



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:38 PM UTC

PDB ID : 7SP5 / pdb_00007sp5
Title : Crystal Structure of a Eukaryotic Phosphate Transporter
Authors : Stroud, R.M.; Pedersen, B.P.; Kumar, H.; Waight, A.B.; Risenmay, A.J.; Roetz, Z.; Chau, B.H.; Schlessinger, A.; Bonomi, M.; Harries, W.; Sali, A.; Johri, A.K.; Finer-Moore, J.
Deposited on : 2021-11-02
Resolution : 2.90 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

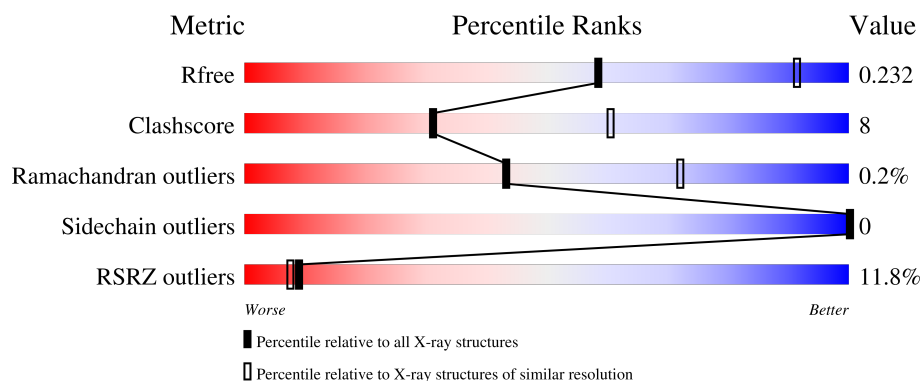
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	530	8% 65% 14% 20%
1	B	530	11% 70% 11% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6669 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 Phosphate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	1
			3240	2138	532	554	16			
1	B	428	Total	C	N	O	S	0	0	0
			3314	2188	546	564	16			

There are 16 discrepancies between the modelled and reference sequences:

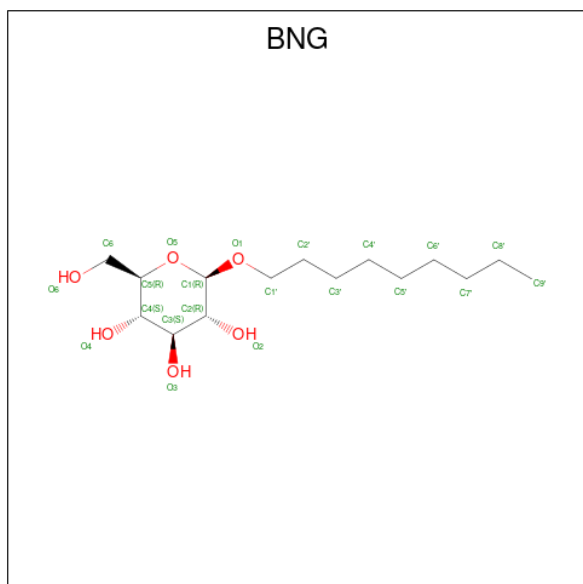
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A8N031
A	0	PRO	-	expression tag	UNP A8N031
A	523	GLY	-	expression tag	UNP A8N031
A	524	GLY	-	expression tag	UNP A8N031
A	525	LEU	-	expression tag	UNP A8N031
A	526	VAL	-	expression tag	UNP A8N031
A	527	PRO	-	expression tag	UNP A8N031
A	528	ARG	-	expression tag	UNP A8N031
B	-1	GLY	-	expression tag	UNP A8N031
B	0	PRO	-	expression tag	UNP A8N031
B	523	GLY	-	expression tag	UNP A8N031
B	524	GLY	-	expression tag	UNP A8N031
B	525	LEU	-	expression tag	UNP A8N031
B	526	VAL	-	expression tag	UNP A8N031
B	527	PRO	-	expression tag	UNP A8N031
B	528	ARG	-	expression tag	UNP A8N031

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: $C_{15}H_{30}O_6$) (labeled as "Ligand of Interest" by depositor).



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

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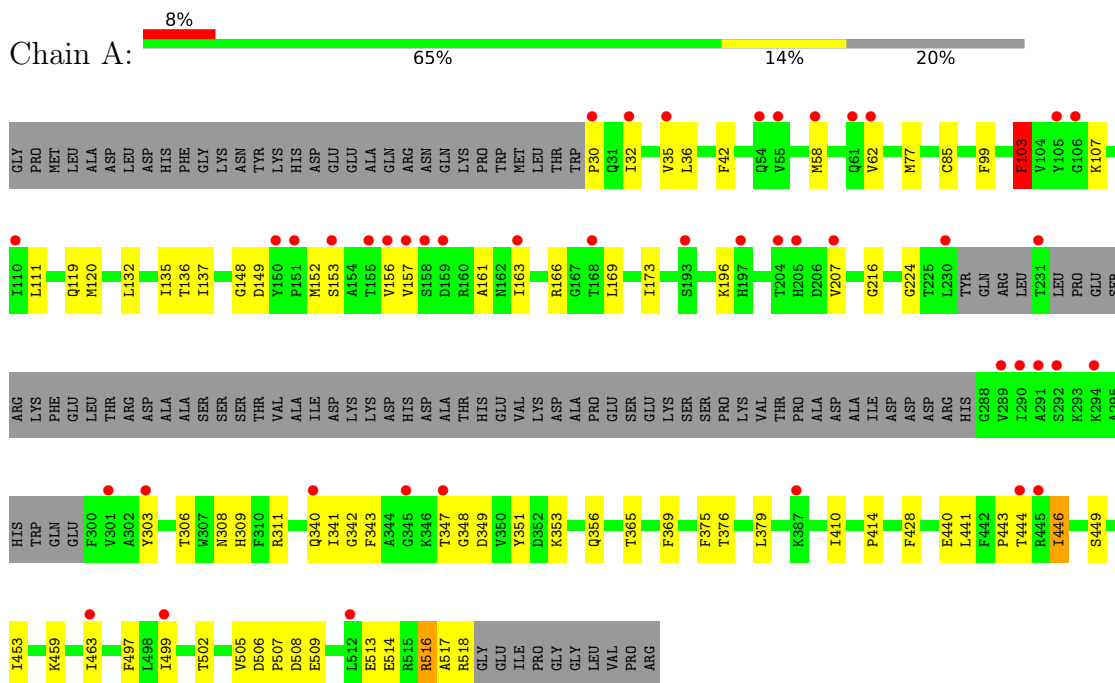
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		

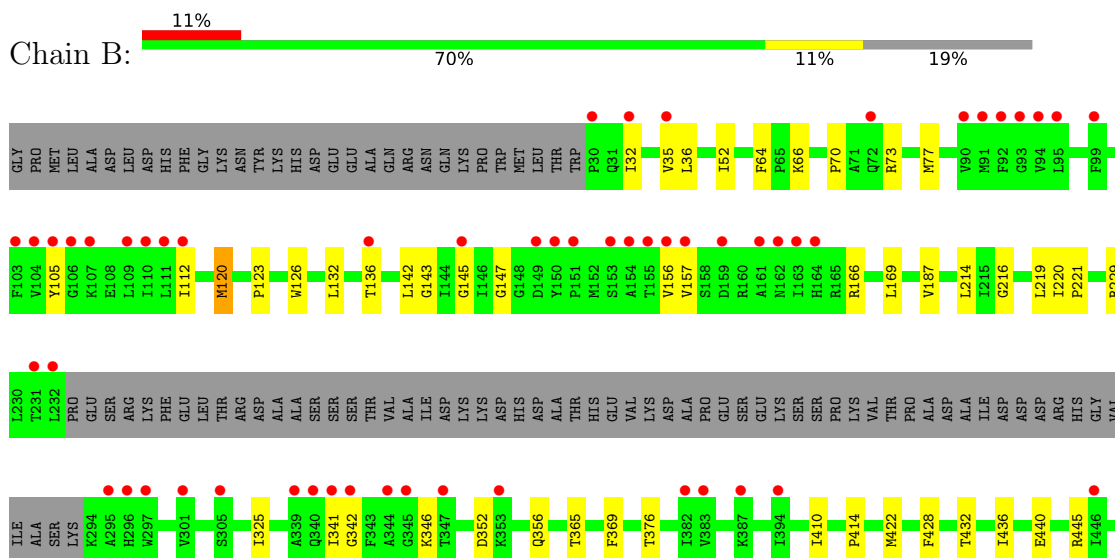
3 Residue-property plots

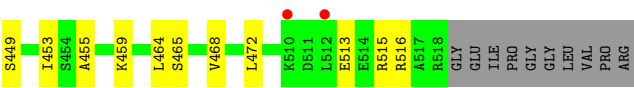
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphate transporter



• Molecule 1: Phosphate transporter





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.51Å 174.51Å 173.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.27 – 2.90 69.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (69.27-2.90) 93.6 (69.27-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.234 , 0.255 (Not available) , 0.232	Depositor DCC
R_{free} test set	1982 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.31	1/3331 (0.0%)	0.63	6/4515 (0.1%)
1	B	0.20	0/3397	0.51	1/4602 (0.0%)
All	All	0.26	1/6728 (0.0%)	0.57	7/9117 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	ILE	CG1-CD1	-6.01	1.28	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	CB-CA-C	-7.68	94.26	110.31
1	A	446	ILE	CA-CB-CG1	-7.43	97.78	110.40
1	A	516	ARG	CD-NE-CZ	-6.54	115.25	124.40
1	A	516	ARG	N-CA-C	-5.59	105.72	112.54
1	B	120	MET	CB-CG-SD	-5.57	95.99	112.70
1	A	103	PHE	CB-CA-C	-5.45	99.27	110.38
1	A	340	GLN	CA-CB-CG	5.17	124.43	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	PHE	Sidechain

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	3240	0	3271	68	0
1	B	3314	0	3346	41	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	63	0	90	5	0
3	B	42	0	60	0	0
All	All	6669	0	6767	109	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 8.

All (109) 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:B:120:MET:HE2	1:B:216:GLY:HA2	1.49	0.95
1:A:85:CYS:SG	1:A:459:LYS:NZ	2.48	0.86
1:A:303:TYR:HE2	1:A:309:HIS:HD1	1.30	0.79
1:A:347:THR:O	1:A:353:LYS:NZ	2.12	0.77
1:A:513:GLU:OE1	1:A:516:ARG:NH2	2.19	0.74
1:A:103:PHE:O	1:A:103:PHE:HD2	1.71	0.74
1:A:303:TYR:HE2	1:A:309:HIS:ND1	1.88	0.72
1:A:311:ARG:HH21	3:A:602:BNG:H5	1.55	0.71
1:B:64:PHE:HA	1:B:66:LYS:NZ	2.07	0.69
1:B:513:GLU:OE2	1:B:516:ARG:NE	2.27	0.68
1:A:513:GLU:HA	1:A:516:ARG:HG2	1.75	0.68
1:B:123:PRO:HG2	1:B:126:TRP:CE2	2.30	0.67
1:B:52:ILE:HD11	1:B:77:MET:HE3	1.78	0.66
1:B:123:PRO:HG2	1:B:126:TRP:CD2	2.33	0.64
1:B:468:VAL:HG22	1:B:472:LEU:HG	1.80	0.64
1:A:62:VAL:HG22	1:A:207:VAL:HG13	1.78	0.64
1:A:513:GLU:OE1	1:A:516:ARG:NE	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:HA	1:A:152:MET:HE3	1.80	0.63
1:A:99:PHE:HB2	1:A:103:PHE:HD1	1.67	0.60
1:B:105:TYR:CE2	1:B:229:ARG:HD3	2.38	0.59
1:A:443:PRO:HG2	1:A:446:ILE:HD11	1.85	0.59
1:A:513:GLU:OE1	1:A:516:ARG:CZ	2.50	0.59
1:B:166:ARG:HH21	1:B:440:GLU:HB3	1.66	0.58
1:B:70:PRO:HG2	1:B:73:ARG:HD2	1.84	0.58
1:A:77:MET:HA	1:A:136:THR:HG22	1.85	0.57
1:A:303:TYR:CE2	1:A:309:HIS:ND1	2.69	0.57
1:A:497:PHE:O	3:A:602:BNG:O2	2.22	0.57
1:B:365:THR:HA	1:B:369:PHE:HB3	1.88	0.56
1:B:445:ARG:HH12	1:B:515:ARG:HD2	1.70	0.56
1:A:306:THR:HB	1:A:309:HIS:CD2	2.41	0.56
1:A:349:ASP:O	1:A:353:LYS:HG2	2.06	0.56
1:A:459:LYS:O	1:A:463:ILE:HG12	2.06	0.56
1:A:103:PHE:O	1:A:103:PHE:CD2	2.58	0.55
1:B:346:LYS:HB2	1:B:356:GLN:HE22	1.72	0.55
1:B:464:LEU:O	1:B:468:VAL:HG12	2.06	0.55
1:A:303:TYR:CD1	1:A:446:ILE:HD13	2.42	0.54
1:A:103:PHE:O	1:A:107:LYS:NZ	2.40	0.54
1:B:143:GLY:O	1:B:147:GLY:N	2.35	0.54
1:A:311:ARG:NH2	3:A:602:BNG:H5	2.23	0.54
1:A:343:PHE:O	1:A:356:GLN:NE2	2.41	0.54
1:A:32:ILE:HG22	1:A:36:LEU:HD11	1.89	0.53
1:A:514:GLU:O	1:A:518:ARG:NH1	2.42	0.53
1:B:120:MET:HE2	1:B:216:GLY:CA	2.32	0.52
1:B:64:PHE:HA	1:B:66:LYS:HZ2	1.74	0.52
1:A:32:ILE:O	1:A:35:VAL:HG22	2.11	0.51
1:A:375:PHE:O	1:A:379:LEU:HD12	2.10	0.51
1:A:308:ASN:HA	1:A:311:ARG:CD	2.41	0.51
1:A:58:MET:O	1:A:62:VAL:HG23	2.10	0.51
1:A:506:ASP:OD2	1:A:509:GLU:N	2.39	0.51
1:B:449:SER:O	1:B:453:ILE:HG12	2.10	0.51
1:A:42:PHE:HE1	1:A:153:SER:HG	1.59	0.51
1:A:410:ILE:HD12	1:A:414:PRO:HB2	1.94	0.50
1:A:30:PRO:HB2	1:A:32:ILE:HD12	1.93	0.50
1:B:120:MET:HE1	1:B:219:LEU:HD11	1.93	0.50
1:B:77:MET:HA	1:B:136:THR:HG22	1.94	0.49
1:B:341:ILE:HG22	1:B:342:GLY:H	1.78	0.49
1:A:99:PHE:HB2	1:A:103:PHE:CD1	2.47	0.49
1:A:449:SER:O	1:A:453:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD12	3:A:603:BNG:H9'1	1.92	0.49
1:A:308:ASN:HA	1:A:311:ARG:HD2	1.94	0.49
1:A:303:TYR:CE1	1:A:446:ILE:CD1	2.96	0.49
1:A:376:THR:OG1	1:A:428:PHE:HA	2.13	0.49
1:B:132:LEU:O	1:B:136:THR:HG23	2.14	0.47
1:A:341:ILE:HG22	1:A:342:GLY:H	1.78	0.47
1:B:32:ILE:HG22	1:B:36:LEU:CD1	2.45	0.46
1:A:516:ARG:HG3	1:A:517:ALA:N	2.29	0.46
1:B:422:MET:HB3	1:B:422:MET:HE2	1.77	0.46
1:A:42:PHE:HE1	1:A:153:SER:OG	1.98	0.46
1:A:103:PHE:O	1:A:107:LYS:HD2	2.15	0.46
1:B:156:VAL:HG23	1:B:157:VAL:HG13	1.97	0.46
1:A:132:LEU:O	1:A:136:THR:HG23	2.15	0.46
1:B:325:ILE:HG23	1:B:465:SER:HB3	1.98	0.45
1:A:119:GLN:HG3	1:A:135:ILE:HG23	1.98	0.45
1:B:32:ILE:O	1:B:35:VAL:HG22	2.16	0.45
1:B:376:THR:OG1	1:B:428:PHE:HA	2.16	0.45
1:A:365:THR:HA	1:A:369:PHE:HB3	1.99	0.45
1:A:161:ALA:HB1	1:A:163:ILE:HG22	1.99	0.45
1:A:306:THR:HB	1:A:309:HIS:HD2	1.82	0.44
1:B:455:ALA:O	1:B:459:LYS:HG3	2.18	0.44
1:A:120:MET:HE2	1:A:216:GLY:HA2	1.99	0.44
1:B:220:ILE:HB	1:B:221:PRO:HD3	1.99	0.44
1:A:32:ILE:HG22	1:A:36:LEU:CD1	2.48	0.44
1:A:196:LYS:HG3	1:A:351:TYR:CZ	2.53	0.43
1:B:346:LYS:CB	1:B:356:GLN:HE22	2.31	0.43
1:A:166:ARG:HH12	1:A:507:PRO:HD3	1.82	0.43
1:A:516:ARG:HH11	1:A:516:ARG:HD2	1.43	0.43
1:A:441:LEU:HD11	1:A:499:ILE:HD12	2.00	0.43
1:A:440:GLU:OE2	1:A:502:THR:OG1	2.27	0.43
1:A:169:LEU:O	1:A:173:ILE:HG13	2.18	0.42
1:A:36:LEU:H	1:A:36:LEU:HD12	1.84	0.42
1:B:169:LEU:HD12	1:B:169:LEU:HA	1.86	0.42
1:A:303:TYR:CE1	1:A:446:ILE:HD13	2.54	0.42
1:B:66:LYS:H	1:B:66:LYS:HG2	1.40	0.41
1:B:410:ILE:HD12	1:B:414:PRO:HB2	2.02	0.41
1:A:152:MET:HE3	1:A:152:MET:HB2	1.84	0.41
1:B:112:ILE:HG22	1:B:142:LEU:HD12	2.02	0.41
1:A:156:VAL:HG23	1:A:157:VAL:HG13	2.03	0.41
1:B:187:VAL:HG12	1:B:214:LEU:HD22	2.02	0.41
1:A:444:THR:HG23	1:A:508:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:HD12	1:B:52:ILE:HA	1.85	0.41
1:A:77:MET:CA	1:A:136:THR:HG22	2.50	0.41
1:A:137:ILE:HG21	3:A:603:BNG:H2'2	2.02	0.41
1:A:99:PHE:CB	1:A:103:PHE:HD1	2.32	0.41
1:A:502:THR:O	1:A:505:VAL:HG22	2.21	0.41
1:B:112:ILE:HG23	1:B:145:GLY:HA3	2.03	0.40
1:B:166:ARG:NH2	1:B:440:GLU:HB3	2.34	0.40
1:B:432:THR:HG22	1:B:436:ILE:HD12	2.04	0.40
1:B:352:ASP:O	1:B:356:GLN:HG3	2.21	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	421/530 (79%)	410 (97%)	9 (2%)	2 (0%)	24	54
1	B	424/530 (80%)	412 (97%)	12 (3%)	0	100	100
All	All	845/1060 (80%)	822 (97%)	21 (2%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	GLY
1	A	348	GLY

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	332/433 (77%)	332 (100%)	0	100	100
1	B	341/433 (79%)	341 (100%)	0	100	100
All	All	673/866 (78%)	673 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	129	ASN
1	A	203	HIS
1	B	61	GLN
1	B	125	HIS
1	B	129	ASN
1	B	298	GLN
1	B	356	GLN
1	B	451	HIS

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 ⓘ

7 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	A	603	-	21,21,21	1.13	2 (9%)	26,26,26	1.34	3 (11%)
2	PO4	B	601	-	4,4,4	0.95	0	6,6,6	0.47	0
2	PO4	A	601	-	4,4,4	0.94	0	6,6,6	0.46	0
3	BNG	B	603	-	21,21,21	1.25	3 (14%)	26,26,26	1.18	3 (11%)
3	BNG	A	602	-	21,21,21	1.12	1 (4%)	26,26,26	1.00	1 (3%)
3	BNG	B	602	-	21,21,21	1.10	2 (9%)	26,26,26	0.98	1 (3%)
3	BNG	A	604	-	21,21,21	1.08	2 (9%)	26,26,26	1.07	2 (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
3	BNG	A	603	-	-	7/12/32/32	0/1/1/1
3	BNG	B	603	-	-	7/12/32/32	0/1/1/1
3	BNG	A	602	-	-	8/12/32/32	0/1/1/1
3	BNG	B	602	-	-	6/12/32/32	0/1/1/1
3	BNG	A	604	-	-	3/12/32/32	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	BNG	O5-C1	3.76	1.51	1.41
3	A	603	BNG	O5-C1	3.60	1.51	1.41
3	A	602	BNG	O5-C1	3.50	1.50	1.41
3	B	602	BNG	O5-C1	3.49	1.50	1.41
3	A	604	BNG	O5-C1	3.28	1.50	1.41
3	B	603	BNG	O1-C1	-2.24	1.36	1.40
3	B	602	BNG	O1-C1	-2.15	1.36	1.40
3	A	604	BNG	O1-C1	-2.11	1.36	1.40
3	A	603	BNG	O1-C1	-2.10	1.36	1.40
3	B	603	BNG	O5-C5	2.05	1.49	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	BNG	C3-C4-C5	3.22	116.08	110.23
3	B	603	BNG	C1-C2-C3	-2.98	103.75	110.01
3	A	603	BNG	O5-C1-C2	2.80	116.13	110.37
3	A	603	BNG	C4-C3-C2	2.73	115.62	110.83
3	B	603	BNG	O5-C5-C4	2.27	113.79	109.70
3	B	603	BNG	C4-C3-C2	-2.26	106.86	110.83
3	A	602	BNG	C5'-C4'-C3'	-2.22	103.13	114.37
3	A	604	BNG	C1-O5-C5	-2.17	109.49	113.72
3	B	602	BNG	C6'-C5'-C4'	-2.12	103.64	114.37
3	A	604	BNG	C3-C4-C5	2.11	114.06	110.23

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	BNG	C2-C1-O1-C1'
3	A	602	BNG	O5-C1-O1-C1'
3	A	603	BNG	O5-C5-C6-O6
3	B	603	BNG	O5-C5-C6-O6
3	B	602	BNG	O5-C1-O1-C1'
3	A	603	BNG	C4-C5-C6-O6
3	B	603	BNG	O1-C1'-C2'-C3'
3	A	603	BNG	O1-C1'-C2'-C3'
3	B	602	BNG	C2-C1-O1-C1'
3	B	602	BNG	C2'-C3'-C4'-C5'
3	A	603	BNG	C2'-C1'-O1-C1
3	B	603	BNG	C2'-C1'-O1-C1
3	B	603	BNG	C1'-C2'-C3'-C4'
3	A	602	BNG	C2'-C3'-C4'-C5'
3	A	602	BNG	C3'-C4'-C5'-C6'
3	A	604	BNG	C2-C1-O1-C1'
3	A	603	BNG	C1'-C2'-C3'-C4'
3	B	602	BNG	C5'-C6'-C7'-C8'
3	A	602	BNG	C2'-C1'-O1-C1
3	B	602	BNG	O1-C1'-C2'-C3'
3	A	602	BNG	C5'-C6'-C7'-C8'
3	A	604	BNG	O5-C1-O1-C1'
3	A	602	BNG	O1-C1'-C2'-C3'
3	B	603	BNG	C4'-C5'-C6'-C7'
3	A	603	BNG	C4'-C5'-C6'-C7'
3	B	603	BNG	C4-C5-C6-O6

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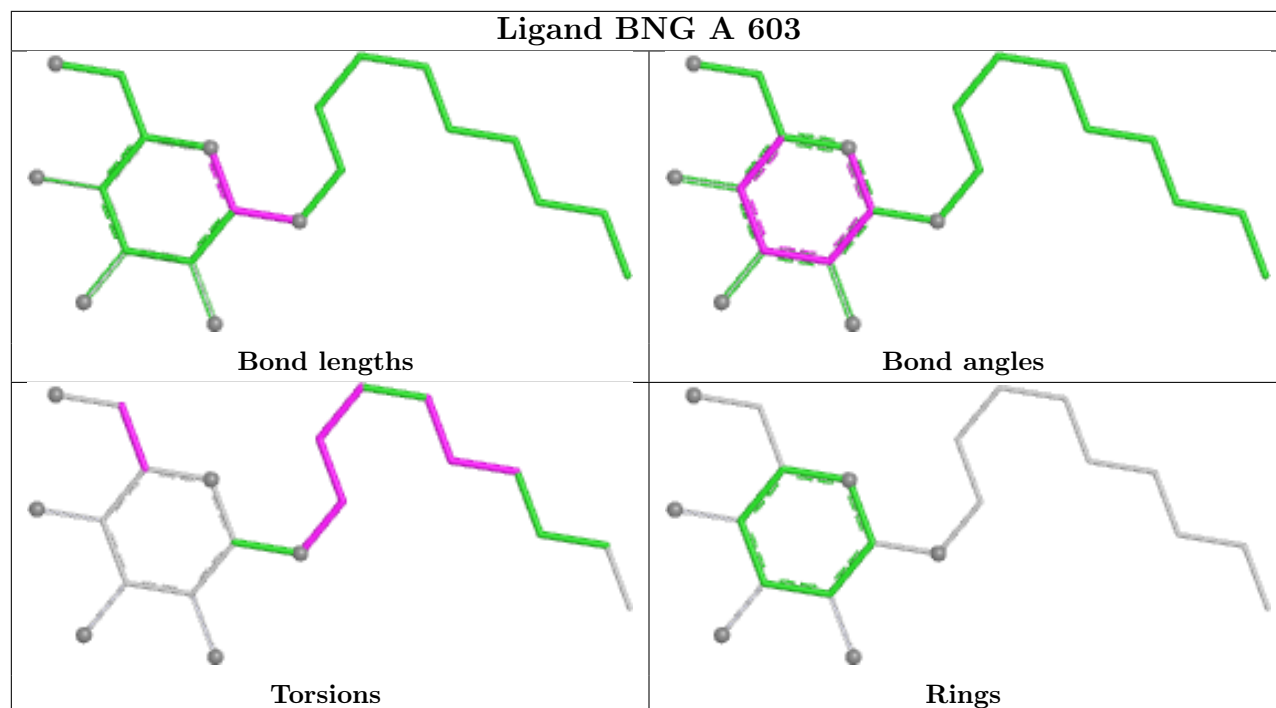
Mol	Chain	Res	Type	Atoms
3	A	603	BNG	C3'-C4'-C5'-C6'
3	A	604	BNG	O5-C5-C6-O6
3	A	602	BNG	C6'-C7'-C8'-C9'
3	B	603	BNG	C3'-C4'-C5'-C6'
3	B	602	BNG	C2'-C1'-O1-C1

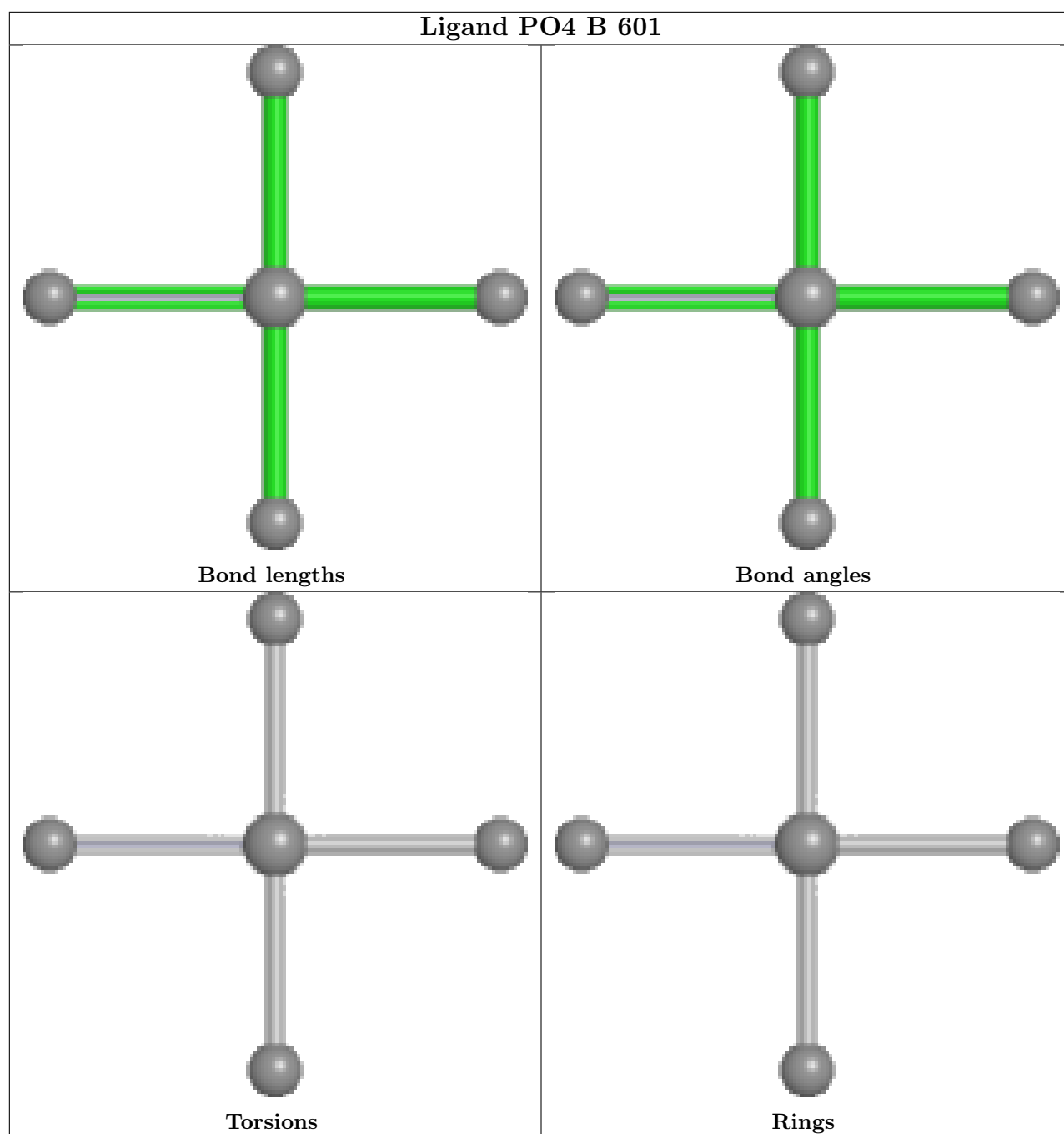
There are no ring outliers.

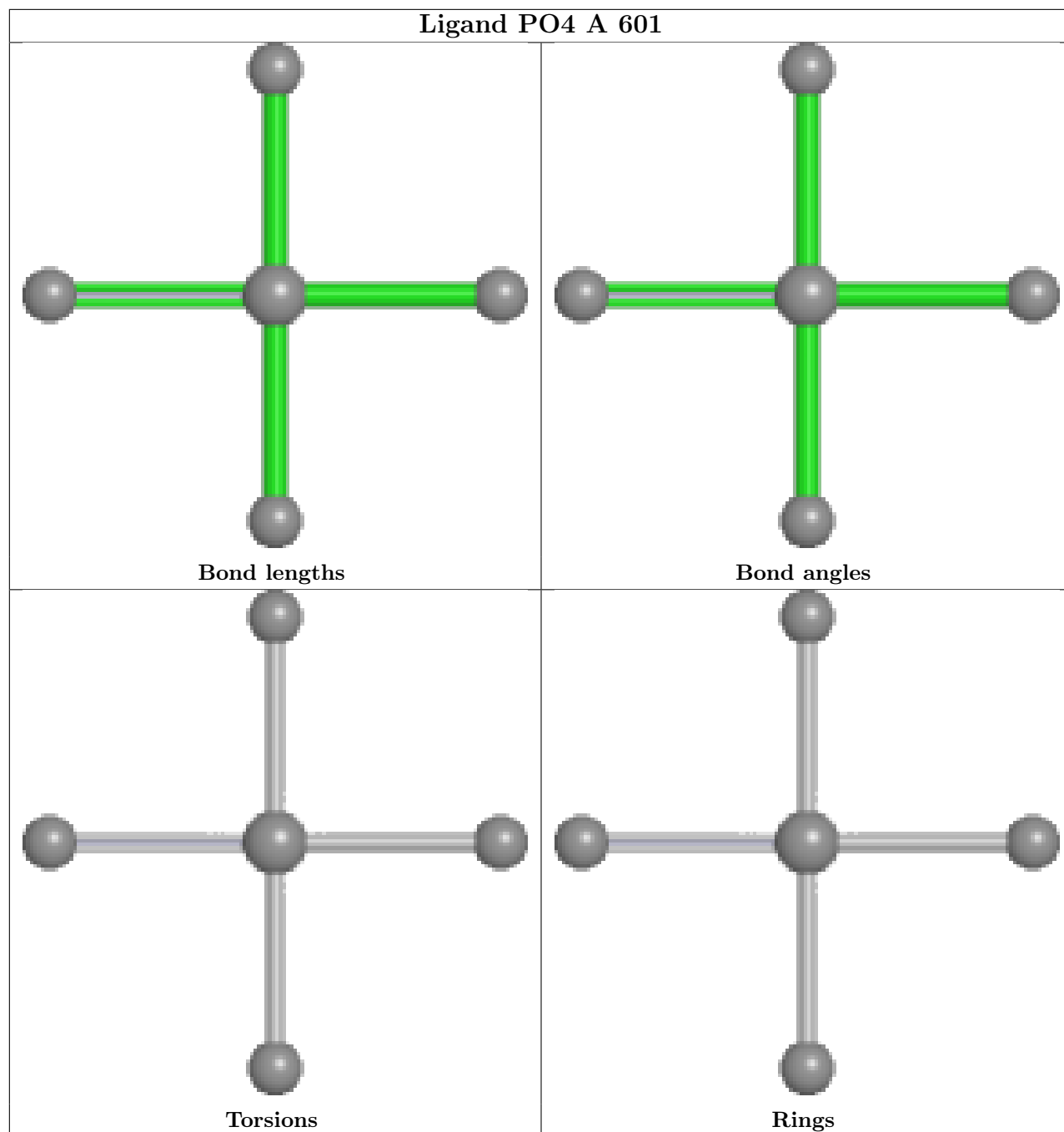
2 monomers are involved in 5 short contacts:

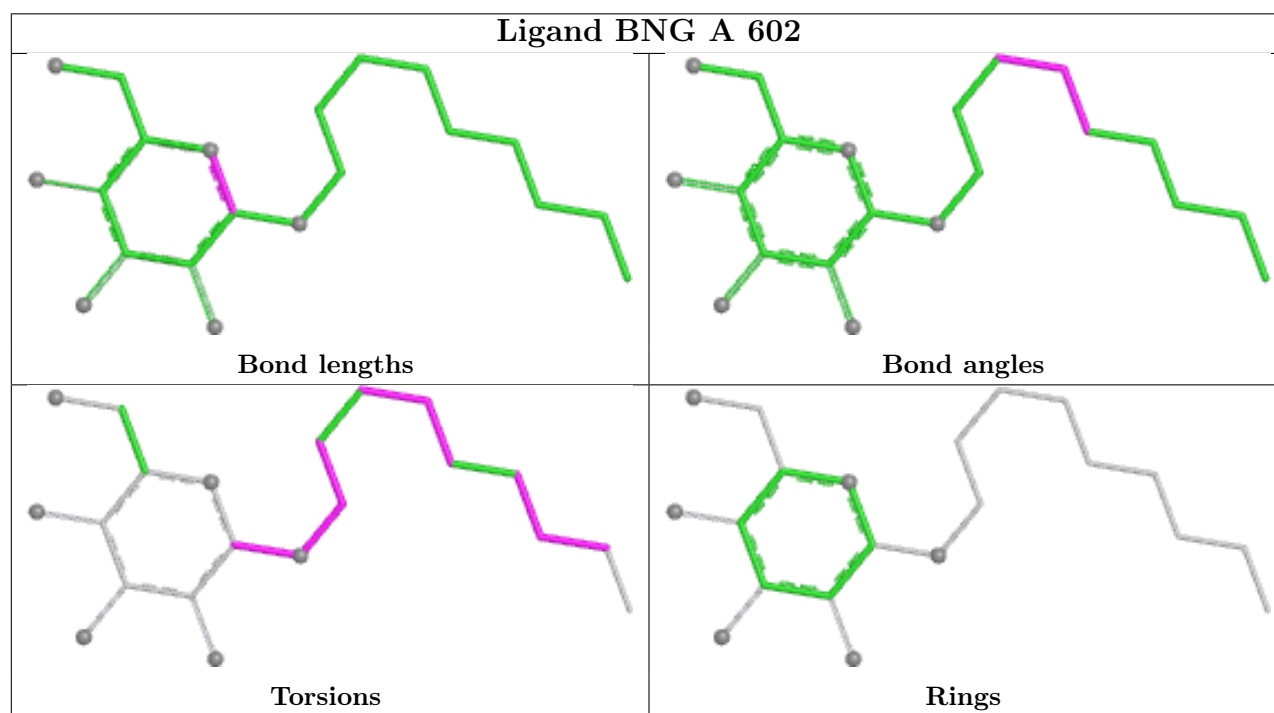
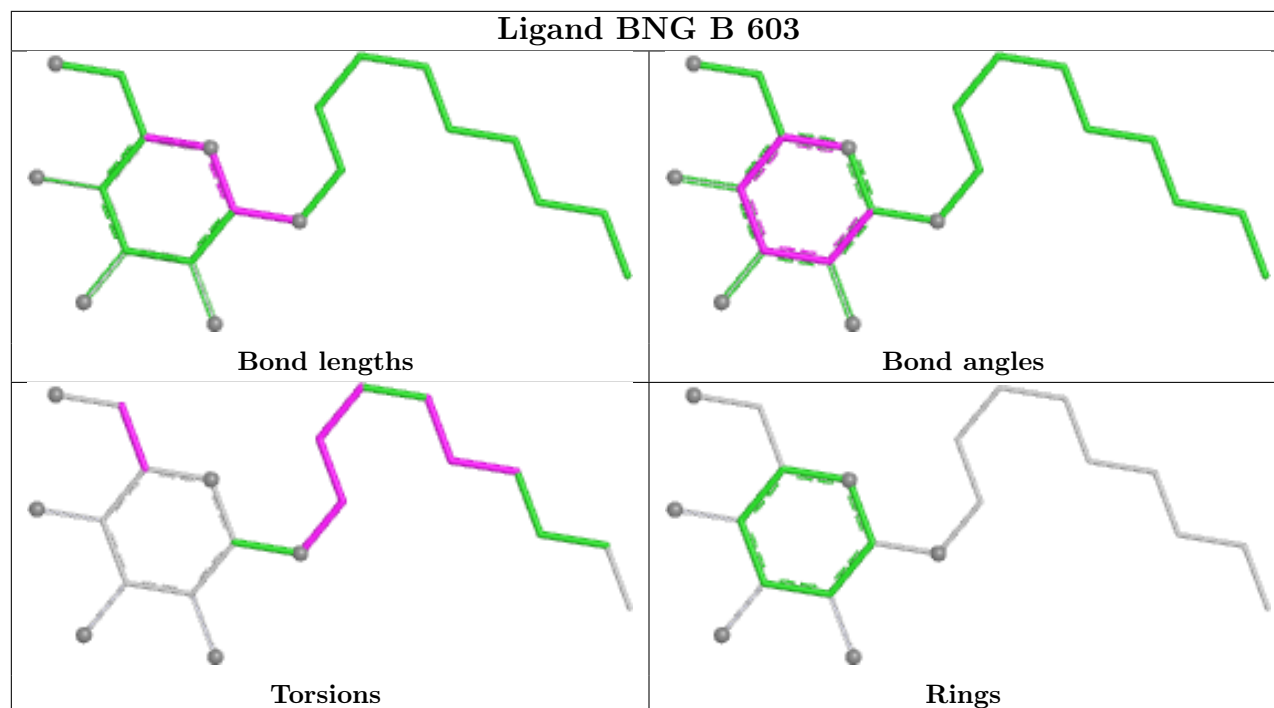
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	BNG	2	0
3	A	602	BNG	3	0

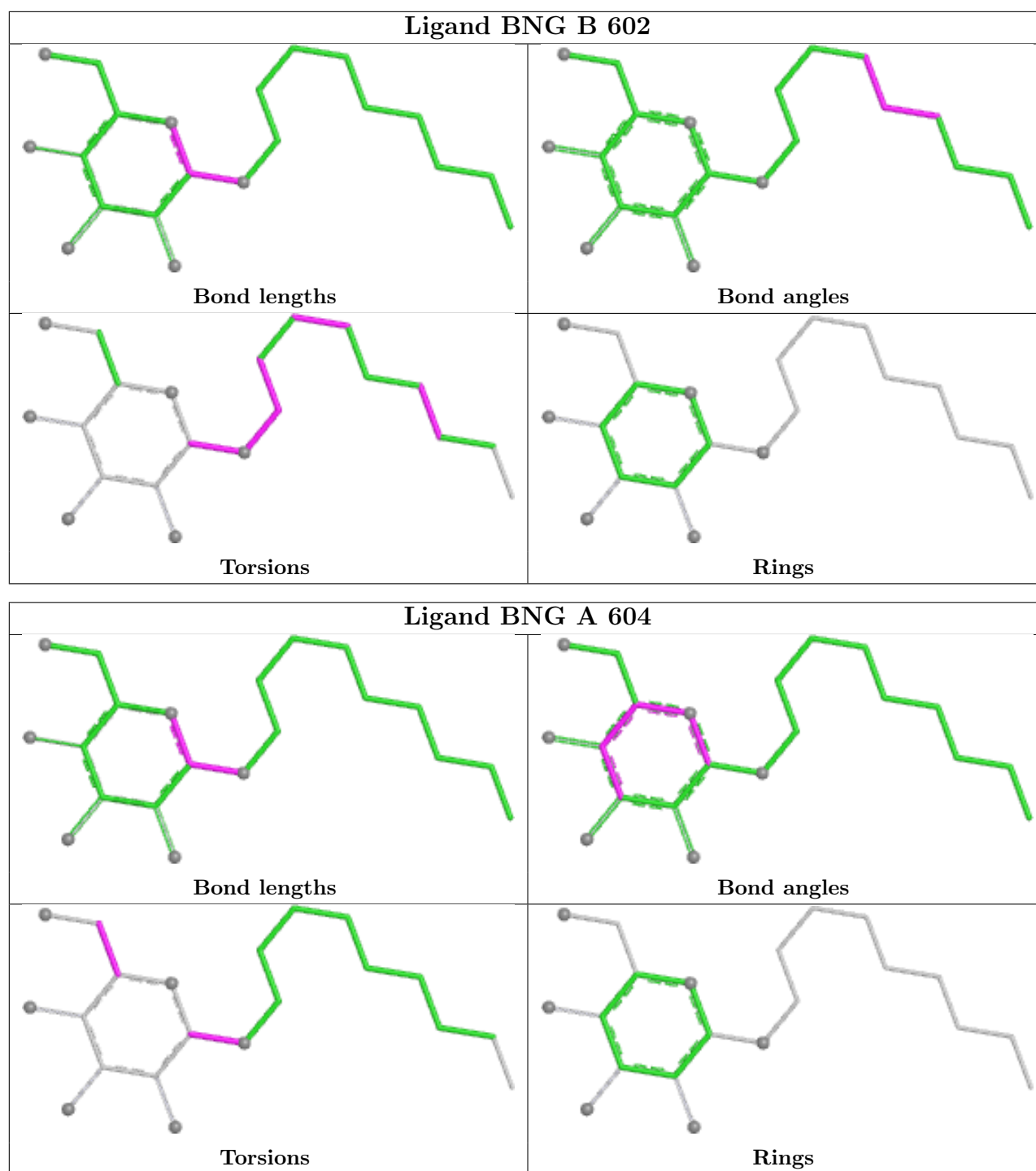
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	423/530 (79%)	0.56	44 (10%)	11 10	53, 80, 166, 258	0
1	B	428/530 (80%)	0.62	57 (13%)	7 6	54, 84, 195, 250	0
All	All	851/1060 (80%)	0.59	101 (11%)	9 7	53, 82, 178, 258	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	VAL	6.8
1	B	155	THR	6.1
1	B	387	LYS	5.4
1	A	106	GLY	5.0
1	B	159	ASP	4.8
1	B	94	VAL	4.7
1	B	296	HIS	4.6
1	A	231	THR	4.4
1	B	163	ILE	4.3
1	B	153	SER	4.2
1	B	95	LEU	4.1
1	A	30	PRO	4.1
1	A	155	THR	4.1
1	A	512	LEU	4.0
1	B	32	ILE	3.9
1	B	30	PRO	3.7
1	B	99	PHE	3.7
1	B	340	GLN	3.7
1	B	297	TRP	3.7
1	A	62	VAL	3.7
1	B	110	ILE	3.6
1	A	150	TYR	3.6
1	A	151	PRO	3.5
1	B	150	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	345	GLY	3.4
1	B	232	LEU	3.4
1	A	61	GLN	3.4
1	A	168	THR	3.3
1	B	164	HIS	3.3
1	B	107	LYS	3.3
1	B	154	ALA	3.3
1	A	291	ALA	3.2
1	A	387	LYS	3.2
1	B	151	PRO	3.2
1	A	444	THR	3.2
1	B	295	ALA	3.1
1	A	32	ILE	3.1
1	B	93	GLY	3.0
1	A	340	GLN	2.9
1	A	193	SER	2.9
1	A	158	SER	2.9
1	B	106	GLY	2.9
1	B	510	LYS	2.9
1	A	197	HIS	2.9
1	A	204	THR	2.9
1	B	156	VAL	2.9
1	A	347	THR	2.9
1	B	105	TYR	2.8
1	B	72	GLN	2.8
1	B	344	ALA	2.7
1	A	157	VAL	2.7
1	B	104	VAL	2.7
1	B	92	PHE	2.6
1	B	512	LEU	2.6
1	A	230	LEU	2.5
1	B	109	LEU	2.5
1	B	90	VAL	2.5
1	A	55	VAL	2.5
1	B	157	VAL	2.5
1	B	103	PHE	2.5
1	A	205	HIS	2.5
1	A	303	TYR	2.4
1	B	231	THR	2.4
1	B	342	GLY	2.3
1	B	382	ILE	2.3
1	A	207	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	301	VAL	2.3
1	B	162	ASN	2.3
1	A	35	VAL	2.3
1	B	111	LEU	2.3
1	A	163	ILE	2.3
1	B	305	SER	2.3
1	B	35	VAL	2.3
1	B	345	GLY	2.3
1	A	105	TYR	2.2
1	A	292	SER	2.2
1	A	58	MET	2.2
1	B	136	THR	2.2
1	B	145	GLY	2.2
1	A	445	ARG	2.2
1	A	499	ILE	2.2
1	B	341	ILE	2.2
1	A	463	ILE	2.2
1	B	149	ASP	2.2
1	A	110	ILE	2.1
1	A	290	ILE	2.1
1	B	353	LYS	2.1
1	A	159	ASP	2.1
1	B	446	ILE	2.1
1	A	289	VAL	2.1
1	B	394	ILE	2.1
1	B	91	MET	2.0
1	B	383	VAL	2.0
1	B	112	ILE	2.0
1	B	347	THR	2.0
1	B	161	ALA	2.0
1	A	294	LYS	2.0
1	A	54	GLN	2.0
1	A	153	SER	2.0
1	A	301	VAL	2.0
1	B	339	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

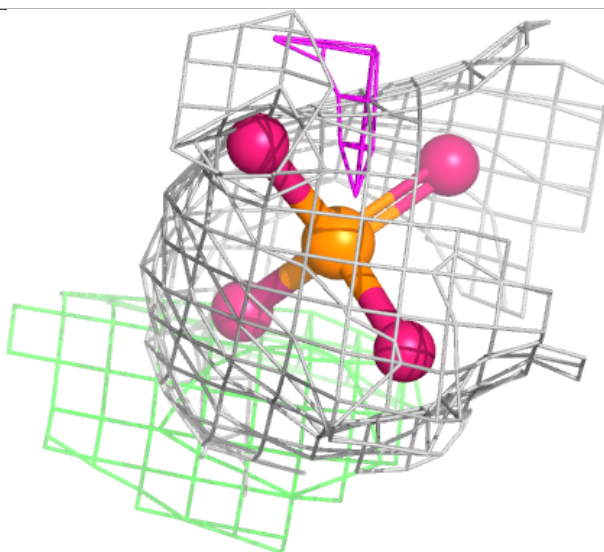
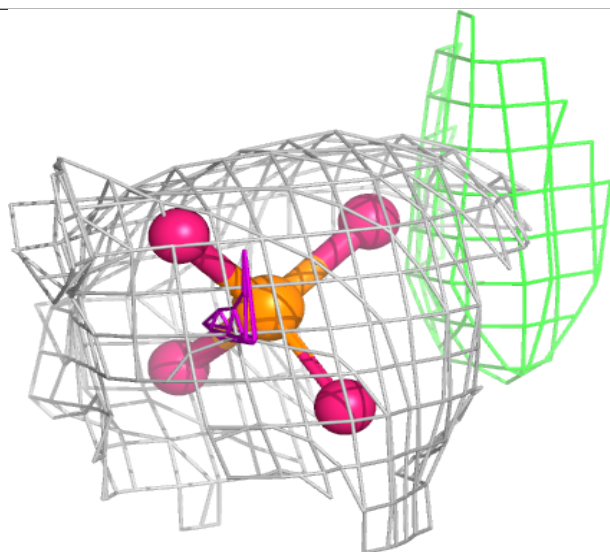
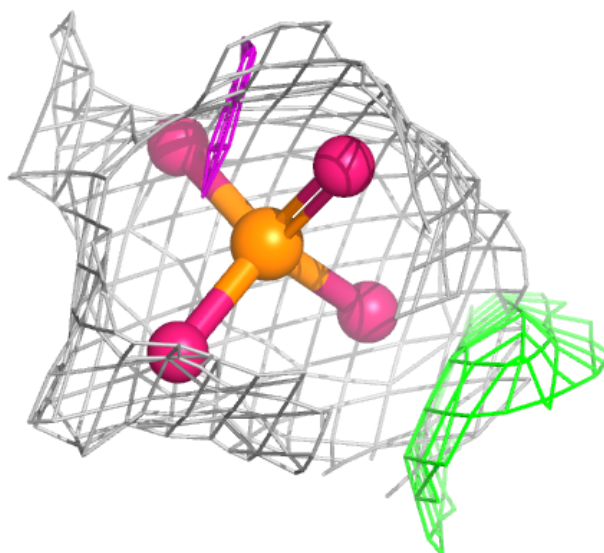
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	A	601	5/5	0.76	0.20	103,103,137,138	0
2	PO4	B	601	5/5	0.86	0.18	80,94,119,125	0
3	BNG	A	604	21/21	0.86	0.14	71,97,113,118	0
3	BNG	B	603	21/21	0.86	0.24	66,90,101,111	0
3	BNG	B	602	21/21	0.87	0.18	68,90,111,115	0
3	BNG	A	603	21/21	0.88	0.16	75,102,120,121	0
3	BNG	A	602	21/21	0.91	0.15	64,93,114,116	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.

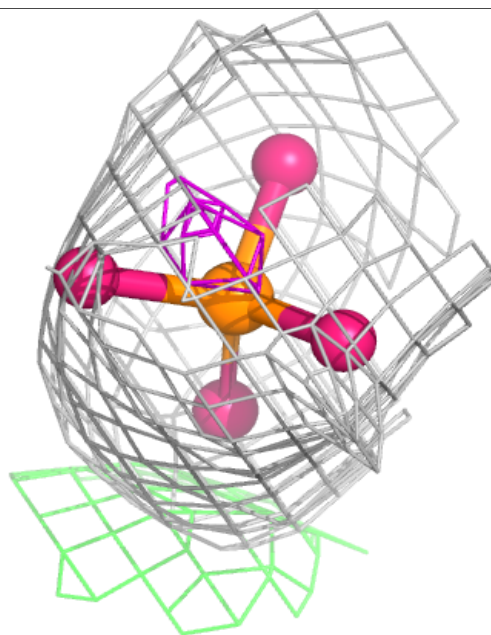
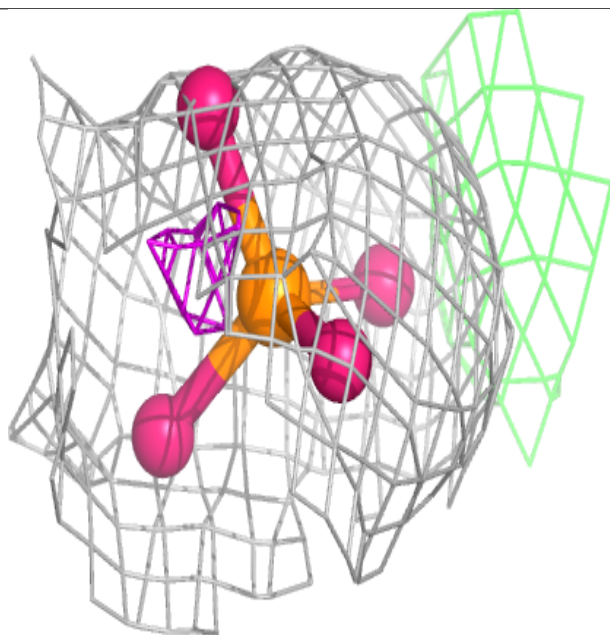
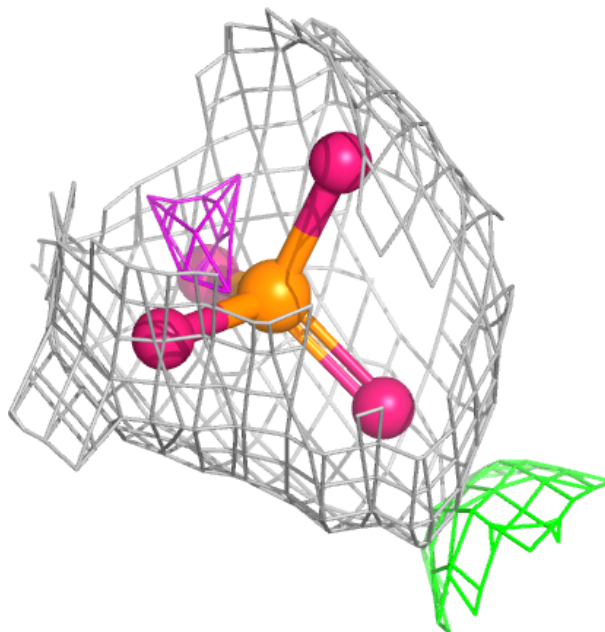
Electron density around PO4 A 601:

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



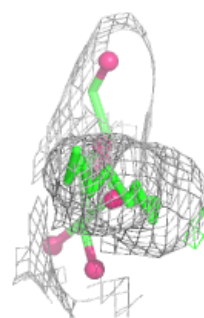
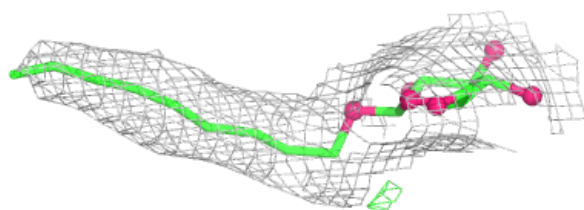
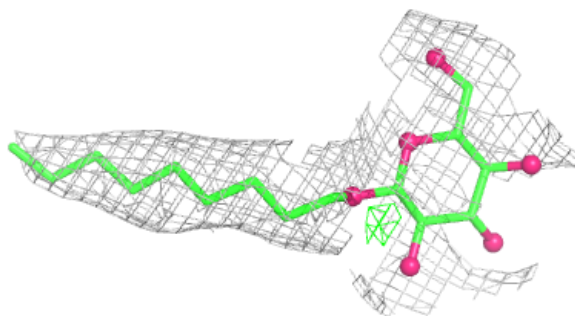
Electron density around PO4 B 601:

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

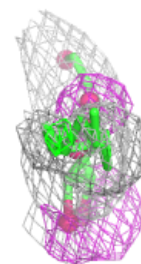
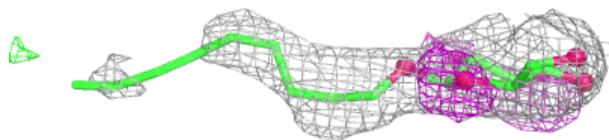
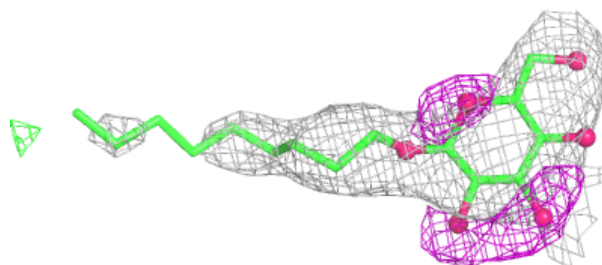


Electron density around BNG A 604:

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

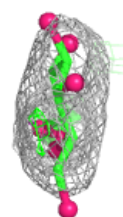
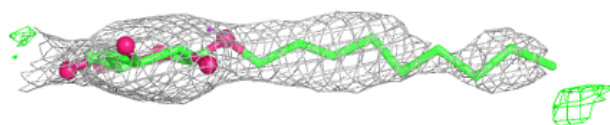
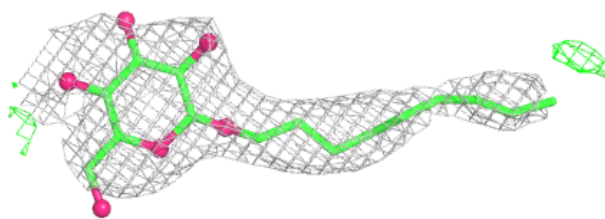
**Electron density around BNG B 603:**

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

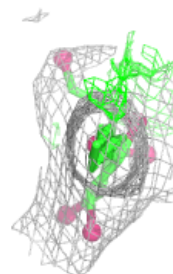
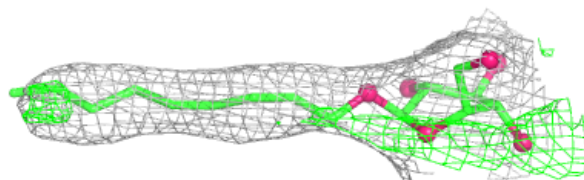
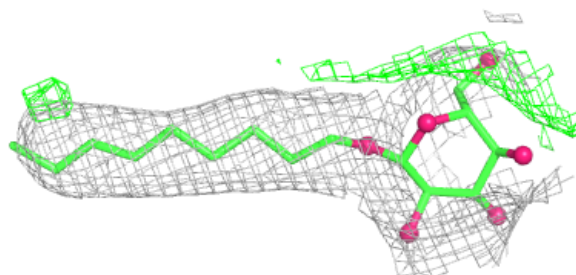


Electron density around BNG B 602:

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and green (positive)

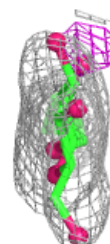
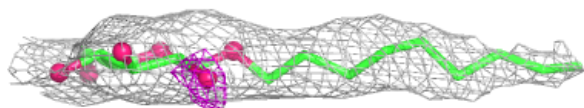
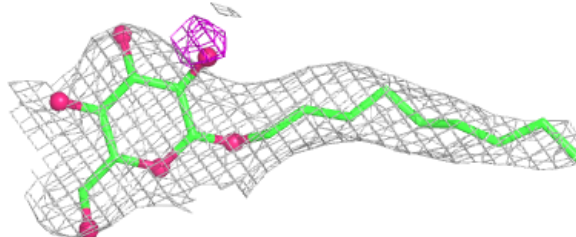
**Electron density around BNG A 603:**

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



Electron density around BNG A 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.