	1	1	0	0

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.

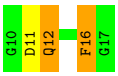
• Molecule 1: Undecaprenyl-diphosphooligosaccharide--protein glycotransferase

Chain A: 8% 70% 22% 7%



• Molecule 2: Substrate mimicking peptide

Chain B: 62% 12% 25%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.94Å 116.18Å 172.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.77 – 2.70 47.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.77-2.70) 100.0 (47.77-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.244 0.217 , 0.242	Depositor DCC
R_{free} test set	2346 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5941	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 9UB, PPN, NA

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	0.49	0/5970	0.64	4/8095 (0.0%)
2	B	0.62	0/43	0.73	0/55
All	All	0.49	0/6013	0.64	4/8150 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	374	LEU	CA-CB-CG	7.84	133.33	115.30
1	A	331	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	147	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	673	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ASN	Peptide

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	5816	0	5847	127	0
2	B	59	0	42	5	0
3	A	2	0	0	0	0
4	A	43	0	0	1	0
5	A	1	0	0	0	0
6	A	19	0	0	1	0
6	B	1	0	0	0	0
All	All	5941	0	5889	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:20:ILE:HG13	1:A:119:ILE:HD11	1.63	0.79
1:A:697:GLU:OE2	1:A:709:ARG:NH1	2.16	0.78
1:A:115:VAL:HG22	1:A:135:ALA:HB1	1.65	0.78
1:A:586:ASN:HB3	1:A:588:GLU:H	1.52	0.74
1:A:552:LYS:HD3	1:A:552:LYS:H	1.53	0.71
1:A:149:MET:HE2	1:A:433:TYR:HE2	1.54	0.71
1:A:31:ARG:NH2	1:A:139:SER:O	2.25	0.69
1:A:609:SER:N	1:A:620:ASN:OD1	2.25	0.69
1:A:19:LEU:HD13	1:A:132:PHE:HB2	1.78	0.66
1:A:54:THR:HA	2:B:12:GLN:HE21	1.60	0.65
1:A:502:ILE:H	1:A:502:ILE:HD12	1.61	0.64
1:A:13:ILE:H	1:A:13:ILE:HD13	1.63	0.64
1:A:54:THR:HG23	2:B:12:GLN:NE2	2.15	0.62
1:A:237:MET:HG3	1:A:280:SER:HB3	1.83	0.60
1:A:155:THR:O	1:A:195:TRP:CZ3	2.54	0.60
1:A:460:VAL:CG1	1:A:476:VAL:HG21	2.32	0.60
1:A:263:PHE:O	1:A:266:ILE:HG13	2.02	0.59
1:A:354:LYS:HD2	1:A:354:LYS:H	1.66	0.59
1:A:660:TYR:HE1	1:A:675:GLU:HG2	1.67	0.59
1:A:144:TYR:HA	1:A:378:ILE:HD11	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HG13	1:A:119:ILE:CD1	2.32	0.58
1:A:354:LYS:O	1:A:357:LEU:HB2	2.03	0.57
1:A:245:ALA:O	1:A:249:LEU:HB2	2.05	0.57
1:A:110:PHE:HA	1:A:113:LEU:HD22	1.86	0.56
1:A:318:MET:HG2	2:B:16:PPN:HB2	1.87	0.56
1:A:507:MET:O	1:A:507:MET:HE2	2.05	0.56
1:A:160:LEU:HD21	1:A:379:TYR:HA	1.87	0.56
1:A:155:THR:O	1:A:195:TRP:HZ3	1.88	0.56
1:A:375:ARG:NH2	4:A:803:9UB:O28	2.38	0.55
1:A:194:TRP:CZ3	1:A:195:TRP:HD1	2.24	0.55
1:A:570:LEU:HD22	1:A:595:PHE:HZ	1.70	0.55
1:A:189:ILE:HD13	1:A:207:ILE:HD11	1.89	0.55
1:A:595:PHE:HA	1:A:672:ILE:O	2.07	0.55
1:A:495:PHE:CD2	1:A:507:MET:HG3	2.42	0.54
1:A:158:LEU:HB2	1:A:195:TRP:CZ3	2.43	0.54
1:A:117:PRO:HB3	1:A:165:LEU:HD23	1.89	0.53
1:A:177:LYS:HE2	1:A:221:GLU:OE2	2.08	0.53
1:A:450:LEU:HG	1:A:707:ILE:HD13	1.90	0.53
1:A:200:TYR:OH	1:A:282:GLY:HA2	2.09	0.52
1:A:331:ARG:HH22	2:B:11:ASP:CG	2.12	0.52
1:A:451:LYS:HB2	1:A:474:SER:HA	1.91	0.52
1:A:625:LEU:O	1:A:631:SER:HA	2.10	0.52
1:A:25:ALA:O	1:A:29:LEU:HB2	2.11	0.51
1:A:516:GLU:HG2	1:A:559:ARG:NH1	2.26	0.51
1:A:341:LEU:HD22	1:A:391:PHE:CZ	2.46	0.50
1:A:185:SER:HB3	1:A:186:PRO:HD3	1.93	0.50
1:A:257:LYS:HG2	1:A:260:LYS:H	1.75	0.50
1:A:57:GLY:HA2	1:A:153:TYR:O	2.12	0.50
1:A:253:ILE:O	1:A:257:LYS:HB3	2.12	0.50
1:A:163:PRO:HD3	1:A:192:TYR:CZ	2.47	0.49
1:A:604:ASP:HB2	1:A:608:GLY:N	2.28	0.49
1:A:44:PHE:CE2	1:A:436:SER:HB2	2.48	0.49
1:A:464:TRP:CZ3	1:A:485:HIS:HD2	2.30	0.49
1:A:525:ASP:HB3	1:A:528:LYS:HB2	1.94	0.49
1:A:14:LYS:O	1:A:18:ILE:HG13	2.13	0.48
1:A:147:ARG:NH1	1:A:156:ASP:OD2	2.32	0.48
1:A:51:MET:HB2	1:A:437:THR:HG21	1.95	0.48
1:A:238:LEU:HD21	1:A:276:ILE:HD13	1.96	0.48
1:A:456:ARG:HD3	1:A:475:ASP:O	2.13	0.48
1:A:354:LYS:H	1:A:354:LYS:CD	2.27	0.48
1:A:313:VAL:O	1:A:316:THR:HB	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HA	1:A:52:ILE:HD12	1.65	0.47
1:A:182:LEU:HD11	1:A:226:LEU:HD13	1.96	0.47
1:A:54:THR:HG23	2:B:12:GLN:HE21	1.79	0.47
1:A:76:ASP:N	1:A:477:LYS:HE2	2.29	0.47
1:A:182:LEU:HD22	1:A:230:LEU:HD12	1.95	0.47
1:A:52:ILE:HG13	1:A:153:TYR:HB3	1.96	0.46
1:A:31:ARG:HG3	1:A:108:THR:HG23	1.97	0.46
1:A:269:LEU:O	1:A:273:SER:HB2	2.16	0.46
1:A:627:ILE:HG22	1:A:628:GLU:HG2	1.98	0.46
1:A:182:LEU:HB3	1:A:251:PHE:HD1	1.80	0.46
1:A:236:SER:O	1:A:243:LYS:NZ	2.40	0.45
1:A:378:ILE:HD12	1:A:378:ILE:HA	1.66	0.45
1:A:437:THR:HG22	1:A:438:VAL:N	2.31	0.45
1:A:508:ALA:HB3	1:A:710:LEU:HD11	1.98	0.45
1:A:320:VAL:HG12	1:A:320:VAL:O	2.16	0.45
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.81	0.45
1:A:507:MET:HG2	1:A:546:LEU:CD1	2.47	0.45
1:A:378:ILE:HG22	1:A:379:TYR:CD1	2.51	0.44
1:A:183:LEU:HD22	1:A:183:LEU:HA	1.76	0.44
1:A:448:ASN:O	1:A:451:LYS:HB3	2.18	0.44
1:A:160:LEU:HD11	1:A:378:ILE:O	2.16	0.44
1:A:241:GLN:H	1:A:241:GLN:HG2	1.33	0.44
1:A:625:LEU:HD13	1:A:672:ILE:HD13	1.98	0.44
1:A:223:ILE:O	1:A:227:THR:HG22	2.18	0.44
1:A:51:MET:HB2	1:A:437:THR:CG2	2.48	0.44
1:A:635:LYS:HE3	1:A:675:GLU:OE2	2.18	0.44
1:A:253:ILE:HG22	1:A:261:ILE:HD11	2.00	0.43
1:A:502:ILE:HB	1:A:503:PRO:HD3	2.00	0.43
1:A:196:TYR:CZ	1:A:198:SER:HB2	2.53	0.43
1:A:228:ILE:O	1:A:232:ILE:HG13	2.19	0.43
1:A:578:GLN:NE2	1:A:593:LEU:HD12	2.34	0.43
1:A:608:GLY:HA2	1:A:620:ASN:HD21	1.84	0.43
1:A:283:LEU:HD12	1:A:286:VAL:HB	2.00	0.43
1:A:323:ILE:HD13	1:A:323:ILE:HA	1.64	0.43
1:A:419:ALA:O	1:A:423:ILE:HB	2.19	0.43
1:A:464:TRP:CE3	1:A:485:HIS:HD2	2.36	0.43
1:A:534:TYR:O	1:A:536:LYS:HD3	2.18	0.42
1:A:13:ILE:H	1:A:13:ILE:CD1	2.31	0.42
1:A:167:LEU:O	1:A:171:ILE:HG12	2.19	0.42
1:A:315:GLU:H	1:A:315:GLU:HG2	1.53	0.42
1:A:632:ILE:HD11	1:A:659:ILE:HG13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:CE1	1:A:356:MET:HE3	2.55	0.42
1:A:366:GLY:HA3	1:A:380:ALA:HB2	2.02	0.42
1:A:31:ARG:HA	6:A:909:HOH:O	2.20	0.42
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.60	0.42
1:A:65:ARG:NH1	1:A:472:TYR:O	2.52	0.42
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.89	0.42
1:A:102:ILE:O	1:A:106:MET:HG3	2.20	0.41
1:A:110:PHE:O	1:A:113:LEU:HB2	2.19	0.41
1:A:456:ARG:HD3	1:A:456:ARG:HA	1.76	0.41
1:A:237:MET:HG3	1:A:280:SER:CB	2.49	0.41
1:A:460:VAL:HG13	1:A:476:VAL:HG21	2.02	0.41
1:A:37:TRP:CH2	1:A:434:LYS:HB3	2.56	0.41
1:A:173:LEU:HD23	1:A:210:PHE:HZ	1.86	0.41
1:A:225:TYR:HB3	1:A:266:ILE:HD13	2.01	0.41
1:A:263:PHE:CD2	1:A:266:ILE:HD11	2.54	0.41
1:A:395:PHE:O	1:A:398:PHE:HB3	2.21	0.41
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.77	0.41
1:A:119:ILE:HG22	1:A:131:GLY:O	2.21	0.41
1:A:583:ASN:CG	1:A:586:ASN:HB2	2.41	0.41
1:A:7:PHE:HD1	1:A:412:ASN:HD21	1.67	0.40
1:A:125:TYR:HE1	1:A:356:MET:HE3	1.85	0.40
1:A:618:ILE:HD13	1:A:661:LEU:HD21	2.02	0.40
1:A:601:LEU:HD13	1:A:601:LEU:HA	1.96	0.40
1:A:642:SER:HB3	1:A:645:ASN:HB2	2.04	0.40
1:A:507:MET:HG2	1:A:546:LEU:HD13	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	703/713 (99%)	656 (93%)	40 (6%)	7 (1%)	15 37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	5/8 (62%)	5 (100%)	0	0	100	100
All	All	708/721 (98%)	661 (93%)	40 (6%)	7 (1%)	15	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ARG
1	A	602	ASP
1	A	282	GLY
1	A	609	SER
1	A	593	LEU
1	A	142	ASN
1	A	378	ILE

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	633/639 (99%)	559 (88%)	74 (12%)	5	12
2	B	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	637/643 (99%)	562 (88%)	75 (12%)	5	12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	20	ILE
1	A	29	LEU
1	A	32	LEU
1	A	40	GLU
1	A	52	ILE
1	A	53	THR
1	A	54	THR
1	A	65	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	94	ILE
1	A	103	ILE
1	A	113	LEU
1	A	114	ILE
1	A	119	ILE
1	A	147	ARG
1	A	149	MET
1	A	155	THR
1	A	159	VAL
1	A	169	THR
1	A	182	LEU
1	A	183	LEU
1	A	185	SER
1	A	192	TYR
1	A	195	TRP
1	A	202	LEU
1	A	220	LYS
1	A	226	LEU
1	A	238	LEU
1	A	241	GLN
1	A	244	LEU
1	A	246	LEU
1	A	249	LEU
1	A	253	ILE
1	A	263	PHE
1	A	265	MET
1	A	269	LEU
1	A	273	SER
1	A	298	SER
1	A	303	LEU
1	A	315	GLU
1	A	323	ILE
1	A	335	SER
1	A	337	LEU
1	A	354	LYS
1	A	363	LEU
1	A	365	LEU
1	A	374	LEU
1	A	378	ILE
1	A	407	SER
1	A	408	LEU
1	A	414	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	423	ILE
1	A	435	SER
1	A	450	LEU
1	A	456	ARG
1	A	460	VAL
1	A	485	HIS
1	A	507	MET
1	A	535	GLN
1	A	536	LYS
1	A	552	LYS
1	A	553	ILE
1	A	555	THR
1	A	570	LEU
1	A	571	ARG
1	A	592	SER
1	A	602	ASP
1	A	604	ASP
1	A	631	SER
1	A	632	ILE
1	A	647	LYS
1	A	652	GLU
1	A	658	GLN
1	A	673	LEU
2	B	12	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	HIS
2	B	12	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)

1 non-standard protein/DNA/RNA residue is 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	PPN	B	16	2	12,14,15	1.14	1 (8%)	13,18,20	1.40	1 (7%)

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	PPN	B	16	2	-	0/7/10/12	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	PPN	CZ-N1	2.32	1.50	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	16	PPN	CB-CA-C	-4.00	103.97	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	16	PPN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are 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	$\#\|Z\| > 2$
4	9UB	A	803	-	41,43,43	2.31	10 (24%)	47,59,59	1.65	13 (27%)

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
4	9UB	A	803	-	-	4/39/62/62	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	9UB	P26-O25	8.11	1.67	1.58
4	A	803	9UB	P26-C29	7.19	1.91	1.80
4	A	803	9UB	C37-C39	-3.58	1.46	1.53
4	A	803	9UB	C41-N40	3.36	1.45	1.34
4	A	803	9UB	C06-C07	2.98	1.57	1.51
4	A	803	9UB	C11-C12	2.67	1.56	1.51
4	A	803	9UB	C16-C17	2.34	1.56	1.51
4	A	803	9UB	C18-C17	2.33	1.56	1.50
4	A	803	9UB	C20-C19	2.09	1.55	1.49
4	A	803	9UB	P26-O27	-2.00	1.51	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	9UB	C18-C17-C16	4.22	122.36	115.27
4	A	803	9UB	C20-C19-C17	-3.50	120.00	126.04
4	A	803	9UB	C01-C02-C03	2.70	120.56	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	9UB	C39-N40-C41	-2.61	116.84	123.18
4	A	803	9UB	C32-O31-C30	2.60	117.71	113.16
4	A	803	9UB	O27-P26-C29	2.43	111.08	105.72
4	A	803	9UB	O31-C32-C35	2.43	114.11	109.69
4	A	803	9UB	C08-C07-C06	2.36	119.24	115.27
4	A	803	9UB	C10-C09-C07	-2.30	122.12	127.66
4	A	803	9UB	C15-C14-C12	-2.30	122.13	127.66
4	A	803	9UB	C18-C17-C19	-2.23	117.96	123.68
4	A	803	9UB	C13-C12-C11	2.21	118.98	115.27
4	A	803	9UB	C33-C32-C35	-2.16	107.94	113.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

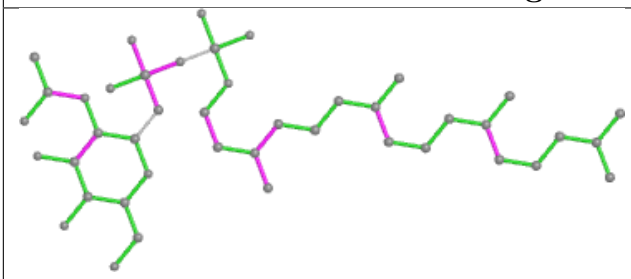
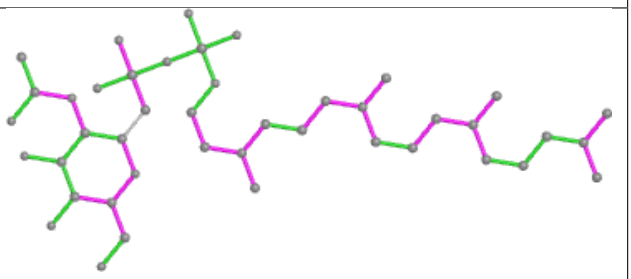
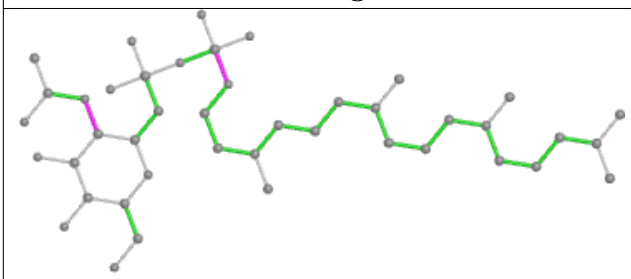
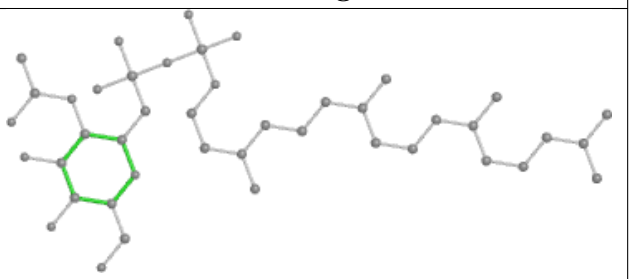
Mol	Chain	Res	Type	Atoms
4	A	803	9UB	C20-O21-P22-O25
4	A	803	9UB	C20-O21-P22-O23
4	A	803	9UB	C20-O21-P22-O24
4	A	803	9UB	C30-C39-N40-C41

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	9UB	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 9UB A 803	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	707/713 (99%)	0.29	56 (7%) 12 10	56, 75, 111, 152	0
2	B	7/8 (87%)	0.42	0 100 100	55, 57, 58, 60	2 (28%)
All	All	714/721 (99%)	0.29	56 (7%) 13 11	55, 74, 111, 152	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	LYS	10.5
1	A	553	ILE	10.0
1	A	653	ILE	8.2
1	A	554	ASP	7.8
1	A	551	PHE	6.7
1	A	535	GLN	6.5
1	A	621	ASP	6.0
1	A	550	ASN	5.9
1	A	623	ARG	5.9
1	A	604	ASP	5.3
1	A	534	TYR	4.7
1	A	555	THR	4.6
1	A	651	ASN	4.5
1	A	549	PRO	4.4
1	A	258	GLU	4.3
1	A	5	GLN	4.3
1	A	652	GLU	4.3
1	A	622	TYR	4.2
1	A	655	SER	3.9
1	A	654	ASP	3.7
1	A	3	LEU	3.7
1	A	557	LYS	3.5
1	A	545	SER	3.5
1	A	300	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	650	TYR	3.4
1	A	259	GLU	3.3
1	A	13	ILE	3.3
1	A	4	GLN	3.2
1	A	299	ASP	3.2
1	A	217	PHE	3.1
1	A	556	PRO	3.1
1	A	302	ASN	3.0
1	A	126	LYS	2.9
1	A	634	LEU	2.8
1	A	80	PHE	2.8
1	A	421	PHE	2.7
1	A	11	ASN	2.7
1	A	620	ASN	2.7
1	A	548	ASP	2.6
1	A	298	SER	2.6
1	A	462	ALA	2.5
1	A	388	PHE	2.5
1	A	695	LEU	2.4
1	A	694	ASP	2.4
1	A	479	LEU	2.3
1	A	536	LYS	2.3
1	A	522	ASN	2.1
1	A	636	ALA	2.1
1	A	301	GLN	2.1
1	A	53	THR	2.1
1	A	637	PHE	2.1
1	A	288	TYR	2.1
1	A	303	LEU	2.1
1	A	12	SER	2.1
1	A	69	ALA	2.0
1	A	70	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
2	PPN	B	16	14/15	0.94	0.15	57,61,63,64	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

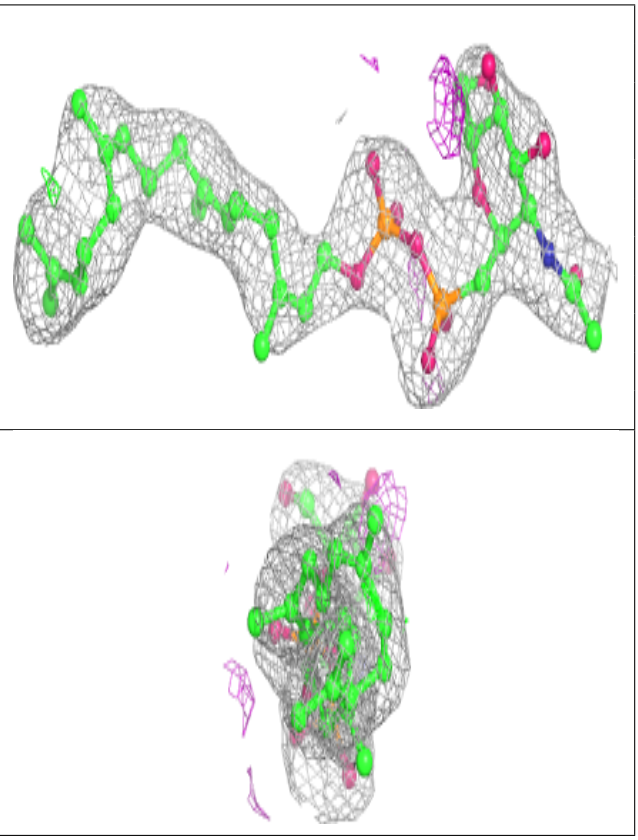
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	A	804	1/1	0.86	0.31	55,55,55,55	0
4	9UB	A	803	43/43	0.94	0.20	72,77,86,91	0
3	MN	A	802	1/1	0.96	0.23	70,70,70,70	1
3	MN	A	801	1/1	0.99	0.20	48,48,48,48	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 9UB A 803:

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.