



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:43 AM UTC

PDB ID : 4ZYR / pdb_00004zyr
Title : Crystal structure of E. coli Lactose permease G46W/G262W bound to p-nitrophenyl alpha-D-galactopyranoside (alpha-NPG)
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Deposited on : 2015-05-22
Resolution : 3.31 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

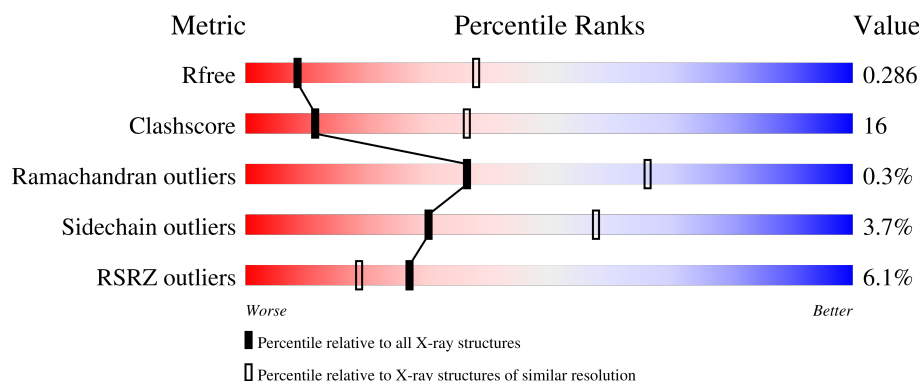
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	417	6% 70% 22% • 7%
1	B	417	5% 62% 28% • 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6271 atoms, of which 30 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.

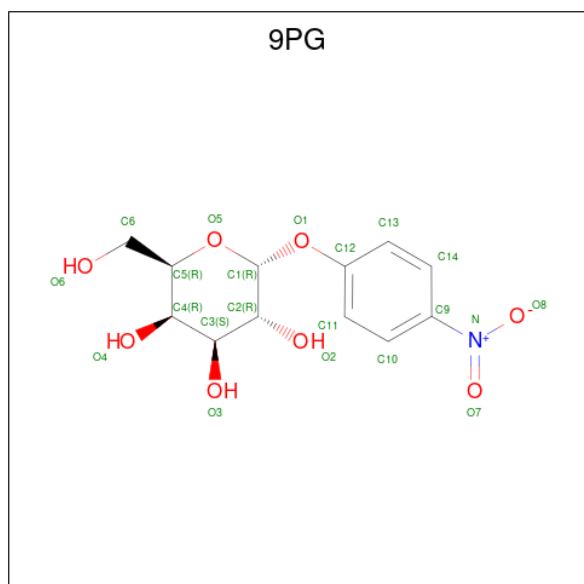
- Molecule 1 is a protein called Lactose permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3086	2102	465	498	21			
1	B	385	Total	C	N	O	S	0	0	0
			3071	2094	463	493	21			

There are 4 discrepancies between the modelled and reference sequences:

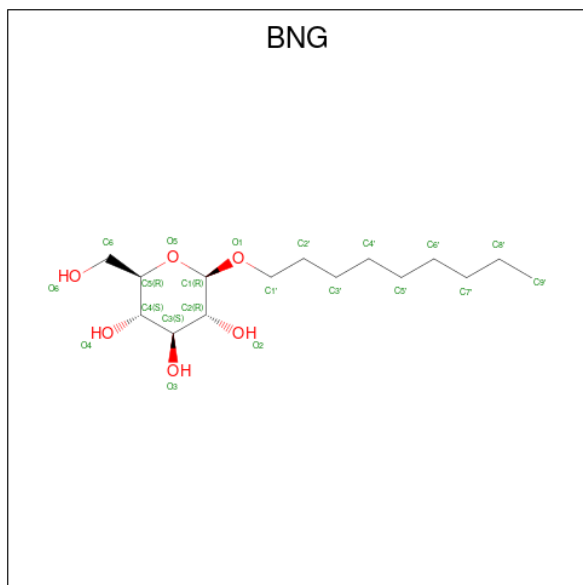
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	TRP	GLY	engineered mutation	UNP P02920
A	262	TRP	GLY	engineered mutation	UNP P02920
B	46	TRP	GLY	engineered mutation	UNP P02920
B	262	TRP	GLY	engineered mutation	UNP P02920

- Molecule 2 is 4-nitrophenyl alpha-D-galactopyranoside (CCD ID: 9PG) (formula: C₁₂H₁₅NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	12	1	8		
2	B	1	Total	C	N	O	0	0
			21	12	1	8		

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			51	15	30	6		
3	B	1	Total	C	O		0	0
			21	15	6			

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.15Å 121.99Å 266.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.04 – 3.31 37.04 – 3.31	Depositor EDS
% Data completeness (in resolution range)	96.1 (37.04-3.31) 81.0 (37.04-3.31)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_1700	Depositor
R, R_{free}	0.259 , 0.278 0.267 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6271	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: 9PG, BNG

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	0.34	0/3182	0.80	2/4312 (0.0%)
1	B	0.34	0/3167	0.84	3/4291 (0.1%)
All	All	0.34	0/6349	0.82	5/8603 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	GLY	N-CA-C	-10.79	99.42	112.48
1	B	135	ARG	N-CA-C	-6.41	106.09	114.04
1	A	144	ARG	N-CA-C	-6.31	104.28	112.23
1	A	286	ILE	N-CA-C	-6.27	103.21	111.05
1	B	110	GLY	N-CA-C	-5.88	105.57	115.62

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	3086	0	3120	92	1
1	B	3071	0	3109	111	1
2	A	21	0	15	2	0
2	B	21	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	30	30	1	0
3	B	21	0	30	6	0
All	All	6241	30	6319	202	1

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 16.

All (202) 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:286:ILE:CD1	1:A:290:ASN:HB2	1.26	1.56
1:A:286:ILE:HD11	1:A:290:ASN:CB	1.35	1.52
1:A:286:ILE:HD12	1:A:286:ILE:O	1.35	1.23
1:A:282:ILE:O	1:A:286:ILE:HG22	1.37	1.21
1:A:282:ILE:O	1:A:286:ILE:CG2	1.97	1.12
1:A:286:ILE:CD1	1:A:290:ASN:CB	2.08	1.04
1:A:337:ILE:HG23	1:A:349:ILE:HD11	1.39	1.02
1:A:286:ILE:HD12	1:A:286:ILE:C	1.88	0.98
1:B:337:ILE:HD12	1:B:349:ILE:HG13	1.51	0.92
1:B:282:ILE:HG22	1:B:286:ILE:CD1	2.00	0.91
1:B:171:TRP:HB3	3:B:502:BNG:H5'1	1.54	0.88
1:B:282:ILE:HG22	1:B:286:ILE:HD12	1.55	0.88
1:B:288:GLY:O	1:B:291:ALA:N	2.09	0.85
1:A:164:ILE:HD13	1:A:164:ILE:N	1.93	0.83
1:B:282:ILE:CG2	1:B:286:ILE:HD11	2.08	0.82
1:A:164:ILE:HD13	1:A:164:ILE:H	1.46	0.81
1:A:103:ILE:HG23	1:A:106:GLY:H	1.46	0.80
1:A:286:ILE:HD13	1:A:290:ASN:CB	2.12	0.78
1:B:286:ILE:HG22	1:B:290:ASN:HB2	1.66	0.76
1:A:161:MET:HA	1:A:164:ILE:CG1	2.14	0.76
1:B:37:ILE:HG13	1:B:38:ASN:ND2	2.03	0.73
1:B:114:LEU:HD23	1:B:114:LEU:H	1.54	0.72
1:B:216:LEU:HD13	1:B:349:ILE:CG2	2.20	0.71
1:B:290:ASN:HD21	1:B:405:PRO:HA	1.55	0.71
1:B:171:TRP:CB	3:B:502:BNG:H5'1	2.21	0.70
1:A:220:PRO:HA	1:A:223:TRP:HD1	1.57	0.69
1:B:282:ILE:CG2	1:B:286:ILE:CD1	2.68	0.69
1:B:33:TRP:CD1	1:B:37:ILE:HD11	2.27	0.68
1:A:160:ILE:O	1:A:164:ILE:HD11	1.94	0.68
1:B:31:PRO:HA	1:B:34:LEU:CD1	2.23	0.68
1:B:105:VAL:HA	1:B:108:ILE:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:HA	1:A:241:GLN:HG3	1.77	0.67
1:A:286:ILE:CD1	1:A:290:ASN:HB3	2.22	0.66
1:A:23:MET:HE2	1:A:118:PHE:HB3	1.77	0.66
1:B:37:ILE:HG13	1:B:38:ASN:HD22	1.59	0.65
1:A:408:LEU:H	1:A:408:LEU:HD23	1.63	0.64
1:A:161:MET:HA	1:A:164:ILE:HD11	1.79	0.63
1:B:70:LEU:HD13	1:B:75:TYR:HB3	1.81	0.62
1:B:160:ILE:HG13	1:B:161:MET:HG2	1.82	0.62
1:A:337:ILE:HG23	1:A:349:ILE:CD1	2.23	0.61
1:B:351:LEU:N	1:B:351:LEU:HD13	2.15	0.61
1:B:104:LEU:O	1:B:108:ILE:HG23	2.00	0.61
1:B:31:PRO:HA	1:B:34:LEU:HD11	1.83	0.61
1:B:19:TYR:O	1:B:22:ILE:HG22	2.01	0.60
1:B:279:ALA:O	1:B:283:ILE:HG12	2.01	0.59
1:B:288:GLY:O	1:B:291:ALA:HB3	2.03	0.59
1:B:288:GLY:O	1:B:289:LYS:C	2.45	0.59
1:A:225:LEU:HD13	1:A:336:TYR:CE2	2.38	0.59
1:A:286:ILE:HG13	1:A:287:GLY:O	2.03	0.58
1:A:161:MET:HA	1:A:164:ILE:CD1	2.33	0.58
1:A:299:MET:HE1	1:A:329:LEU:HD22	1.86	0.58
1:A:299:MET:CE	1:A:329:LEU:HD22	2.33	0.58
1:A:23:MET:HE1	1:A:122:ALA:HB2	1.85	0.57
1:B:282:ILE:HG23	1:B:286:ILE:HD11	1.85	0.57
1:A:406:LEU:HD23	1:A:406:LEU:H	1.69	0.57
1:B:290:ASN:HD21	1:B:405:PRO:CA	2.18	0.57
1:B:30:PHE:N	1:B:31:PRO:HD2	2.19	0.56
1:A:271:LEU:O	1:A:275:ILE:HG12	2.05	0.56
1:A:99:LEU:HA	1:A:107:SER:OG	2.05	0.56
1:A:142:ARG:O	1:A:143:ALA:HB3	2.05	0.55
1:A:279:ALA:O	1:A:283:ILE:HG12	2.06	0.55
1:A:142:ARG:HE	1:A:277:PHE:HE2	1.53	0.55
1:A:299:MET:O	1:A:303:ILE:HG13	2.06	0.55
1:A:391:GLY:O	1:A:395:ILE:HG13	2.07	0.54
1:B:209:SER:OG	1:B:212:LEU:HG	2.06	0.54
1:A:161:MET:CA	1:A:164:ILE:HD11	2.38	0.54
1:B:286:ILE:CG2	1:B:290:ASN:HB2	2.35	0.54
1:B:237:ASP:O	1:B:241:GLN:HG3	2.07	0.54
1:A:164:ILE:N	1:A:164:ILE:CD1	2.63	0.54
1:B:122:ALA:N	1:B:123:PRO:HD2	2.23	0.54
1:A:164:ILE:H	1:A:164:ILE:CD1	2.11	0.53
1:A:363:ILE:O	1:A:367:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PHE:C	1:B:208:PHE:CD1	2.86	0.53
1:B:283:ILE:HD12	1:B:291:ALA:CB	2.39	0.53
1:A:153:LEU:O	1:A:157:ILE:HG12	2.08	0.53
1:B:391:GLY:O	1:B:395:ILE:HG12	2.09	0.53
1:B:216:LEU:HD23	1:B:219:GLN:OE1	2.08	0.53
1:A:48:ILE:HA	1:A:108:ILE:HD11	1.91	0.53
1:A:48:ILE:CG1	1:A:108:ILE:HD11	2.38	0.53
1:B:176:CYS:HA	1:B:179:ILE:HG22	1.91	0.53
1:B:406:LEU:HD12	1:B:407:SER:H	1.73	0.52
1:A:350:TYR:HD2	1:A:351:LEU:HD22	1.75	0.52
1:B:34:LEU:HD23	1:B:48:ILE:HD13	1.90	0.52
1:A:143:ALA:HA	1:A:146:PHE:HD1	1.72	0.52
1:A:88:ALA:HB3	1:A:89:PRO:HD3	1.91	0.52
1:A:122:ALA:N	1:A:123:PRO:HD2	2.25	0.52
1:A:286:ILE:HD11	1:A:290:ASN:CA	2.30	0.52
1:B:296:GLY:HA2	1:B:299:MET:HE3	1.92	0.51
1:A:220:PRO:HA	1:A:223:TRP:CD1	2.43	0.51
1:B:406:LEU:HD12	1:B:407:SER:N	2.25	0.51
1:A:143:ALA:HA	1:A:146:PHE:CD1	2.46	0.51
1:A:229:VAL:HG11	1:A:353:CYS:O	2.10	0.51
1:B:171:TRP:CD1	3:B:502:BNG:H3'1	2.46	0.51
1:B:253:THR:O	1:B:256:GLN:HG2	2.12	0.50
1:B:303:ILE:CG2	1:B:386:GLY:HA2	2.41	0.50
1:B:27:PHE:HB3	1:B:28:PRO:HD3	1.92	0.50
1:A:46:TRP:CD1	1:A:47:ILE:HG12	2.46	0.50
1:B:300:SER:OG	1:B:390:LEU:HB2	2.12	0.50
1:B:288:GLY:C	1:B:291:ALA:H	2.14	0.49
1:A:79:ILE:HD13	1:B:93:PHE:CE1	2.47	0.49
1:A:99:LEU:HA	1:A:107:SER:CB	2.42	0.49
1:B:351:LEU:HD13	1:B:351:LEU:H	1.77	0.49
1:A:161:MET:HA	1:A:164:ILE:HG12	1.93	0.49
1:B:111:GLY:HA2	1:B:114:LEU:HD21	1.94	0.49
1:B:64:GLY:HA2	1:B:351:LEU:HD21	1.94	0.48
1:B:226:SER:O	1:B:230:ILE:HD12	2.13	0.48
1:A:130:GLU:HG3	1:A:334:PHE:CD1	2.48	0.48
1:B:92:ILE:HG23	1:B:167:GLN:HE21	1.79	0.48
1:A:178:LEU:HB2	3:B:502:BNG:H8'2	1.96	0.48
1:B:349:ILE:HA	1:B:352:VAL:HG22	1.94	0.48
1:B:33:TRP:HD1	1:B:37:ILE:HD11	1.78	0.48
1:B:326:VAL:N	1:B:327:PRO:HD2	2.29	0.47
1:A:337:ILE:O	1:A:341:PHE:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HG3	3:A:502:BNG:H7'1	1.96	0.47
1:A:343:VAL:C	1:A:345:PHE:H	2.21	0.47
1:A:368:LEU:HD12	1:A:368:LEU:O	2.15	0.47
1:B:272:ASN:OD1	1:B:327:PRO:HD3	2.14	0.47
1:B:167:GLN:NE2	3:B:502:BNG:O3	2.48	0.46
1:B:32:ILE:HD12	1:B:32:ILE:N	2.30	0.46
1:B:79:ILE:HD12	1:B:79:ILE:N	2.30	0.46
1:B:81:THR:HG22	1:B:180:LEU:HD23	1.97	0.46
1:B:212:LEU:HD12	1:B:344:ARG:HH12	1.80	0.46
1:B:350:TYR:HB3	1:B:351:LEU:HD13	1.97	0.46
1:B:230:ILE:HD11	1:B:357:PHE:HB3	1.97	0.46
1:A:23:MET:HE2	1:A:118:PHE:CB	2.45	0.46
1:A:30:PHE:N	1:A:31:PRO:HD2	2.30	0.46
1:B:288:GLY:O	1:B:291:ALA:CB	2.63	0.46
1:B:32:ILE:HD12	1:B:32:ILE:H	1.80	0.46
1:B:74:LYS:HB3	1:B:184:LEU:HD21	1.98	0.46
1:B:79:ILE:HD12	1:B:79:ILE:H	1.80	0.46
1:B:337:ILE:HG23	1:B:349:ILE:HD11	1.97	0.46
1:A:160:ILE:O	1:A:164:ILE:CD1	2.64	0.46
1:B:303:ILE:HG23	1:B:386:GLY:HA2	1.98	0.46
1:B:384:VAL:O	1:B:388:VAL:HG23	2.15	0.46
1:B:34:LEU:H	1:B:34:LEU:HD12	1.81	0.46
1:B:303:ILE:HD11	1:B:385:LEU:HB3	1.98	0.46
1:A:279:ALA:N	1:A:280:PRO:HD2	2.31	0.45
1:B:154:CYS:O	1:B:158:VAL:HG23	2.17	0.45
1:B:172:LEU:HD13	1:B:172:LEU:O	2.16	0.45
1:A:92:ILE:HD11	1:A:170:PHE:CD1	2.51	0.45
1:B:348:THR:O	1:B:352:VAL:HG13	2.17	0.45
1:A:181:ALA:HB2	1:B:171:TRP:CZ3	2.51	0.45
1:A:272:ASN:OD1	1:A:327:PRO:HD3	2.17	0.45
1:A:88:ALA:HB3	1:A:89:PRO:CD	2.47	0.45
1:B:51:ALA:HB2	1:B:108:ILE:HG13	1.98	0.45
1:A:37:ILE:HG22	1:A:37:ILE:O	2.17	0.45
1:A:161:MET:HA	1:A:164:ILE:HG13	1.97	0.44
1:A:276:MET:HA	1:A:279:ALA:HB2	1.99	0.44
1:B:183:LEU:H	1:B:183:LEU:HD13	1.83	0.44
1:A:48:ILE:HG12	1:A:108:ILE:CD1	2.48	0.44
1:B:103:ILE:HG13	1:B:106:GLY:H	1.82	0.44
1:A:130:GLU:HG3	1:A:334:PHE:CG	2.52	0.44
1:A:326:VAL:HB	1:A:327:PRO:HD3	2.00	0.44
1:B:348:THR:O	1:B:352:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:O	1:A:92:ILE:HG12	2.18	0.44
1:A:326:VAL:N	1:A:327:PRO:HD2	2.32	0.44
1:B:394:LEU:O	1:B:397:VAL:HG22	2.18	0.44
1:A:134:ARG:NH1	1:A:343:VAL:HG11	2.33	0.43
1:B:238:VAL:HG13	1:B:362:MET:HG3	2.00	0.43
1:B:299:MET:HG3	1:B:325:GLU:HG3	2.00	0.43
1:A:238:VAL:HA	1:A:241:GLN:CG	2.45	0.43
1:B:35:HIS:O	1:B:39:HIS:HA	2.18	0.43
1:B:42:LYS:HA	1:B:45:THR:HG23	1.99	0.43
1:B:283:ILE:HD12	1:B:291:ALA:HB2	1.99	0.43
1:B:299:MET:CG	1:B:325:GLU:HG3	2.48	0.43
1:B:171:TRP:HB3	3:B:502:BNG:C5'	2.37	0.43
1:A:230:ILE:O	1:A:234:CYS:HB3	2.18	0.43
1:A:286:ILE:HD13	1:A:290:ASN:HB3	1.92	0.43
1:B:130:GLU:O	1:B:133:SER:HB3	2.19	0.43
1:A:178:LEU:O	1:A:182:VAL:HG23	2.18	0.43
1:B:164:ILE:HD12	1:B:164:ILE:N	2.34	0.43
1:A:48:ILE:HG13	1:A:108:ILE:HD11	2.01	0.43
1:B:9:PHE:CD2	1:B:9:PHE:C	2.96	0.43
1:B:30:PHE:N	1:B:31:PRO:CD	2.82	0.43
1:B:60:GLN:N	1:B:61:PRO:HD2	2.34	0.43
1:B:108:ILE:C	1:B:111:GLY:H	2.27	0.43
1:A:11:MET:HE2	1:A:11:MET:HA	2.01	0.42
1:A:216:LEU:HD11	1:A:345:PHE:CG	2.54	0.42
1:B:88:ALA:HB3	1:B:89:PRO:HD3	2.00	0.42
1:B:282:ILE:O	1:B:286:ILE:HG13	2.18	0.42
1:A:238:VAL:O	1:A:241:GLN:HB2	2.19	0.42
1:B:70:LEU:HD12	1:B:76:LEU:HB2	2.01	0.42
1:B:337:ILE:CD1	1:B:349:ILE:HG13	2.37	0.42
1:B:288:GLY:O	1:B:291:ALA:CA	2.67	0.42
1:B:358:LYS:O	1:B:362:MET:HB2	2.20	0.42
1:A:266:THR:O	1:A:270:LEU:HD23	2.20	0.42
1:A:16:PHE:CZ	1:A:129:ILE:HD12	2.55	0.41
1:B:16:PHE:CE2	1:B:129:ILE:HG21	2.55	0.41
1:A:15:PHE:CE1	1:A:180:LEU:HG	2.55	0.41
1:A:297:THR:O	1:A:301:VAL:HG23	2.20	0.41
1:A:151:TRP:CH2	2:A:501:9PG:H10	2.55	0.41
1:B:9:PHE:HD1	1:B:138:PHE:HB2	1.86	0.41
1:B:72:LEU:CD2	1:B:135:ARG:HG3	2.51	0.41
1:B:109:VAL:O	1:B:112:ILE:HG13	2.20	0.41
2:A:501:9PG:H9	2:A:501:9PG:H7	1.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:CD1	1:B:114:LEU:HD11	2.51	0.41
1:B:20:PHE:CD2	1:B:23:MET:CE	3.05	0.40
1:B:351:LEU:H	1:B:351:LEU:HD22	1.85	0.40
1:B:151:TRP:CE3	2:B:501:9PG:H3	2.55	0.40
1:A:229:VAL:CG1	1:A:358:LYS:HB2	2.51	0.40
1:A:68:ASP:OD1	1:A:347:ALA:HB3	2.21	0.40
1:B:247:PHE:CE2	1:B:251:PHE:HE1	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH1	1:B:215:GLU:OE1[5_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/417 (92%)	364 (95%)	18 (5%)	1 (0%)	36	66
1	B	381/417 (91%)	366 (96%)	14 (4%)	1 (0%)	36	66
All	All	764/834 (92%)	730 (96%)	32 (4%)	2 (0%)	36	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ILE
1	B	376	ILE

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	325/348 (93%)	317 (98%)	8 (2%)	42	64
1	B	323/348 (93%)	307 (95%)	16 (5%)	22	50
All	All	648/696 (93%)	624 (96%)	24 (4%)	30	58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	36	ASP
1	A	108	ILE
1	A	164	ILE
1	A	169	VAL
1	A	286	ILE
1	A	344	ARG
1	A	408	LEU
1	B	34	LEU
1	B	69	LYS
1	B	108	ILE
1	B	114	LEU
1	B	162	PHE
1	B	169	VAL
1	B	172	LEU
1	B	183	LEU
1	B	184	LEU
1	B	208	PHE
1	B	230	ILE
1	B	242	GLN
1	B	276	MET
1	B	284	ASN
1	B	351	LEU
1	B	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	379	GLN
1	B	38	ASN
1	B	137	ASN
1	B	165	ASN
1	B	167	GLN
1	B	290	ASN

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 ⓘ

4 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	BNG	B	502	-	21,21,21	0.50	0	26,26,26	0.82	1 (3%)
2	9PG	A	501	-	22,22,22	1.00	2 (9%)	29,31,31	1.21	1 (3%)
2	9PG	B	501	-	22,22,22	1.02	2 (9%)	29,31,31	1.33	1 (3%)
3	BNG	A	502	-	21,21,21	0.52	0	26,26,26	0.65	0

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	BNG	B	502	-	-	1/12/32/32	0/1/1/1
2	9PG	A	501	-	-	4/8/30/30	0/2/2/2
2	9PG	B	501	-	-	2/8/30/30	0/2/2/2
3	BNG	A	502	-	-	0/12/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	9PG	O7-N	-2.80	1.18	1.22
2	B	501	9PG	O7-N	-2.79	1.18	1.22
2	A	501	9PG	O8-N	-2.60	1.17	1.35
2	B	501	9PG	O8-N	-2.59	1.18	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	9PG	C12-O1-C1	-6.21	109.07	117.82
2	A	501	9PG	C12-O1-C1	-5.35	110.28	117.82
3	B	502	BNG	O1-C1-C2	2.53	112.12	108.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	9PG	C14-C9-N-O7
2	A	501	9PG	O5-C1-O1-C12
2	B	501	9PG	C10-C9-N-O7
2	A	501	9PG	C4-C5-C6-O6
2	A	501	9PG	C2-C1-O1-C12
2	A	501	9PG	O5-C5-C6-O6
3	B	502	BNG	C2'-C1'-O1-C1

There are no ring outliers.

4 monomers are involved in 10 short contacts:

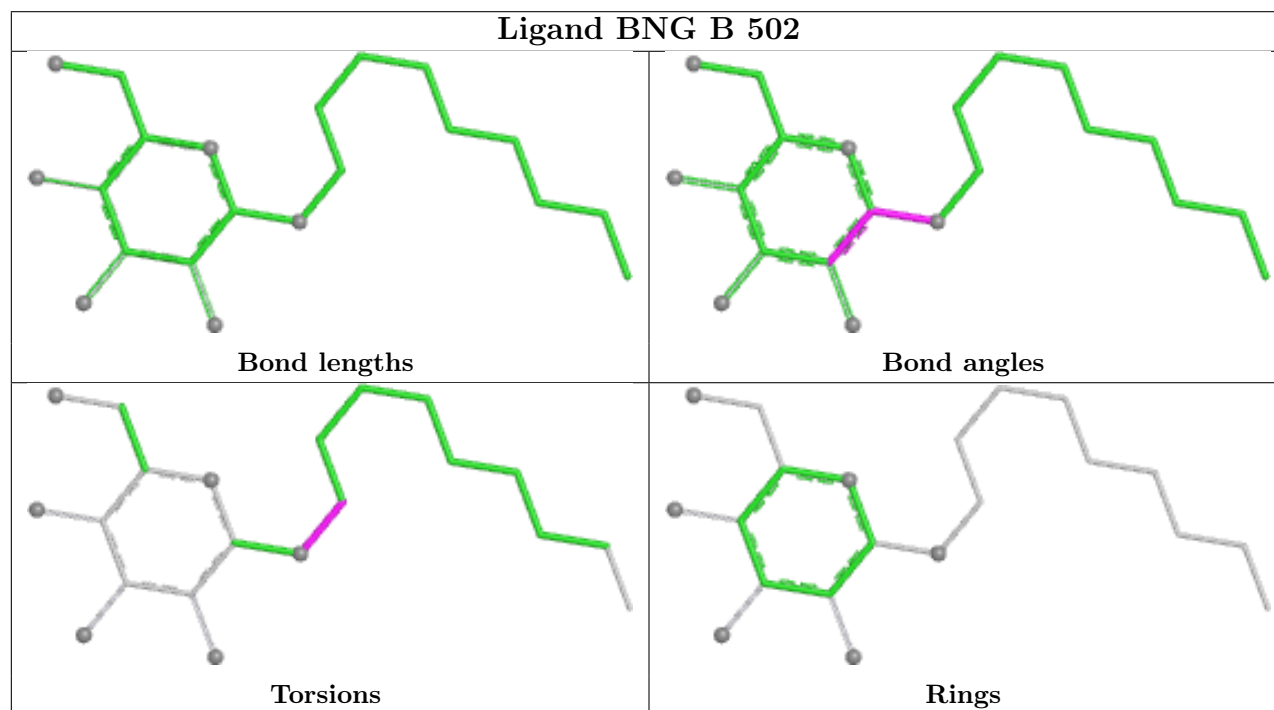
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	BNG	6	0
2	A	501	9PG	2	0
2	B	501	9PG	1	0

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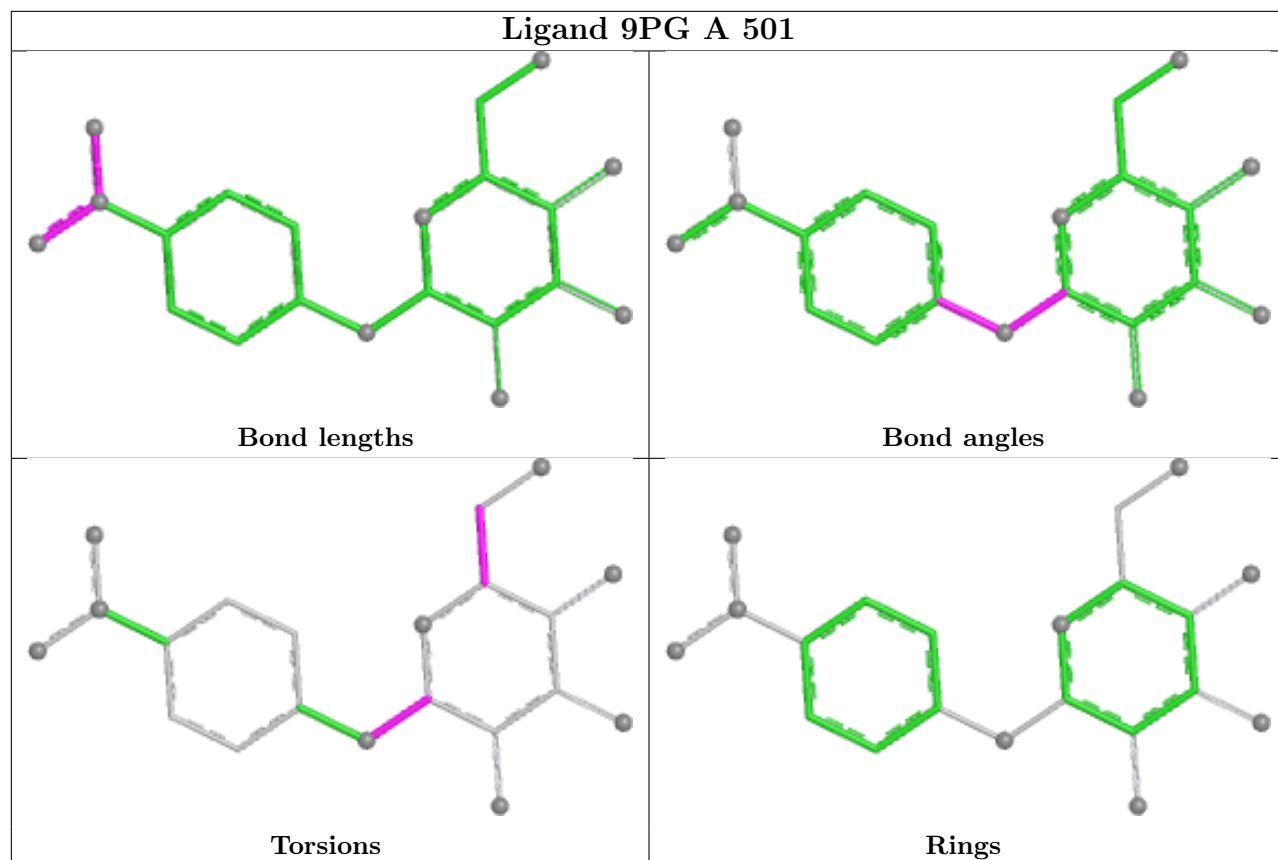
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	BNG	1	0

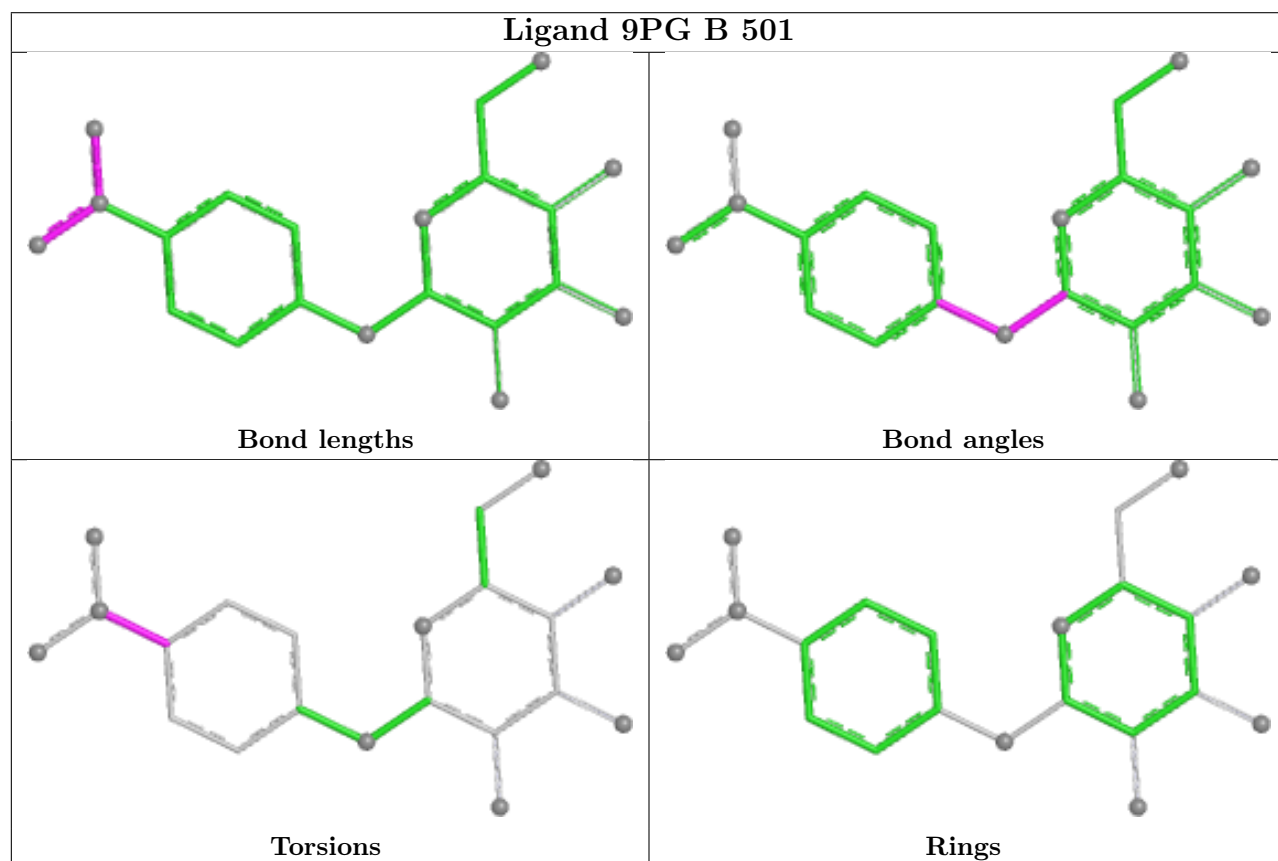
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 9PG A 501



Ligand 9PG B 501



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	387/417 (92%)	0.36	25 (6%)	25 17	30, 140, 209, 243	0
1	B	385/417 (92%)	0.32	22 (5%)	29 20	88, 135, 183, 220	0
All	All	772/834 (92%)	0.34	47 (6%)	27 19	30, 137, 200, 243	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	GLY	6.3
1	A	186	PHE	5.0
1	A	33	TRP	4.9
1	B	39	HIS	4.9
1	B	333	CYS	4.0
1	A	240	ASP	4.0
1	B	334	PHE	3.8
1	B	126	GLU	3.8
1	B	27	PHE	3.5
1	A	244	ALA	3.2
1	A	171	TRP	3.2
1	B	146	PHE	3.1
1	A	346	SER	3.1
1	A	190	ASP	3.0
1	B	380	GLY	3.0
1	B	28	PRO	3.0
1	A	313	LEU	2.9
1	B	350	TYR	2.9
1	B	240	ASP	2.8
1	A	28	PRO	2.8
1	A	212	LEU	2.8
1	A	243	PHE	2.7
1	B	265	THR	2.7
1	A	217	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	354	PHE	2.7
1	A	215	GLU	2.6
1	A	380	GLY	2.6
1	B	383	LEU	2.6
1	A	340	GLN	2.6
1	A	76	LEU	2.5
1	B	398	PHE	2.4
1	B	401	SER	2.4
1	A	210	LEU	2.4
1	A	160	ILE	2.4
1	A	161	MET	2.4
1	B	399	THR	2.3
1	B	375	SER	2.3
1	A	376	ILE	2.3
1	A	50	ALA	2.2
1	B	149	VAL	2.2
1	A	241	GLN	2.2
1	A	11	MET	2.1
1	B	368	LEU	2.1
1	B	209	SER	2.1
1	B	232	VAL	2.1
1	B	316	VAL	2.1
1	A	339	SER	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.

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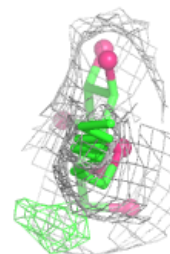
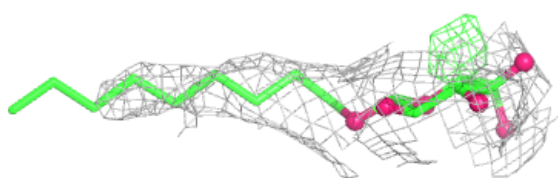
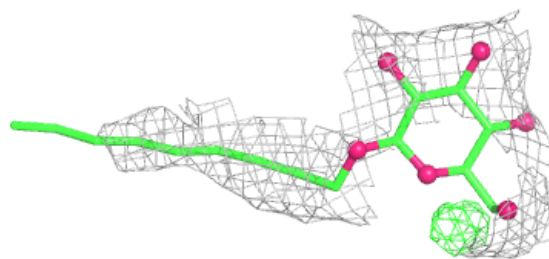
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BNG	A	502	21/21	0.78	0.15	16,16,168,168	0
3	BNG	B	502	21/21	0.87	0.14	82,127,173,194	0
2	9PG	A	501	21/21	0.94	0.10	107,127,171,197	0
2	9PG	B	501	21/21	0.94	0.15	98,122,169,210	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.

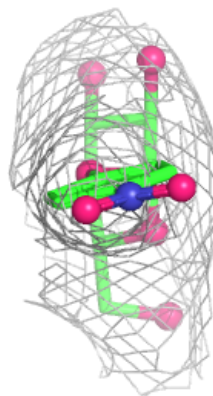
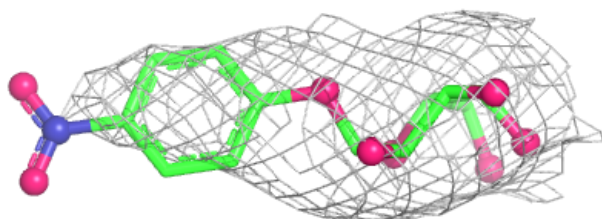
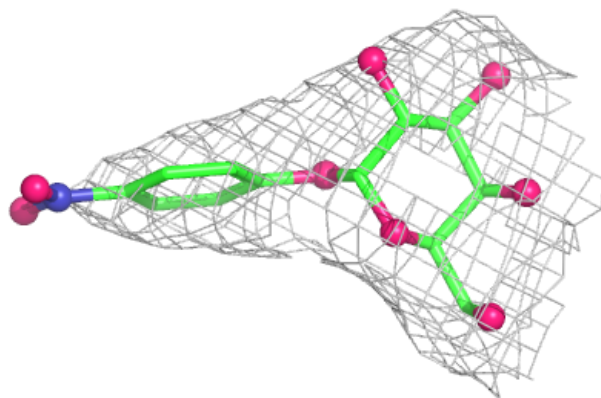
Electron density around BNG B 502:

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

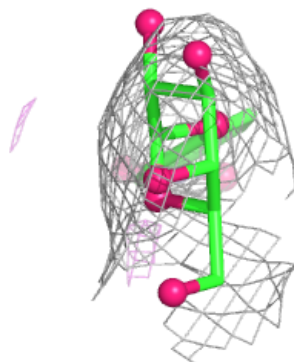
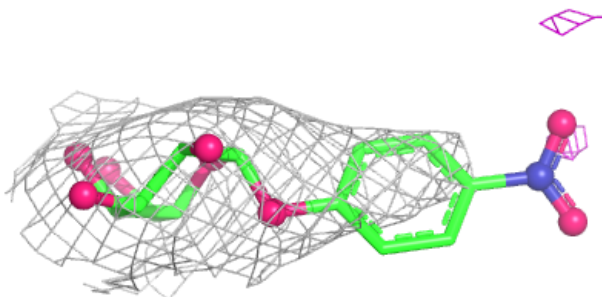
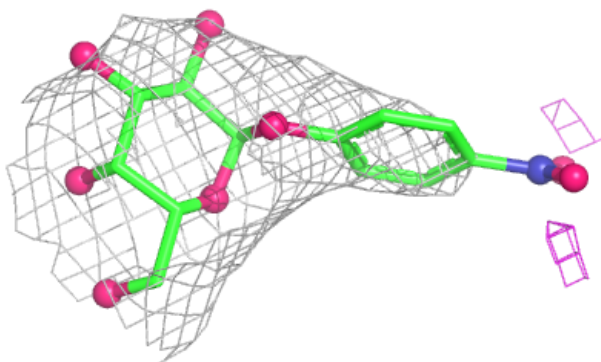


Electron density around 9PG A 501:

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

**Electron density around 9PG B 501:**

$2mF_o-DF_c$ (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.