



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:45 AM UTC

PDB ID : 4PL0 / pdb_00004pl0
Title : Crystal structure of the antibacterial peptide ABC transporter McjD in an outward occluded state
Authors : Choudhury, H.G.; Beis, K.
Deposited on : 2014-05-15
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

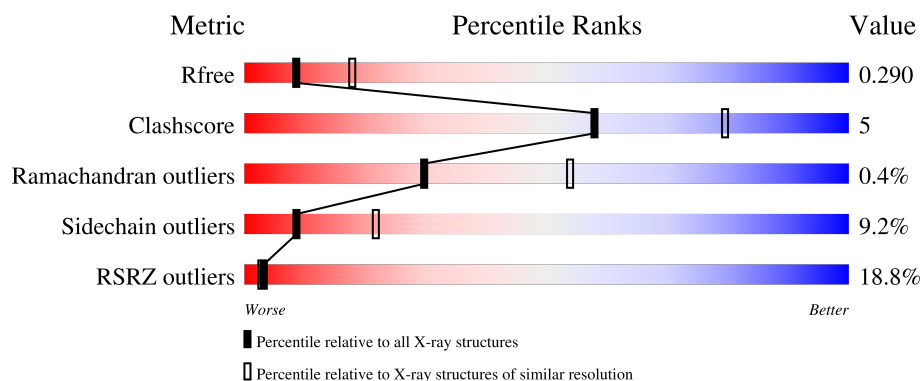
1 Overall quality at a glance

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	580	18% 79% 17% ..
1	B	580	19% 79% 18% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9213 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 Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4527	2920	739	850	18			
1	B	576	Total	C	N	O	S	0	2	0
			4580	2954	750	858	18			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

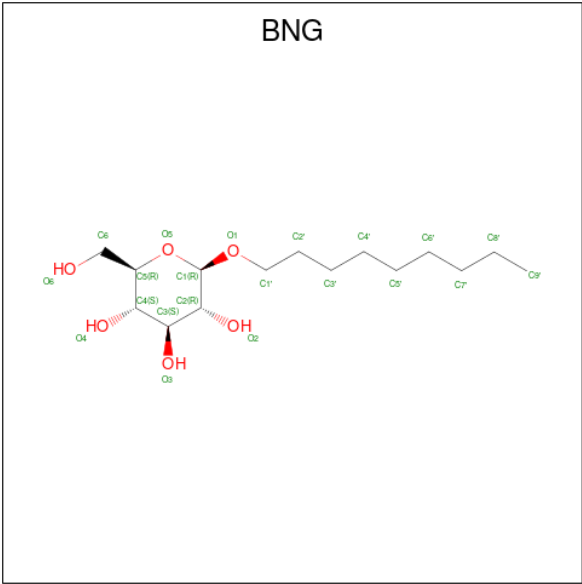


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	15	6		
4	B	1	Total	C	O	0	0
			21	15	6		

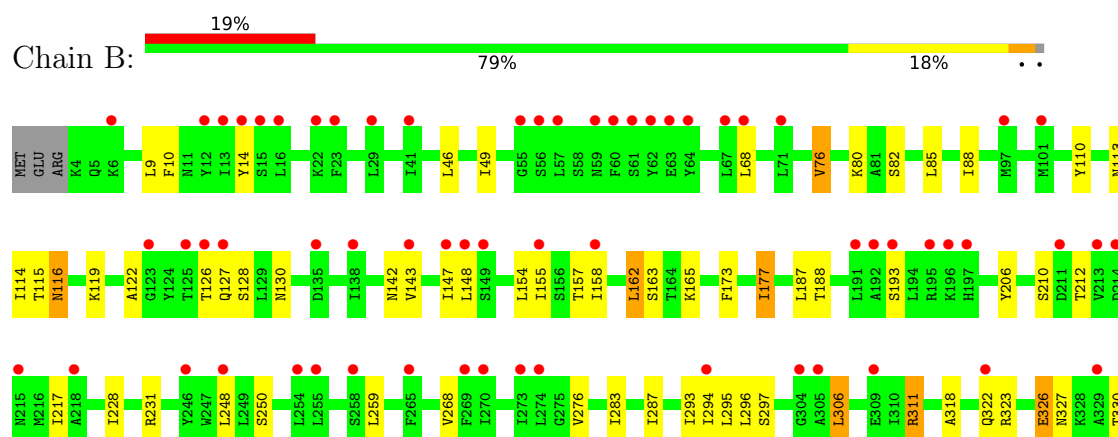
3 Residue-property plots

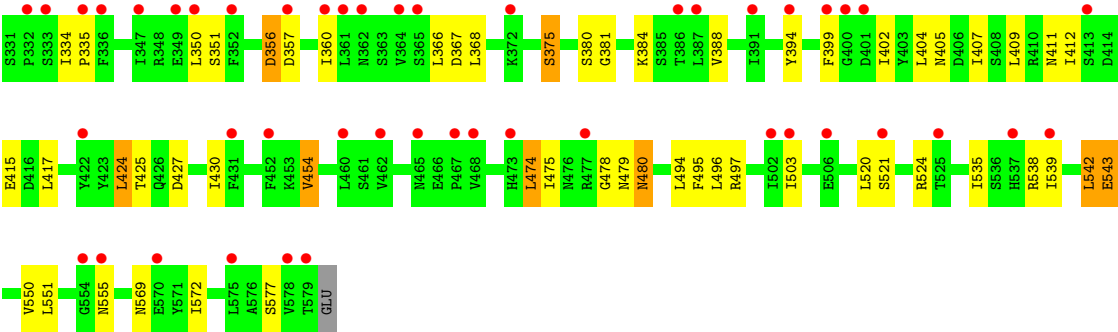
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD



- Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.83Å 107.92Å 232.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.70 48.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.96-2.70) 99.6 (48.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.247 , 0.266 0.267 , 0.290	Depositor DCC
R_{free} test set	2891 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: ANP, MG, 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	0.88	0/4603	1.34	14/6234 (0.2%)
1	B	0.88	0/4663	1.36	18/6313 (0.3%)
All	All	0.88	0/9266	1.35	32/12547 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	173	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	538	ARG	CA-C-N	6.02	128.37	120.60
1	B	538	ARG	C-N-CA	6.02	128.37	120.60
1	A	567	VAL	CA-C-N	5.71	128.39	120.63
1	A	567	VAL	C-N-CA	5.71	128.39	120.63
1	B	479	ASN	CA-C-N	5.52	131.38	121.66
1	B	479	ASN	C-N-CA	5.52	131.38	121.66
1	A	567	VAL	N-CA-C	-5.52	106.81	111.56
1	B	480	ASN	N-CA-C	-5.45	106.47	113.23
1	A	424	LEU	CA-C-N	5.42	128.93	120.75
1	A	424	LEU	C-N-CA	5.42	128.93	120.75
1	B	543	GLU	CA-C-N	5.36	127.99	120.28
1	B	543	GLU	C-N-CA	5.36	127.99	120.28
1	B	424	LEU	CA-C-N	5.32	128.79	120.75
1	B	424	LEU	C-N-CA	5.32	128.79	120.75
1	A	113	ASN	CA-C-N	5.27	127.96	120.53
1	A	113	ASN	C-N-CA	5.27	127.96	120.53
1	A	566	MET	CA-C-N	5.25	128.38	123.08
1	A	566	MET	C-N-CA	5.25	128.38	123.08
1	B	113	ASN	CA-C-N	5.20	127.86	120.53
1	B	113	ASN	C-N-CA	5.20	127.86	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	542	LEU	CA-C-N	5.16	127.14	120.44
1	B	542	LEU	C-N-CA	5.16	127.14	120.44
1	A	541	LEU	CA-C-N	5.08	127.50	120.29
1	A	541	LEU	C-N-CA	5.08	127.50	120.29
1	B	318	ALA	CA-C-N	5.08	125.72	120.03
1	B	318	ALA	C-N-CA	5.08	125.72	120.03
1	A	479	ASN	CA-C-N	5.05	129.98	121.14
1	A	479	ASN	C-N-CA	5.05	129.98	121.14
1	B	480	ASN	CA-CB-CG	5.03	117.63	112.60

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	4527	0	4638	45	0
1	B	4580	0	4701	48	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	30	1	0
4	B	21	0	30	0	0
All	All	9213	0	9425	84	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 5.

All (84) 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:48:LYS:HB3	1:A:68:LEU:HD21	1.69	0.75
1:A:143:VAL:HA	1:A:147:ILE:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HA	1:B:147:ILE:HD12	1.75	0.68
1:B:188:THR:HG23	1:B:311:ARG:HE	1.58	0.67
1:A:188:THR:HG23	1:A:308:SER:HA	1.78	0.64
1:A:32:THR:HG21	1:A:145:GLN:HA	1.81	0.62
1:B:454:VAL:HG22	1:B:495:PHE:HB2	1.81	0.62
1:A:454:VAL:HG22	1:A:495:PHE:HB2	1.83	0.61
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.66	0.60
1:B:10:PHE:O	1:B:14:TYR:HD2	1.84	0.59
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.85	0.58
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.86	0.57
1:B:569:ASN:HD22	1:B:572:ILE:H	1.53	0.57
1:A:76:VAL:HG11	1:B:294:ILE:HG12	1.86	0.56
1:A:308:SER:O	1:A:312:GLN:HG2	2.06	0.56
1:B:366:LEU:HD23	1:B:368:LEU:HD11	1.87	0.56
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.87	0.56
1:A:158:ILE:O	1:A:162:LEU:HB2	2.06	0.56
1:B:384:LYS:HD2	1:B:535:ILE:HG23	1.87	0.56
1:B:351:SER:HB2	1:B:399:PHE:HB2	1.88	0.55
1:A:366:LEU:HD23	1:A:368:LEU:HD11	1.87	0.55
1:A:384:LYS:HD2	1:A:535:ILE:HG23	1.87	0.55
1:B:454:VAL:HG22	1:B:495:PHE:CB	2.36	0.55
1:A:475:ILE:HB	1:A:480:ASN:HB2	1.89	0.54
1:B:454:VAL:HG21	1:B:496:LEU:HG	1.90	0.54
1:B:475:ILE:HB	1:B:480:ASN:HB2	1.89	0.53
1:A:454:VAL:HG21	1:A:496:LEU:HG	1.91	0.52
1:A:430:ILE:HG21	1:A:474:LEU:HD22	1.90	0.52
1:A:188:THR:HG22	1:A:311:ARG:HG2	1.92	0.52
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.91	0.51
1:B:116:ASN:HA	1:B:119:LYS:HD3	1.92	0.51
1:A:27:SER:O	1:A:31:ILE:HD12	2.10	0.51
1:A:62:TYR:CE1	1:B:283:ILE:HD11	2.46	0.51
1:B:430:ILE:HG21	1:B:474:LEU:HD22	1.91	0.51
1:A:116:ASN:HA	1:A:119:LYS:HD3	1.92	0.51
1:B:217:ILE:HD12	1:B:217:ILE:H	1.76	0.50
1:A:217:ILE:HD12	1:A:217:ILE:H	1.75	0.50
1:A:454:VAL:HG22	1:A:495:PHE:CB	2.41	0.49
1:A:225:LEU:HB2	1:B:110:TYR:CZ	2.48	0.49
1:B:375:SER:HB3	1:B:542:LEU:HD23	1.95	0.48
1:A:136:ILE:HG13	1:A:317:LEU:HD21	1.96	0.48
1:A:334:ILE:HG12	1:A:337:LEU:HB2	1.96	0.48
1:A:294:ILE:HG12	1:B:76:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:HA	1:A:293:ILE:HD12	1.95	0.48
1:B:356:ASP:O	1:B:357:ASP:HB2	2.12	0.48
1:A:210:SER:HB2	1:B:122:ALA:HB1	1.97	0.47
1:B:268:VAL:HG12	1:B:293:ILE:HD11	1.95	0.47
1:A:122:ALA:HB1	1:B:210:SER:HB2	1.97	0.47
1:A:32:THR:HG22	1:A:149:SER:HB2	1.96	0.47
1:A:286:PHE:O	1:A:290:THR:HG23	2.15	0.46
1:A:195:ARG:HD2	1:A:312:GLN:HB2	1.98	0.46
1:B:475:ILE:H	1:B:480:ASN:HD22	1.65	0.45
1:A:355:SER:C	1:A:357:ASP:H	2.24	0.45
4:A:603:BNG:H4'1	1:B:46:LEU:HD11	1.97	0.45
1:B:322:GLN:O	1:B:326:GLU:HB2	2.16	0.45
1:A:80:LYS:HE3	1:B:297:SER:HB2	1.99	0.45
1:B:154:LEU:HD22	1:B:177:ILE:HD13	1.99	0.45
1:B:157:THR:HG21	1:B:296:LEU:HD21	1.98	0.45
1:A:146:ASN:O	1:A:306:LEU:HD22	2.16	0.44
1:A:388:VAL:HB	1:A:503:ILE:HD13	2.00	0.44
1:B:158:ILE:O	1:B:162:LEU:HB2	2.18	0.43
1:B:334:ILE:HG12	1:B:411:ASN:O	2.18	0.43
1:B:388:VAL:HB	1:B:503:ILE:HD13	2.00	0.43
1:B:142:ASN:OD1	1:B:306:LEU:HA	2.19	0.43
1:B:114:ILE:HD13	1:B:394:TYR:HA	2.01	0.43
1:A:212:THR:HG21	1:A:228:ILE:HG23	2.01	0.42
1:B:381:GLY:HA2	2:B:601:ANP:H3'	2.00	0.42
1:A:130:ASN:ND2	1:B:206:TYR:OH	2.53	0.42
1:B:49:ILE:HG13	1:B:68:LEU:HB3	2.01	0.42
1:A:114:ILE:HD13	1:A:394:TYR:HA	2.02	0.41
1:A:47:ALA:HB2	1:A:288:MET:HB2	2.03	0.41
1:A:409:LEU:HD22	1:A:417:LEU:HD11	2.02	0.41
1:B:350:LEU:HD22	1:B:402:ILE:HD11	2.01	0.41
1:B:550:VAL:HG11	1:B:569:ASN:HD21	1.85	0.41
1:B:478:GLY:C	1:B:480:ASN:H	2.28	0.41
1:A:127:GLN:HG2	1:A:206:TYR:CD2	2.56	0.41
1:A:228:ILE:HD13	1:A:228:ILE:HA	1.84	0.41
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.89	0.41
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.03	0.41
1:A:488:ARG:NH2	1:B:380:SER:HB3	2.36	0.40
1:B:127:GLN:HG2	1:B:206:TYR:CD2	2.56	0.40
1:A:52:LEU:HD21	1:A:64:TYR:CD2	2.56	0.40
1:A:163:SER:C	1:A:165:LYS:H	2.30	0.40
1:B:163:SER:C	1:B:165:LYS:H	2.30	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	569/580 (98%)	531 (93%)	36 (6%)	2 (0%)	30	54
1	B	576/580 (99%)	535 (93%)	38 (7%)	3 (0%)	24	48
All	All	1145/1160 (99%)	1066 (93%)	74 (6%)	5 (0%)	30	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	PRO
1	B	327	ASN
1	A	356	ASP
1	B	323	ARG
1	B	335	PRO

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	520/529 (98%)	472 (91%)	48 (9%)	8	22
1	B	527/529 (100%)	479 (91%)	48 (9%)	9	22
All	All	1047/1058 (99%)	951 (91%)	96 (9%)	8	22

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	46	LEU
1	A	52	LEU
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
1	A	76	VAL
1	A	80	LYS
1	A	82	SER
1	A	85	LEU
1	A	88	ILE
1	A	115	THR
1	A	116	ASN
1	A	126	THR
1	A	128	SER
1	A	130	ASN
1	A	162	LEU
1	A	177	ILE
1	A	193	SER
1	A	228	ILE
1	A	248	LEU
1	A	250	SER
1	A	259	LEU
1	A	276	VAL
1	A	287	ILE
1	A	289	ILE
1	A	290	THR
1	A	295	LEU
1	A	310	ILE
1	A	311	ARG
1	A	330	THR
1	A	367	ASP
1	A	375	SER
1	A	404	LEU
1	A	407	ILE
1	A	425	THR
1	A	427	ASP
1	A	430	ILE
1	A	454	VAL
1	A	457	LEU
1	A	474	LEU
1	A	497	ARG
1	A	520	LEU

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Mol	Chain	Res	Type
1	A	522	SER
1	A	524	ARG
1	A	540	ASN
1	A	551	LEU
1	A	555	ASN
1	B	9	LEU
1	B	76	VAL
1	B	80	LYS
1	B	82	SER
1	B	85	LEU
1	B	88	ILE
1	B	115	THR
1	B	116	ASN
1	B	126	THR
1	B	128	SER
1	B	130	ASN
1	B	148	LEU
1	B	155	ILE
1	B	162	LEU
1	B	177	ILE
1	B	187	LEU
1	B	193	SER
1	B	228	ILE
1	B	248	LEU
1	B	250	SER
1	B	259	LEU
1	B	276	VAL
1	B	287	ILE
1	B	295	LEU
1	B	306	LEU
1	B	311	ARG
1	B	326	GLU
1	B	330	THR
1	B	356	ASP
1	B	360	ILE
1	B	367	ASP
1	B	375	SER
1	B	404	LEU
1	B	407	ILE
1	B	415	GLU
1	B	425	THR
1	B	427	ASP

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Mol	Chain	Res	Type
1	B	454	VAL
1	B	474	LEU
1	B	497	ARG
1	B	520	LEU
1	B	521	SER
1	B	524	ARG
1	B	539	ILE
1	B	543	GLU
1	B	551	LEU
1	B	555	ASN
1	B	577	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	96	ASN
1	A	111	ASN
1	A	130	ASN
1	A	131	GLN
1	A	134	ASN
1	A	142	ASN
1	A	145	GLN
1	A	146	ASN
1	A	153	GLN
1	A	215	ASN
1	A	223	ASN
1	A	285	HIS
1	A	362	ASN
1	A	411	ASN
1	A	459	ASN
1	A	479	ASN
1	A	487	GLN
1	A	515	ASN
1	A	534	ASN
1	A	555	ASN
1	B	98	GLN
1	B	111	ASN
1	B	116	ASN
1	B	127	GLN
1	B	130	ASN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	134	ASN
1	B	153	GLN
1	B	223	ASN
1	B	285	HIS
1	B	362	ASN
1	B	411	ASN
1	B	459	ASN
1	B	464	ASN
1	B	473	HIS
1	B	479	ASN
1	B	480	ASN
1	B	515	ASN
1	B	569	ASN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	BNG	B	603	-	21,21,21	0.22	0	26,26,26	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BNG	A	603	-	21,21,21	0.23	0	26,26,26	0.27	0
2	ANP	B	601	3	33,33,33	2.43	6 (18%)	45,52,52	1.54	5 (11%)
2	ANP	A	601	3	33,33,33	2.31	6 (18%)	45,52,52	1.50	4 (8%)

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	BNG	B	603	-	-	4/12/32/32	0/1/1/1
4	BNG	A	603	-	-	6/12/32/32	0/1/1/1
2	ANP	B	601	3	-	6/18/38/38	0/3/3/3
2	ANP	A	601	3	-	4/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ANP	PB-O1B	8.36	1.58	1.46
2	A	601	ANP	PB-O1B	8.11	1.58	1.46
2	B	601	ANP	PG-O1G	7.98	1.58	1.46
2	A	601	ANP	PG-O1G	7.67	1.57	1.46
2	B	601	ANP	PB-O3A	-4.35	1.53	1.59
2	B	601	ANP	PA-O3A	-3.98	1.55	1.59
2	A	601	ANP	PA-O3A	-3.96	1.55	1.59
2	A	601	ANP	PB-O3A	-3.81	1.54	1.59
2	A	601	ANP	PB-O2B	-3.31	1.48	1.56
2	B	601	ANP	PB-O2B	-3.29	1.48	1.56
2	B	601	ANP	PG-O3G	-3.03	1.48	1.56
2	A	601	ANP	PG-O3G	-2.39	1.50	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ANP	O2G-PG-O1G	-7.28	95.20	113.45
2	A	601	ANP	O2G-PG-O1G	-6.75	96.53	113.45
2	A	601	ANP	O2G-PG-O3G	4.04	118.44	107.59
2	B	601	ANP	O2G-PG-O3G	3.92	118.14	107.59
2	A	601	ANP	O1B-PB-N3B	-3.50	106.62	111.77
2	B	601	ANP	O1B-PB-N3B	-3.01	107.34	111.77
2	A	601	ANP	O2B-PB-O1B	2.58	115.41	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ANP	O3A-PA-O1A	-2.50	103.17	110.70
2	B	601	ANP	O3G-PG-O1G	-2.07	108.27	113.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PB-N3B-PG-O1G
2	A	601	ANP	PG-N3B-PB-O1B
2	B	601	ANP	PB-N3B-PG-O1G
2	B	601	ANP	PG-N3B-PB-O1B
2	B	601	ANP	C5'-O5'-PA-O1A
2	B	601	ANP	C5'-O5'-PA-O3A
4	A	603	BNG	C2-C1-O1-C1'
4	B	603	BNG	C2'-C3'-C4'-C5'
4	A	603	BNG	O5-C1-O1-C1'
4	A	603	BNG	C3'-C4'-C5'-C6'
4	B	603	BNG	O5-C5-C6-O6
4	A	603	BNG	C5'-C6'-C7'-C8'
4	A	603	BNG	C2'-C3'-C4'-C5'
4	B	603	BNG	C1'-C2'-C3'-C4'
4	B	603	BNG	C4'-C5'-C6'-C7'
2	A	601	ANP	PA-O3A-PB-O2B
2	B	601	ANP	PA-O3A-PB-O2B
4	A	603	BNG	C4'-C5'-C6'-C7'
2	A	601	ANP	PA-O3A-PB-O1B
2	B	601	ANP	PA-O3A-PB-O1B

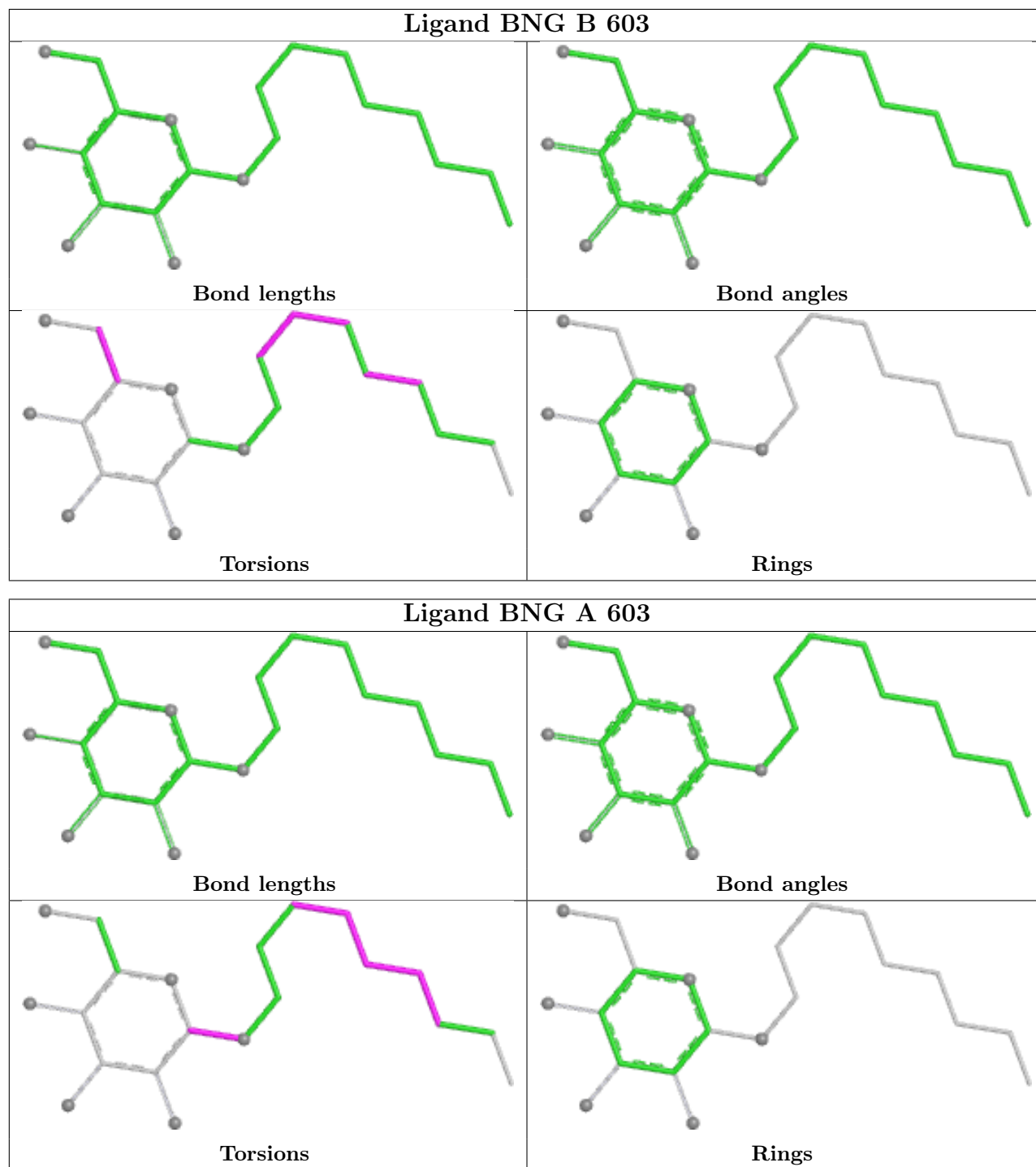
There are no ring outliers.

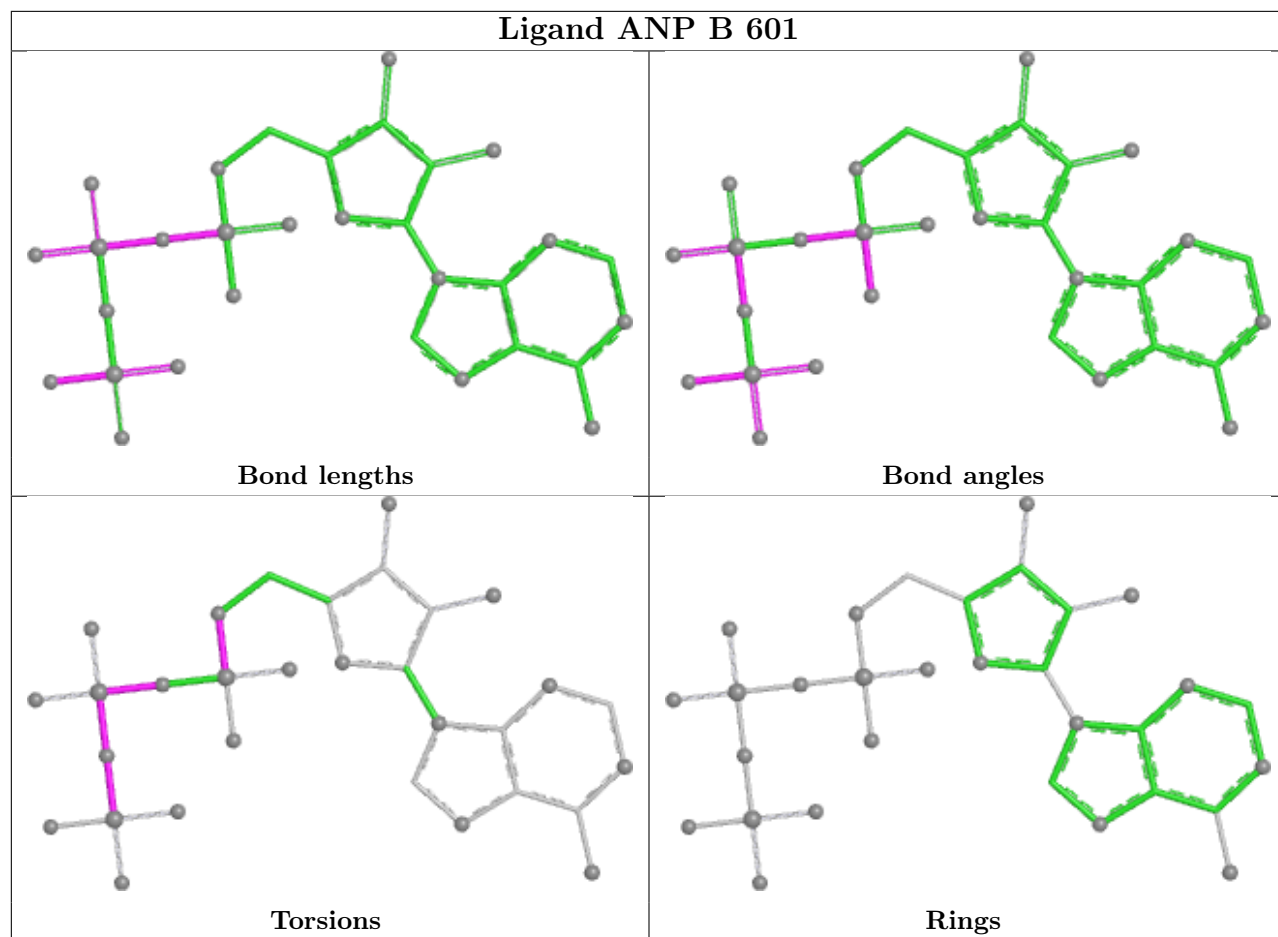
2 monomers are involved in 2 short contacts:

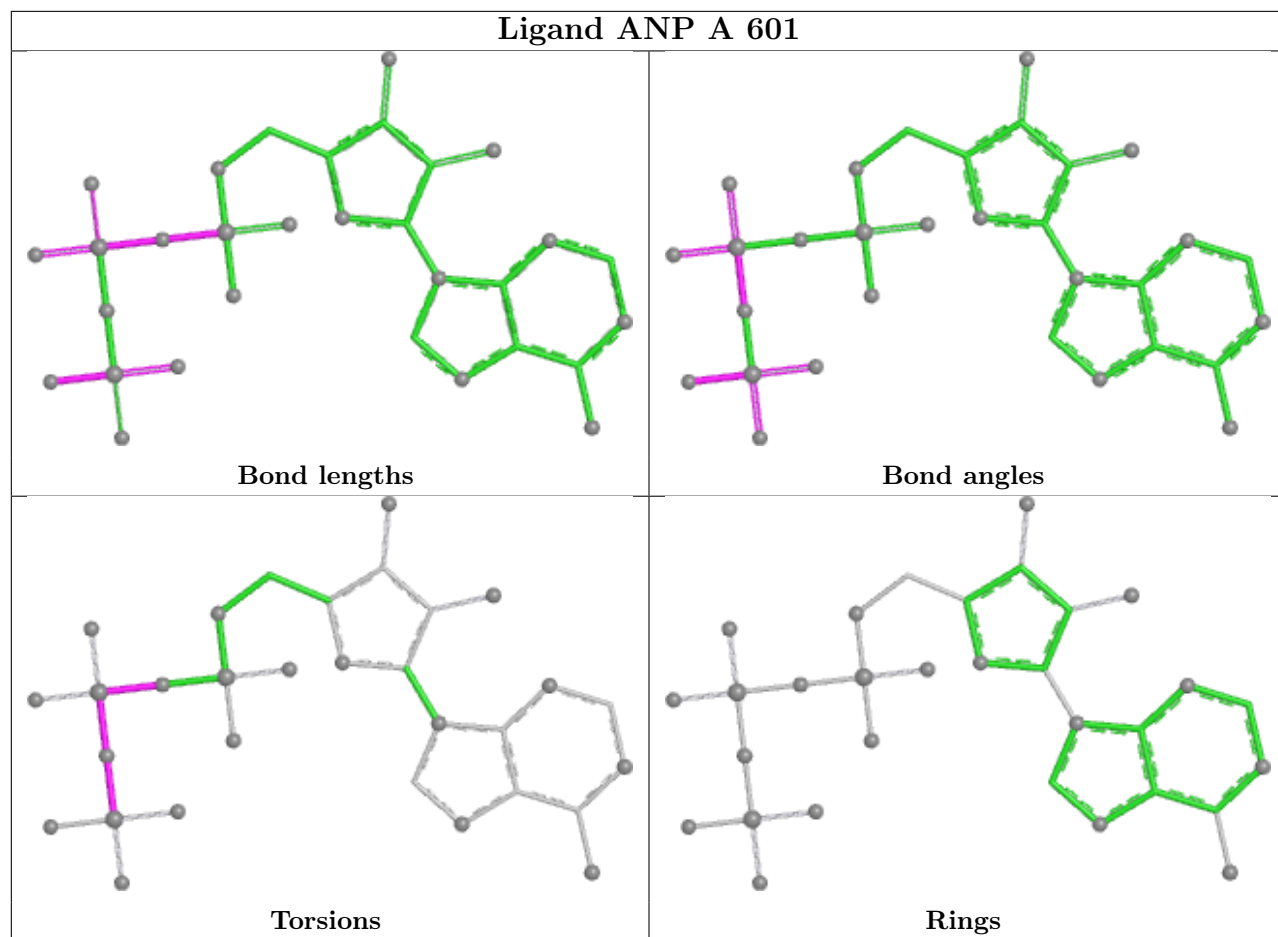
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	BNG	1	0
2	B	601	ANP	1	0

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.







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	571/580 (98%)	1.12	107 (18%) 3 3	61, 95, 135, 202	0
1	B	576/580 (99%)	1.10	109 (18%) 3 3	55, 92, 134, 184	2 (0%)
All	All	1147/1160 (98%)	1.11	216 (18%) 3 3	55, 94, 135, 202	2 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	ARG	20.5
1	B	64	TYR	9.3
1	A	342	LYS	8.5
1	A	476	ASN	8.1
1	A	529	ASP	7.2
1	A	498	LYS	6.4
1	A	477	ARG	6.3
1	A	9	LEU	6.2
1	A	336	PHE	6.1
1	A	500	ALA	6.1
1	B	246	TYR	6.0
1	B	357	ASP	6.0
1	B	578	VAL	5.9
1	A	429	TYR	5.7
1	A	527	PHE	5.5
1	B	350	LEU	5.4
1	A	77	ILE	5.3
1	A	430	ILE	5.3
1	B	349	GLU	5.3
1	B	16	LEU	5.2
1	B	147	ILE	5.2
1	B	364	VAL	5.2
1	A	74	PHE	5.2
1	B	61	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	340	GLU	5.1
1	A	503	ILE	5.1
1	A	499	PRO	5.0
1	A	334	ILE	5.0
1	A	431	PHE	5.0
1	B	59	ASN	4.8
1	A	71	LEU	4.8
1	A	357	ASP	4.8
1	B	63	GLU	4.7
1	B	12	TYR	4.7
1	B	193	SER	4.7
1	B	468	VAL	4.7
1	B	579	THR	4.6
1	B	148	LEU	4.6
1	A	355	SER	4.6
1	A	464	ASN	4.6
1	A	70	CYS	4.5
1	A	337	LEU	4.5
1	A	478	GLY	4.5
1	A	14	TYR	4.5
1	A	579	THR	4.4
1	B	214	ASP	4.4
1	A	80	LYS	4.4
1	A	329	ALA	4.4
1	A	76	VAL	4.4
1	B	126	THR	4.2
1	B	213	VAL	4.2
1	A	528	PRO	4.1
1	A	533	ILE	4.0
1	B	506	GLU	3.9
1	A	362	ASN	3.9
1	A	463	VAL	3.9
1	A	13	ILE	3.9
1	B	537	HIS	3.9
1	B	422	TYR	3.9
1	B	465	ASN	3.9
1	A	338	ASN	3.8
1	A	419	ASP	3.8
1	B	127	GLN	3.8
1	A	420	ALA	3.8
1	B	67	LEU	3.8
1	B	149	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	305	ALA	3.7
1	A	12	TYR	3.7
1	B	372	LYS	3.7
1	B	304	GLY	3.7
1	A	504	ILE	3.6
1	B	329	ALA	3.6
1	B	191	LEU	3.6
1	A	73	MET	3.6
1	B	123	GLY	3.5
1	B	294	ILE	3.5
1	B	215	ASN	3.5
1	A	10	PHE	3.4
1	B	360	ILE	3.4
1	A	501	ILE	3.4
1	A	424	LEU	3.4
1	A	328	LYS	3.3
1	A	126	THR	3.3
1	A	348	ARG	3.3
1	B	155	ILE	3.3
1	A	339	MET	3.3
1	B	575	LEU	3.3
1	B	101	MET	3.2
1	B	467	PRO	3.2
1	A	147	ILE	3.2
1	B	197	HIS	3.2
1	A	452	PHE	3.2
1	B	473	HIS	3.1
1	A	127	GLN	3.1
1	B	400	GLY	3.1
1	A	392	SER	3.1
1	B	394	TYR	3.1
1	A	148	LEU	3.1
1	A	421	ILE	3.1
1	B	138	ILE	3.1
1	A	422	TYR	3.1
1	A	428	ASP	3.1
1	B	525	THR	3.1
1	B	62	TYR	3.0
1	A	320	PHE	3.0
1	B	391	ILE	3.0
1	A	578	VAL	3.0
1	B	462	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	149	SER	2.9
1	A	72	TYR	2.9
1	B	211	ASP	2.9
1	B	554	GLY	2.9
1	A	330	THR	2.9
1	B	274	LEU	2.9
1	B	361	LEU	2.9
1	B	196	LYS	2.9
1	B	335	PRO	2.9
1	A	156	SER	2.9
1	B	13	ILE	2.9
1	B	192	ALA	2.9
1	A	553	GLU	2.9
1	B	365	SER	2.9
1	B	273	ILE	2.9
1	A	564	ASP	2.9
1	B	258	SER	2.8
1	A	204	ASN	2.8
1	B	539	ILE	2.8
1	A	479	ASN	2.8
1	A	350	LEU	2.7
1	A	453	LYS	2.7
1	B	347	ILE	2.7
1	B	97	MET	2.7
1	B	158	ILE	2.7
1	A	59	ASN	2.7
1	B	502	ILE	2.7
1	B	477	ARG	2.7
1	B	362	ASN	2.7
1	A	359	LYS	2.7
1	A	343	LEU	2.6
1	B	6	LYS	2.6
1	A	118	SER	2.6
1	A	567	VAL	2.6
1	B	431	PHE	2.6
1	B	503	ILE	2.6
1	A	284	GLY	2.6
1	B	555	ASN	2.6
1	B	332	PRO	2.6
1	B	333	SER	2.6
1	A	67	LEU	2.6
1	B	68	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	563	ARG	2.6
1	A	400	GLY	2.6
1	B	521	SER	2.6
1	B	14	TYR	2.6
1	B	218	ALA	2.6
1	A	55	GLY	2.5
1	A	197	HIS	2.5
1	B	387	LEU	2.5
1	B	336	PHE	2.5
1	A	408	SER	2.5
1	B	15	SER	2.5
1	B	135	ASP	2.5
1	B	570	GLU	2.5
1	B	269	PHE	2.5
1	B	452	PHE	2.5
1	B	254	LEU	2.4
1	B	22	LYS	2.4
1	B	23	PHE	2.4
1	B	60	PHE	2.4
1	A	323	ARG	2.4
1	B	255[A]	LEU	2.4
1	A	534	ASN	2.4
1	A	75	CYS	2.4
1	B	322	GLN	2.4
1	B	386	THR	2.3
1	A	346	SER	2.3
1	A	158	ILE	2.3
1	A	200	ASP	2.3
1	B	56	SER	2.3
1	B	143	VAL	2.3
1	B	399	PHE	2.3
1	A	263	ILE	2.3
1	B	41	ILE	2.3
1	A	29	LEU	2.3
1	B	71	LEU	2.3
1	B	265	PHE	2.3
1	A	423	TYR	2.2
1	A	438	ASN	2.2
1	B	401	ASP	2.2
1	B	29	LEU	2.2
1	A	321	ILE	2.2
1	A	347	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	416	ASP	2.2
1	A	175	LEU	2.2
1	A	530	ALA	2.2
1	A	157	THR	2.2
1	B	125	THR	2.2
1	A	410	ARG	2.2
1	A	152	ILE	2.2
1	A	332	PRO	2.2
1	A	494	LEU	2.2
1	B	248	LEU	2.2
1	B	413	SER	2.2
1	B	352	PHE	2.2
1	A	570	GLU	2.1
1	B	55	GLY	2.1
1	B	460	LEU	2.1
1	A	270	ILE	2.1
1	A	155	ILE	2.1
1	A	399	PHE	2.1
1	B	309	GLU	2.1
1	B	57	LEU	2.1
1	A	398	TYR	2.1
1	A	84	PHE	2.1
1	B	270	ILE	2.0
1	B	195	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

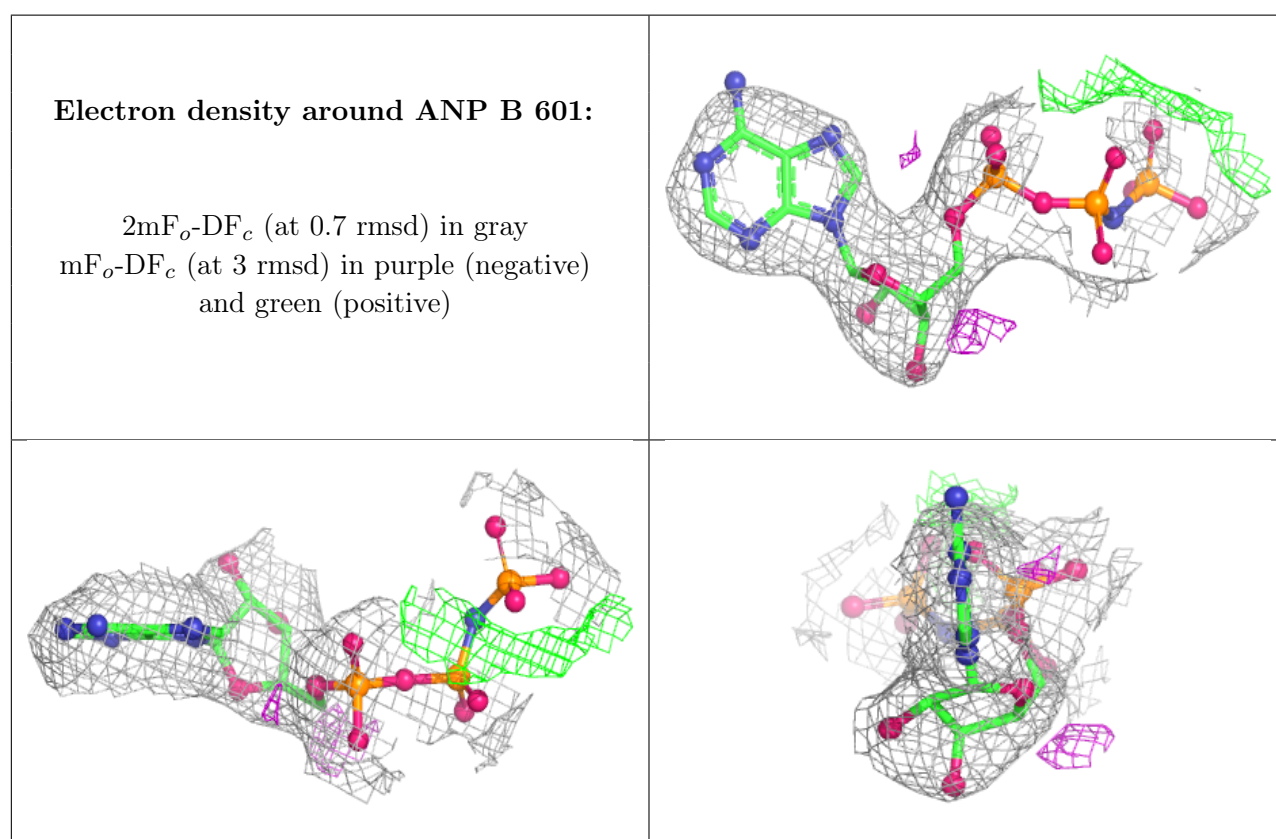
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

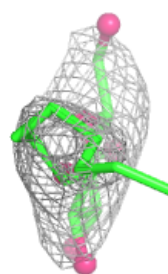
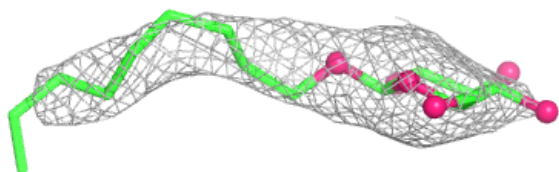
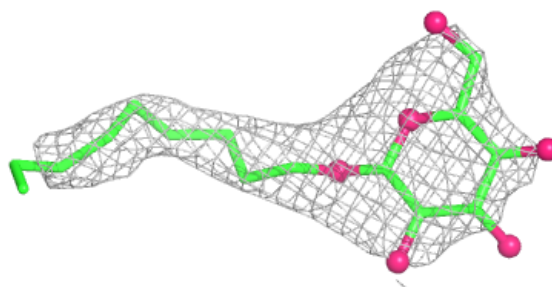
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	B	601	31/31	0.91	0.10	81,88,94,94	0
3	MG	B	602	1/1	0.92	0.15	68,68,68,68	0
4	BNG	A	603	21/21	0.92	0.17	92,123,129,129	0
4	BNG	B	603	21/21	0.92	0.18	96,111,120,124	0
3	MG	A	602	1/1	0.94	0.18	69,69,69,69	0
2	ANP	A	601	31/31	0.94	0.08	91,103,107,109	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.

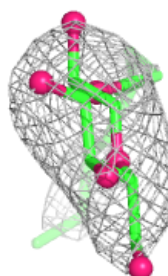
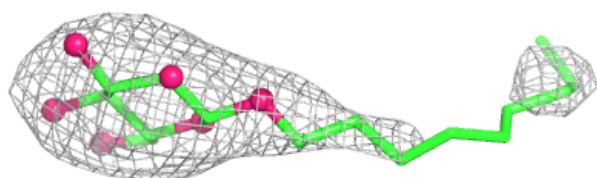
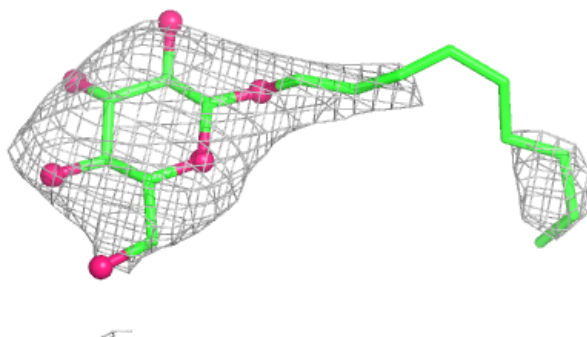


Electron density around BNG A 603:

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

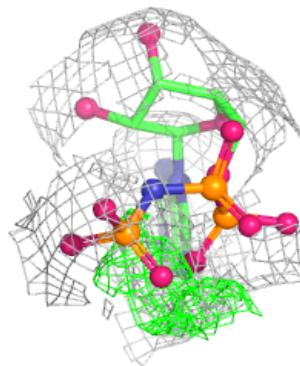
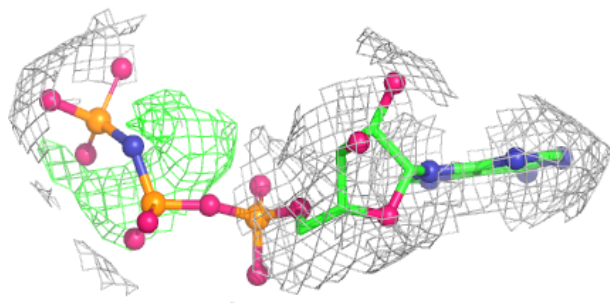
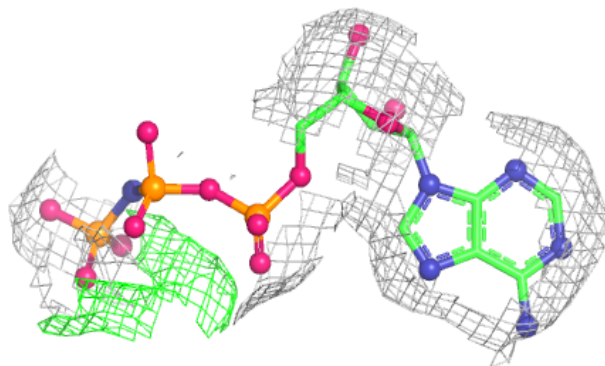
**Electron density around BNG B 603:**

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



Electron density around ANP A 601:

$2mF_o-DF_c$ (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.