



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:28 AM UTC

PDB ID : 2DKD / pdb_00002dkd
Title : Crystal structure of N-acetylglucosamine-phosphate mutase, a member of the alpha-D-phosphohexomutase superfamily, in the product complex
Authors : Nishitani, Y.; Maruyama, D.; Nonaka, T.; Kita, A.; Fukami, T.A.; Mio, T.; Yamada-Okabe, H.; Yamada-Okabe, T.; Miki, K.
Deposited on : 2006-04-07
Resolution : 2.10 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)
Xtrriage (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

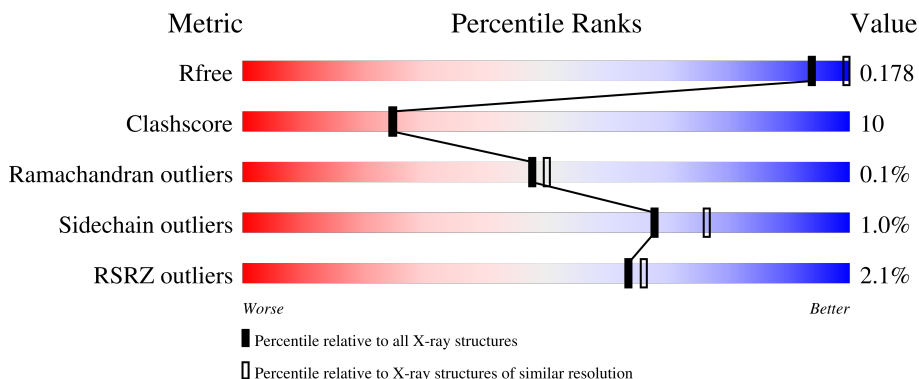
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


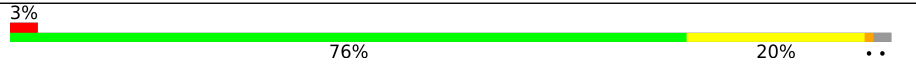
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	544	 78% 19% ..
1	B	544	 76% 20% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NG1	A	901	X	-	-	-
2	NG1	B	902	X	-	-	-

2 Entry composition [i](#)

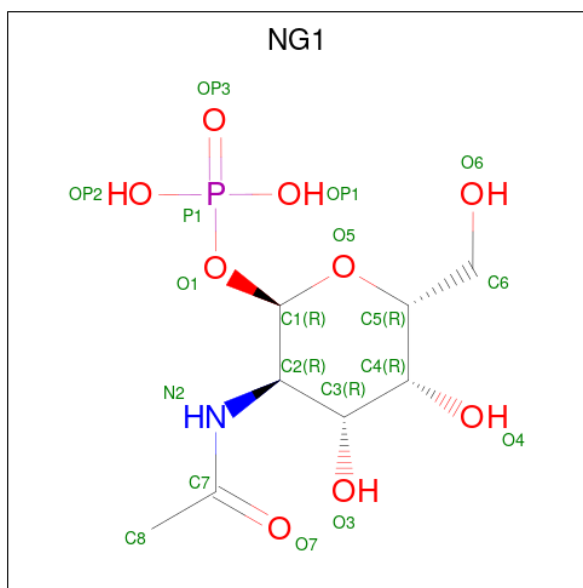
There are 5 unique types of molecules in this entry. The entry contains 9296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoacetylglucosamine mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	Total 4183	C 2662	N 691	O 821	S 9	0	0	0
1	B	535	Total 4173	C 2654	N 688	O 823	S 8	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-1-O-phosphono-alpha-D-galactopyranose (CCD ID: NG1) (formula: C₈H₁₆NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 19	C 8	N 1	O 9	P 1	0	0
2	B	1	Total 19	C 8	N 1	O 9	P 1	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	454	Total O 454 454	0	0
5	B	436	Total O 436 436	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.19Å 129.52Å 81.25Å 90.00° 109.22° 90.00°	Depositor
Resolution (Å)	36.59 – 2.10 36.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.59-2.10) 98.5 (36.59-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.181 , 0.225 0.183 , 0.178	Depositor DCC
R_{free} test set	3367 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9296	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: NG1, PO4, ZN

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	0.38	0/4268	0.88	11/5800 (0.2%)
1	B	0.38	0/4257	0.90	14/5787 (0.2%)
All	All	0.38	0/8525	0.89	25/11587 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	VAL	N-CA-C	-7.22	97.96	108.71
1	B	291	GLY	N-CA-C	6.93	121.29	112.83
1	A	314	LYS	N-CA-C	-6.71	104.04	111.82
1	A	452	SER	N-CA-C	-6.59	101.53	110.36
1	A	387	GLU	N-CA-C	-6.55	99.62	110.17
1	B	452	SER	N-CA-C	-6.24	102.23	110.40
1	B	290	ASP	N-CA-C	-6.16	100.87	110.17
1	B	171	THR	N-CA-C	-6.08	102.35	110.55
1	A	291	GLY	N-CA-C	6.00	119.90	112.64
1	B	387	GLU	N-CA-C	-6.00	100.52	110.17
1	B	314	LYS	N-CA-C	-5.93	104.94	111.82
1	A	171	THR	N-CA-C	-5.89	102.60	110.55
1	A	290	ASP	N-CA-C	-5.87	101.31	110.17
1	B	154	ASP	N-CA-C	-5.75	105.14	111.82
1	B	280	PRO	N-CA-C	5.75	120.36	111.21
1	A	245	SER	N-CA-C	-5.48	100.47	109.40
1	A	381	ASP	N-CA-C	-5.41	105.47	111.36
1	A	244	ILE	N-CA-C	5.38	116.48	108.46
1	B	221	ILE	N-CA-C	5.26	115.54	108.17
1	B	244	ILE	N-CA-C	5.25	116.22	108.45
1	A	69	PRO	CA-C-N	5.21	126.35	119.84
1	A	69	PRO	C-N-CA	5.21	126.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLN	CA-C-N	5.10	125.39	119.47
1	B	255	GLN	C-N-CA	5.10	125.39	119.47
1	B	311	ASP	N-CA-C	5.07	117.70	109.79

There are no chirality outliers.

There are no planarity outliers.

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	4183	0	4138	78	0
1	B	4173	0	4113	87	0
2	A	19	0	14	0	0
2	B	19	0	14	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	454	0	0	6	0
5	B	436	0	0	8	0
All	All	9296	0	8279	163	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 10.

All (163) 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:338:ASN:HD21	1:B:381:ASP:H	1.05	0.92
1:A:397:ASN:OD1	1:A:399:GLU:HG2	1.70	0.90
1:B:338:ASN:C	1:B:338:ASN:HD22	1.81	0.89
1:A:338:ASN:HD21	1:A:381:ASP:H	1.22	0.86
1:B:338:ASN:ND2	1:B:381:ASP:H	1.74	0.84
1:B:20:VAL:HG12	1:B:21:THR:H	1.46	0.81
1:A:338:ASN:HD22	1:A:338:ASN:C	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLN:O	1:A:533:GLU:HG2	1.84	0.77
1:B:348:ASN:HD21	1:B:463:LEU:H	1.30	0.76
1:A:475:ARG:HE	1:A:518:ASP:HA	1.52	0.74
1:A:482:ASN:HD21	1:A:485:ARG:HH21	1.32	0.74
1:A:338:ASN:ND2	1:A:381:ASP:H	1.87	0.72
1:B:482:ASN:ND2	1:B:485:ARG:HH21	1.89	0.70
1:B:482:ASN:HD21	1:B:485:ARG:HH21	1.40	0.70
1:A:482:ASN:ND2	1:A:485:ARG:HH21	1.91	0.68
1:B:338:ASN:HD21	1:B:381:ASP:N	1.85	0.68
1:B:20:VAL:HG12	1:B:21:THR:N	2.09	0.68
1:B:32:LYS:HD3	1:B:72:ASP:OD1	1.95	0.67
1:B:411:ASN:ND2	1:B:413:ASN:HB2	2.10	0.67
1:B:221:ILE:HD13	1:B:232:ILE:HG12	1.77	0.66
1:A:348:ASN:HD21	1:A:463:LEU:H	1.44	0.66
1:B:342:VAL:HG12	1:B:373:LEU:HD23	1.77	0.65
1:A:204:GLN:O	1:A:208:THR:HG23	1.97	0.65
1:A:136:VAL:HG12	1:A:165:GLN:HB3	1.80	0.64
1:A:276:LYS:HG2	1:A:277:ASN:OD1	1.99	0.62
1:A:12:PRO:HG2	5:A:1325:HOH:O	2.00	0.62
1:B:273:LYS:HB2	1:B:273:LYS:NZ	2.14	0.62
1:A:32:LYS:HD3	1:A:72:ASP:OD1	2.00	0.61
1:A:241:HIS:HB3	5:A:1238:HOH:O	2.01	0.60
1:B:331:ASP:OD1	1:B:333:THR:HG22	2.02	0.60
1:A:310:LEU:HA	1:A:314:LYS:HG3	1.83	0.60
1:B:31:MET:HE2	1:B:35:LYS:HB2	1.83	0.60
1:B:163:LYS:N	1:B:163:LYS:HD2	2.18	0.59
1:B:411:ASN:HD21	1:B:413:ASN:HB2	1.67	0.59
1:B:348:ASN:HD22	1:B:350:SER:H	1.50	0.58
1:B:355:VAL:HG11	1:B:363:VAL:HG22	1.86	0.58
1:B:254:LYS:HB2	5:B:947:HOH:O	2.04	0.57
1:A:370:VAL:HG11	1:A:391:HIS:CD2	2.39	0.57
1:B:348:ASN:ND2	1:B:463:LEU:H	2.02	0.57
1:B:11:LEU:N	1:B:12:PRO:HD2	2.19	0.57
1:A:282:ASN:ND2	1:A:301:GLN:HE21	2.03	0.57
1:A:338:ASN:C	1:A:338:ASN:ND2	2.62	0.56
1:B:282:ASN:ND2	1:B:301:GLN:HE21	2.04	0.56
1:B:280:PRO:HA	1:B:286:TYR:OH	2.06	0.56
1:A:327:PHE:HA	1:A:330:ILE:HG12	1.89	0.55
1:A:86:GLU:OE1	1:B:375:HIS:HE1	1.89	0.55
1:A:476:SER:O	1:A:479:LYS:HE3	2.06	0.55
1:A:496:GLU:HG2	1:A:542:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HB3	5:A:927:HOH:O	2.07	0.54
1:B:370:VAL:HG11	1:B:391:HIS:CD2	2.41	0.54
1:B:34:ASP:OD1	1:B:35:LYS:HG3	2.08	0.54
1:B:368:THR:HG22	5:B:1331:HOH:O	2.09	0.53
1:B:162:THR:C	1:B:163:LYS:HD2	2.33	0.53
1:B:399:GLU:HB2	5:B:1350:HOH:O	2.09	0.52
1:B:147:ALA:HA	1:B:150:MET:HE3	1.91	0.52
1:B:274:LEU:HD11	1:B:280:PRO:HG3	1.92	0.52
1:B:482:ASN:HD21	1:B:485:ARG:NH2	2.07	0.52
1:A:169:LEU:HD22	1:A:227:VAL:HG23	1.92	0.52
1:B:31:MET:HE2	1:B:35:LYS:CB	2.40	0.52
1:B:138:ALA:HB1	1:B:170:PHE:HB2	1.91	0.52
1:A:434:ASP:HB3	1:A:437:SER:HB3	1.92	0.51
1:B:68:ASN:HB3	1:B:69:PRO:HD2	1.92	0.51
1:B:338:ASN:C	1:B:338:ASN:ND2	2.54	0.51
1:A:534:GLU:HA	1:A:537:LYS:CE	2.41	0.51
1:B:65:ALA:HB3	1:B:142:ARG:CZ	2.41	0.51
1:B:434:ASP:HB3	1:B:437:SER:HB3	1.93	0.51
1:B:310:LEU:HA	1:B:314:LYS:HG3	1.93	0.50
1:B:355:VAL:CG1	1:B:363:VAL:HG22	2.41	0.50
1:A:411:ASN:ND2	1:A:414:GLU:H	2.09	0.50
1:B:411:ASN:HD22	1:B:413:ASN:H	1.59	0.50
1:A:11:LEU:N	1:A:12:PRO:HD2	2.27	0.50
1:A:410:ASN:C	1:A:410:ASN:HD22	2.19	0.49
1:A:501:VAL:HG13	1:A:507:GLY:C	2.37	0.49
1:B:36:LEU:HD23	1:B:148:LEU:HD13	1.94	0.49
1:A:31:MET:O	1:A:72:ASP:HB3	2.13	0.49
1:B:495:ASP:O	1:B:499:LYS:HG3	2.12	0.49
1:A:534:GLU:HA	1:A:537:LYS:HE2	1.94	0.49
1:A:38:TYR:O	1:A:41:PHE:HB3	2.13	0.49
1:A:348:ASN:ND2	1:A:350:SER:H	2.10	0.49
1:A:327:PHE:O	1:A:330:ILE:HG12	2.13	0.49
1:A:65:ALA:HB3	1:A:142:ARG:CZ	2.43	0.48
1:B:20:VAL:CG1	1:B:21:THR:H	2.22	0.48
1:B:102:SER:OG	1:B:103:PRO:HD2	2.13	0.48
1:B:115:VAL:O	1:B:119:LYS:HG3	2.12	0.48
1:B:22:PHE:HE2	1:B:31:MET:HE1	1.78	0.48
1:A:335:ILE:HG13	1:A:337:LEU:HG	1.95	0.48
1:A:432:VAL:HG22	1:A:433:GLY:N	2.29	0.48
1:A:125:LEU:O	1:A:126:LYS:HB2	2.14	0.48
1:A:274:LEU:CD1	1:A:280:PRO:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:O	1:B:208:THR:HG23	2.14	0.48
1:B:416:LYS:O	1:B:420:VAL:HG23	2.14	0.47
1:A:138:ALA:HB1	1:A:170:PHE:HB2	1.96	0.47
1:A:276:LYS:O	1:A:277:ASN:HB2	2.14	0.47
1:B:282:ASN:HD21	1:B:301:GLN:HE21	1.62	0.47
1:B:272:GLN:HB3	5:B:1203:HOH:O	2.15	0.47
1:A:463:LEU:O	1:A:464:PRO:C	2.56	0.47
1:A:136:VAL:HG11	1:A:182:LEU:CD1	2.45	0.46
1:A:409:PRO:HB3	1:A:414:GLU:HG2	1.98	0.46
1:A:464:PRO:HD2	1:A:526:ALA:O	2.15	0.46
1:A:180:ARG:HG3	1:A:180:ARG:HH11	1.81	0.46
1:A:368:THR:HG22	5:A:1034:HOH:O	2.15	0.46
1:B:273:LYS:HB2	1:B:273:LYS:HZ3	1.80	0.46
1:B:489:GLU:HA	1:B:490:PRO:C	2.41	0.46
1:B:331:ASP:CG	1:B:333:THR:HG22	2.40	0.45
1:A:414:GLU:O	1:A:418:ILE:HG12	2.17	0.45
1:B:212:SER:C	1:B:214:ASN:H	2.24	0.45
1:A:475:ARG:NE	1:A:518:ASP:HA	2.25	0.45
1:A:268:VAL:HG23	1:A:297:ILE:HG21	1.99	0.44
1:A:530:ASN:O	1:A:534:GLU:HG2	2.17	0.44
1:A:348:ASN:HD22	1:A:350:SER:H	1.65	0.44
1:B:205:GLU:HB3	1:B:423:ASN:ND2	2.32	0.44
1:B:331:ASP:HA	1:B:332:PRO:HD2	1.91	0.44
1:A:65:ALA:HB2	1:A:73:ASN:HA	1.99	0.44
1:B:20:VAL:CG1	1:B:21:THR:N	2.79	0.44
1:A:171:THR:HG23	1:A:231:LYS:HG3	1.99	0.44
1:B:38:TYR:O	1:B:41:PHE:HB3	2.17	0.44
1:A:266:ASP:OD1	1:A:295:ARG:NH1	2.51	0.44
1:B:113:SER:HB3	1:B:116:GLU:HG2	2.00	0.44
1:B:287:ALA:HB1	1:B:296:LEU:HD11	2.00	0.44
1:B:135:VAL:O	1:B:164:TYR:HA	2.18	0.44
1:B:361:ILE:HD11	5:B:1232:HOH:O	2.18	0.44
1:A:43:VAL:O	1:A:46:ILE:HG22	2.18	0.43
1:B:25:GLY:C	1:B:27:ALA:H	2.25	0.43
1:B:257:ASN:HB3	5:B:1188:HOH:O	2.17	0.43
1:A:537:LYS:HG3	5:A:1257:HOH:O	2.17	0.43
1:B:475:ARG:NH1	5:B:1048:HOH:O	2.51	0.43
1:A:464:PRO:HB3	1:A:529:GLN:NE2	2.34	0.43
1:B:43:VAL:O	1:B:46:ILE:HG22	2.18	0.43
1:B:327:PHE:HA	1:B:330:ILE:HG12	2.00	0.43
1:B:348:ASN:ND2	1:B:350:SER:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ILE:HD12	5:B:1033:HOH:O	2.17	0.43
1:B:441:ALA:O	1:B:445:VAL:HG23	2.18	0.43
1:B:145:SER:HB2	1:B:146:PRO:HD3	2.01	0.43
1:A:135:VAL:O	1:A:164:TYR:HA	2.19	0.43
1:A:361:ILE:HG23	1:A:362:PRO:HD2	1.99	0.43
1:B:472:VAL:HB	1:B:473:PRO:HD2	2.01	0.42
1:A:409:PRO:HG2	1:A:415:ALA:HA	2.00	0.42
1:A:224:ALA:HA	1:A:263:CYS:SG	2.59	0.42
1:B:488:VAL:HG12	1:B:489:GLU:HG3	2.01	0.42
1:B:276:LYS:O	1:B:277:ASN:HB2	2.19	0.42
1:B:463:LEU:O	1:B:464:PRO:C	2.60	0.42
1:A:413:ASN:HB2	5:A:1349:HOH:O	2.20	0.42
1:B:172:THR:HB	1:B:173:PRO:HD3	2.03	0.41
1:B:201:LYS:O	1:B:205:GLU:HG2	2.19	0.41
1:A:441:ALA:O	1:A:445:VAL:HG23	2.20	0.41
1:A:489:GLU:HA	1:A:490:PRO:C	2.46	0.41
1:B:370:VAL:HG11	1:B:391:HIS:HD2	1.85	0.41
1:A:115:VAL:O	1:A:119:LYS:HG3	2.20	0.41
1:A:465:ASN:HA	1:A:532:VAL:HG21	2.03	0.41
1:A:348:ASN:ND2	1:A:463:LEU:H	2.14	0.41
1:B:353:LYS:HE3	1:B:353:LYS:HB3	1.91	0.41
1:A:279:LYS:HA	1:A:280:PRO:HD2	1.85	0.40
1:A:370:VAL:CG1	1:A:391:HIS:CD2	3.03	0.40
1:B:327:PHE:CE1	1:B:339:ILE:HD11	2.56	0.40
1:A:175:LEU:C	1:A:175:LEU:HD13	2.46	0.40
1:A:212:SER:C	1:A:214:ASN:H	2.28	0.40
1:A:356:GLU:OE2	1:B:126:LYS:HE3	2.21	0.40
1:A:456:TRP:CD1	1:A:456:TRP:C	2.99	0.40
1:B:255:GLN:HA	1:B:256:PRO:HD2	1.86	0.40
1:B:370:VAL:CG1	1:B:391:HIS:HD2	2.35	0.40
1:A:530:ASN:O	1:A:533:GLU:HB2	2.22	0.40
1:B:411:ASN:OD1	1:B:414:GLU:HG3	2.21	0.40
1:A:36:LEU:HD23	1:A:148:LEU:HD13	2.04	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	532/544 (98%)	514 (97%)	17 (3%)	1 (0%)	43	44
1	B	529/544 (97%)	510 (96%)	19 (4%)	0	100	100
All	All	1061/1088 (98%)	1024 (96%)	36 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ASP

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	466/480 (97%)	461 (99%)	5 (1%)	65	74
1	B	465/480 (97%)	461 (99%)	4 (1%)	70	78
All	All	931/960 (97%)	922 (99%)	9 (1%)	68	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	PHE
1	A	338	ASN
1	A	343	GLN
1	A	410	ASN
1	A	534	GLU

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Mol	Chain	Res	Type
1	B	170	PHE
1	B	273	LYS
1	B	338	ASN
1	B	464	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	112	ASN
1	A	257	ASN
1	A	260	ASN
1	A	271	ASN
1	A	282	ASN
1	A	338	ASN
1	A	343	GLN
1	A	348	ASN
1	A	372	HIS
1	A	374	HIS
1	A	375	HIS
1	A	410	ASN
1	A	411	ASN
1	A	482	ASN
1	A	529	GLN
1	B	5	GLN
1	B	9	GLN
1	B	14	HIS
1	B	68	ASN
1	B	112	ASN
1	B	134	ASN
1	B	165	GLN
1	B	255	GLN
1	B	257	ASN
1	B	277	ASN
1	B	282	ASN
1	B	325	GLN
1	B	338	ASN
1	B	348	ASN
1	B	375	HIS
1	B	411	ASN
1	B	413	ASN
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	482	ASN
1	B	503	GLN
1	B	529	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](#)

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$
3	PO4	B	912	4	4,4,4	1.80	2 (50%)	6,6,6	0.46	0
2	NG1	B	902	-	18,19,19	1.76	6 (33%)	28,28,28	0.98	1 (3%)
2	NG1	A	901	-	18,19,19	1.80	5 (27%)	28,28,28	1.04	1 (3%)
3	PO4	A	911	4	4,4,4	1.71	0	6,6,6	0.47	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
2	NG1	B	902	-	1/1/7/8	2/10/31/31	0/1/1/1
2	NG1	A	901	-	1/1/7/8	1/10/31/31	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	NG1	C2-N2	4.51	1.52	1.45
2	A	901	NG1	C2-N2	4.39	1.52	1.45
2	A	901	NG1	C1-C2	2.82	1.57	1.53
2	B	902	NG1	C1-C2	2.48	1.57	1.53
2	B	902	NG1	O5-C1	2.42	1.48	1.41
2	A	901	NG1	P1-OP3	2.32	1.57	1.50
2	B	902	NG1	P1-OP3	2.26	1.57	1.50
3	B	912	PO4	P-O2	-2.17	1.48	1.54
2	A	901	NG1	O5-C1	2.16	1.47	1.41
2	A	901	NG1	C3-C2	2.14	1.57	1.53
2	B	902	NG1	C3-C2	2.05	1.56	1.53
2	B	902	NG1	C4-C5	2.03	1.57	1.53
3	B	912	PO4	P-O4	-2.01	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	NG1	O5-C1-O1	-2.93	107.53	111.36
2	A	901	NG1	O5-C1-O1	-2.88	107.60	111.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	901	NG1	C4
2	B	902	NG1	C4

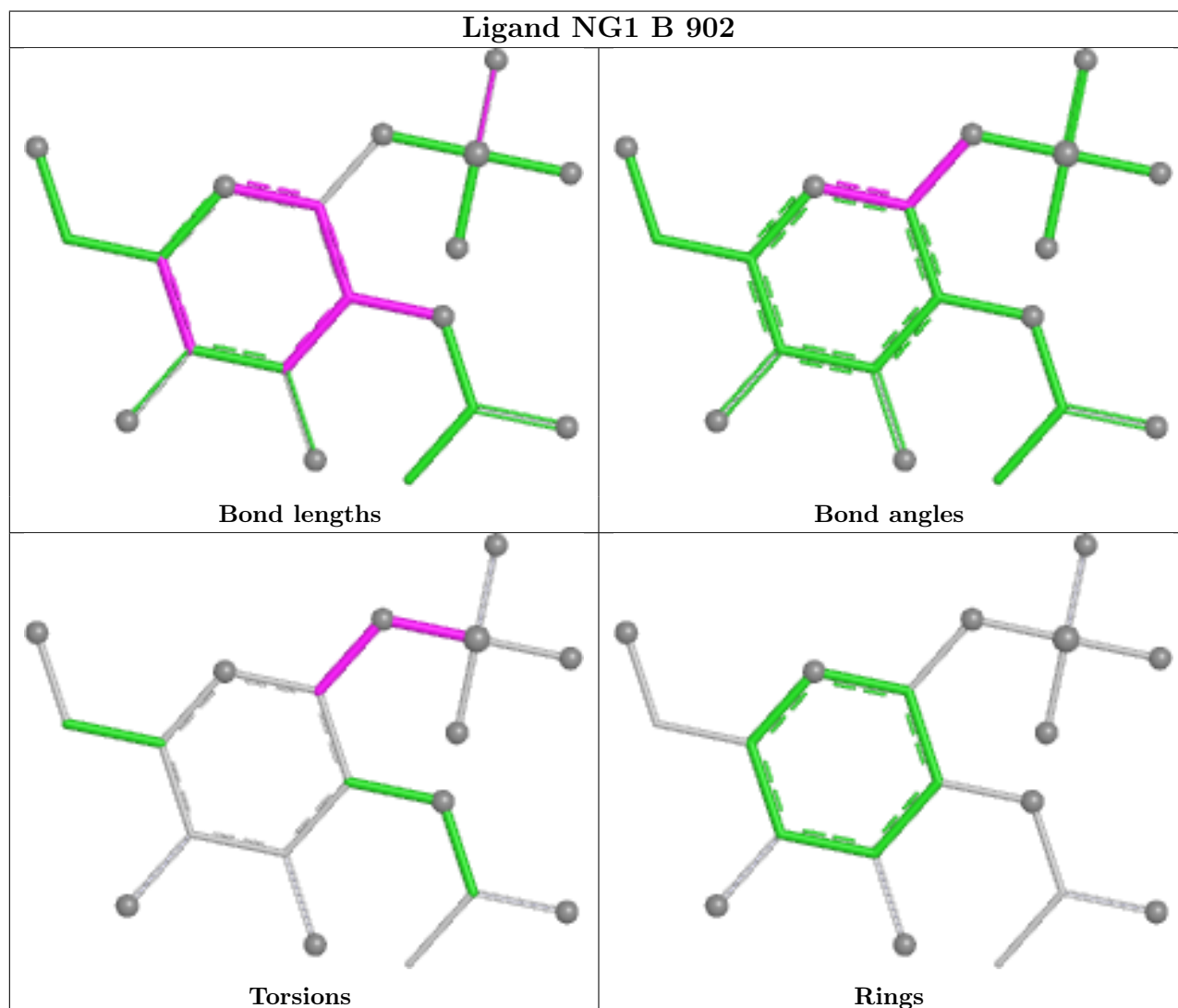
All (3) torsion outliers are listed below:

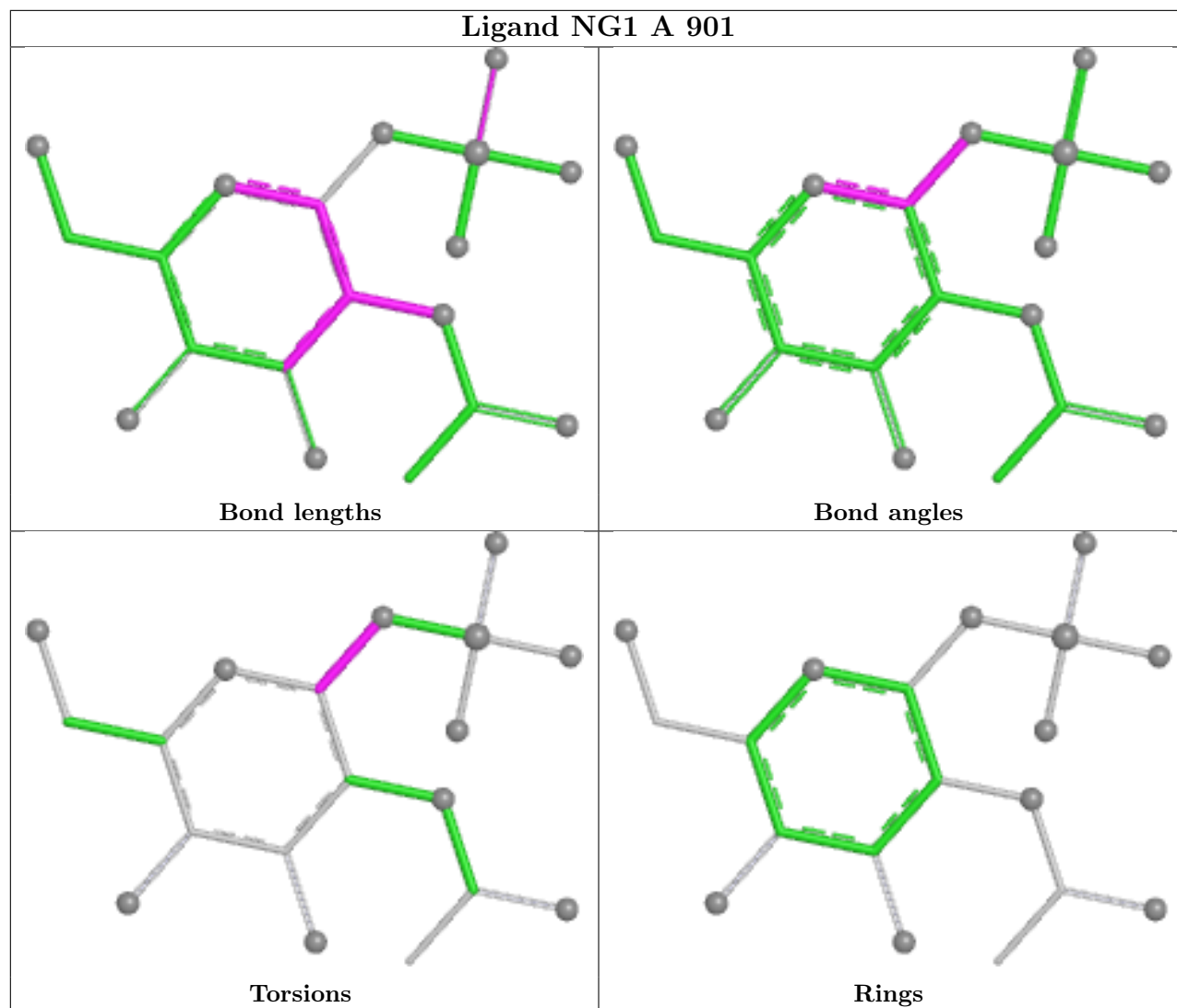
Mol	Chain	Res	Type	Atoms
2	A	901	NG1	O5-C1-O1-P1
2	B	902	NG1	O5-C1-O1-P1
2	B	902	NG1	C1-O1-P1-OP3

There are no ring outliers.

No monomer is involved in short contacts.

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	536/544 (98%)	-0.18	8 (1%) 72 74	7, 16, 39, 61	0
1	B	535/544 (98%)	-0.10	15 (2%) 55 57	7, 17, 41, 60	0
All	All	1071/1088 (98%)	-0.14	23 (2%) 63 66	7, 17, 40, 61	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	THR	5.2
1	B	20	VAL	4.9
1	A	213	ASN	4.5
1	B	18	GLN	3.8
1	B	103	PRO	3.3
1	A	214	ASN	3.2
1	A	330	ILE	3.2
1	B	17	PRO	3.1
1	B	67	HIS	2.9
1	B	333	THR	2.8
1	B	113	SER	2.6
1	B	27	ALA	2.5
1	B	26	THR	2.5
1	B	330	ILE	2.4
1	B	335	ILE	2.4
1	B	69	PRO	2.4
1	A	211	GLU	2.3
1	A	212	SER	2.3
1	A	335	ILE	2.1
1	B	35	LYS	2.1
1	B	409	PRO	2.1
1	A	409	PRO	2.0
1	B	209	ILE	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](#)

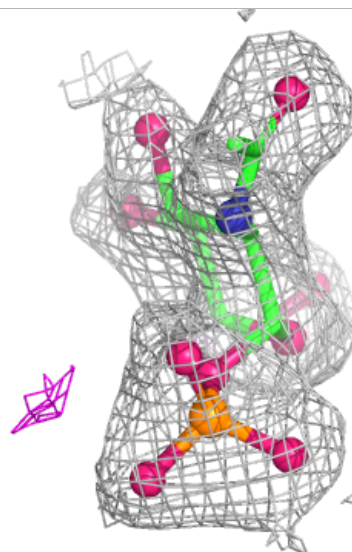
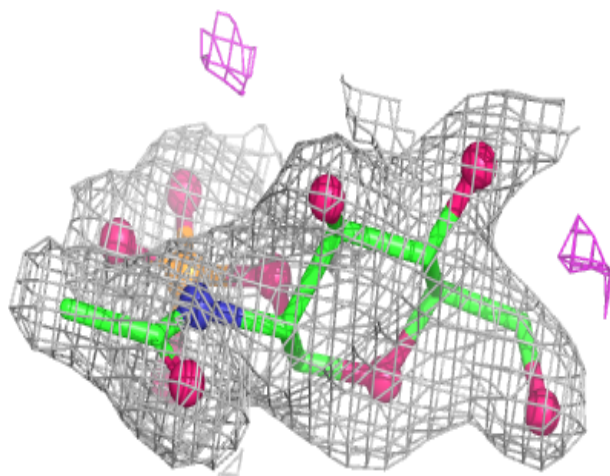
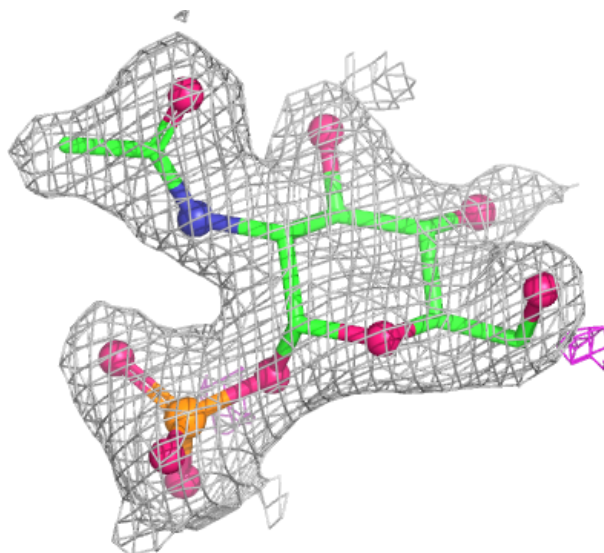
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

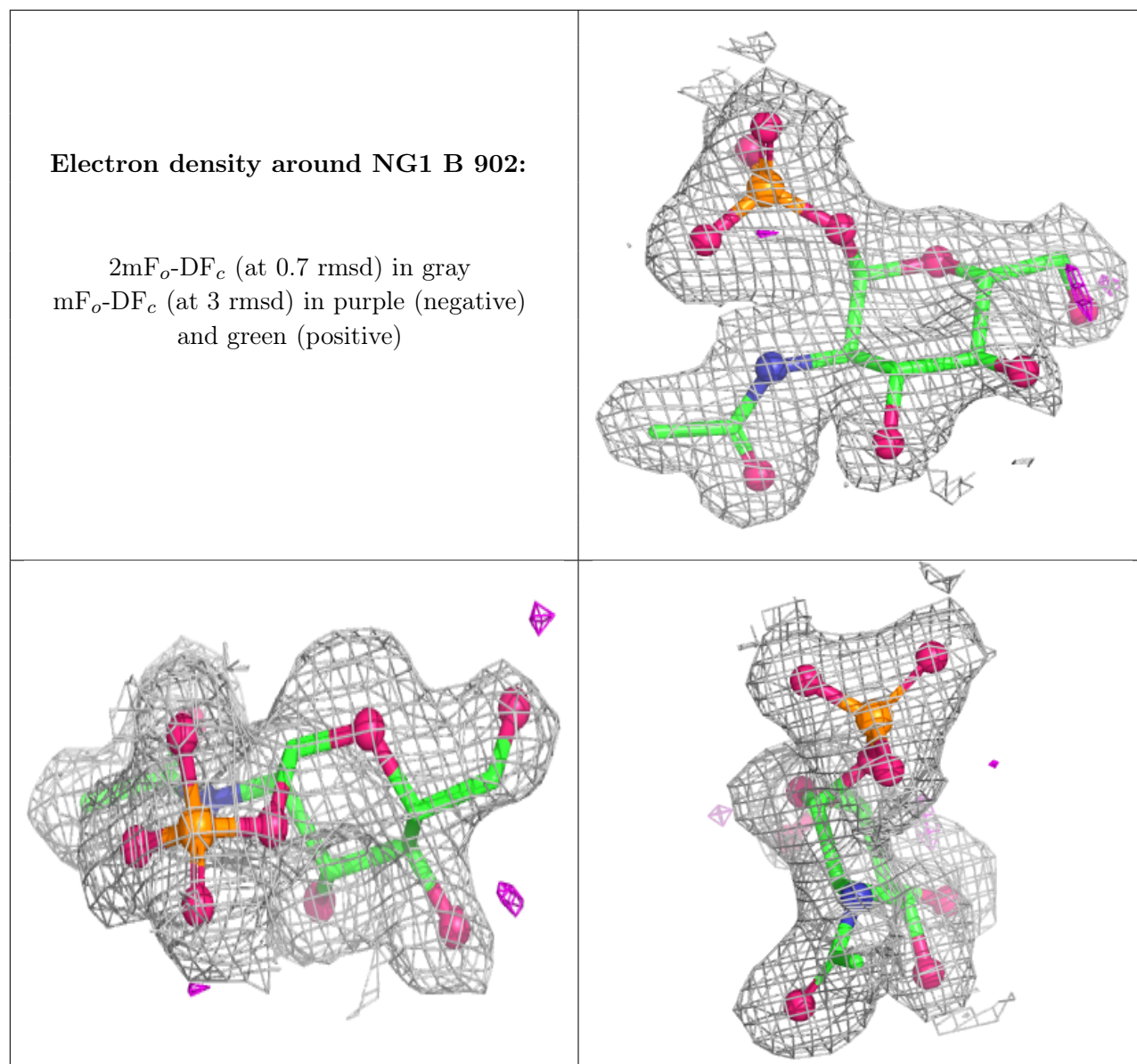
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	911	5/5	0.77	0.21	30,30,31,32	5
3	PO4	B	912	5/5	0.80	0.24	37,37,38,39	5
2	NG1	A	901	19/19	0.96	0.08	21,26,32,34	0
2	NG1	B	902	19/19	0.96	0.07	16,25,34,37	0
4	ZN	A	921	1/1	1.00	0.02	24,24,24,24	0
4	ZN	B	922	1/1	1.00	0.03	26,26,26,26	0

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 NG1 A 901:

$2mF_o-DF_c$ (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.