Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 11:49 pm GMT

PDB ID	:	2VZU
Title	:	Complex of Amycolatopsis orientalis exo-chitosanase CsxA D469A with PNP -beta-D-glucosamine
Authors	:	Lammerts van Bueren, A.; Ghinet, M.G.; Gregg, K.; Fleury, A.; Brzezinski, R.; Boraston, A.B.
Deposited on	:	2008-08-05
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:

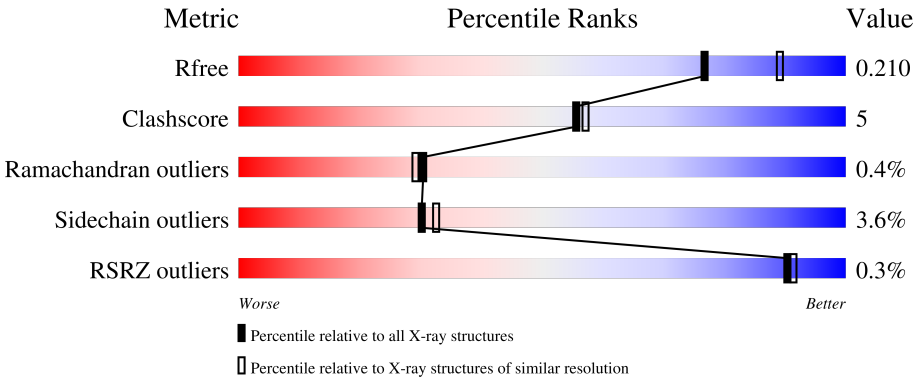
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 <=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	1032	74% 7% • 18%
1	B	1032	73% 8% • 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13943 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 EXO-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	851	Total	C	N	O	S	4	0	1
			6506	4088	1126	1275	17			
1	B	851	Total	C	N	O	S	0	0	1
			6506	4088	1126	1275	17			

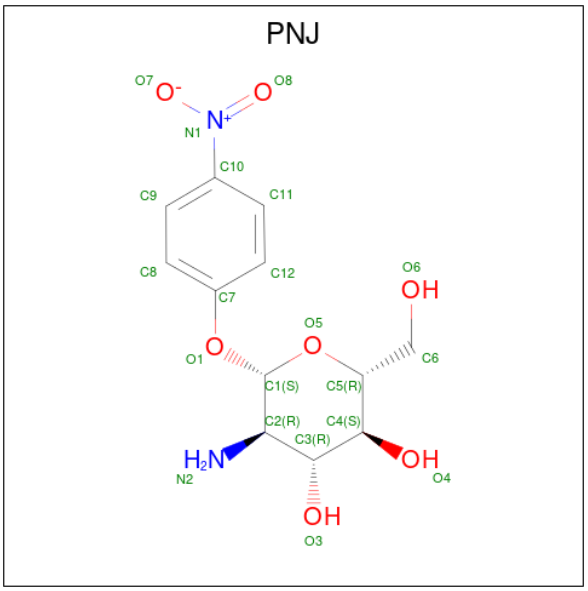
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	ALA	ASP	engineered mutation	UNP Q56F26
A	750	ASN	TRP	conflict	UNP Q56F26
B	469	ALA	ASP	engineered mutation	UNP Q56F26
B	750	ASN	TRP	conflict	UNP Q56F26

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

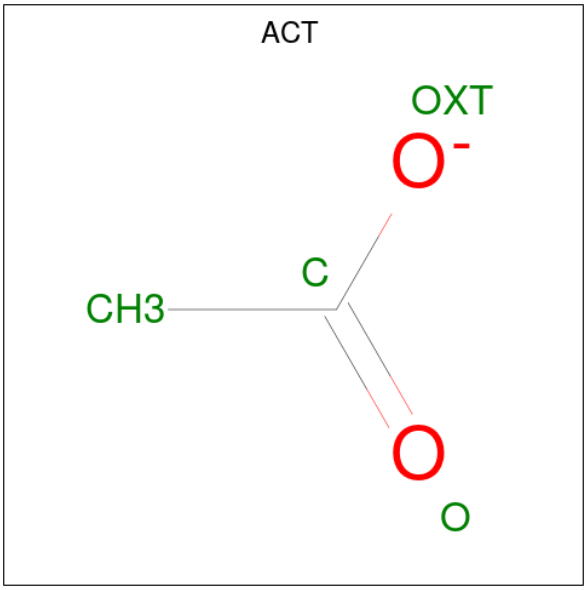
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		
2	B	4	Total	Cd	0	0
			4	4		

- Molecule 3 is 4-nitrophenyl 2-amino-2-deoxy-beta-D-glucopyranoside (three-letter code: PNJ) (formula: $C_{12}H_{16}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	12	2	7		
3	B	1	Total	C	N	O	0	0
			21	12	2	7		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

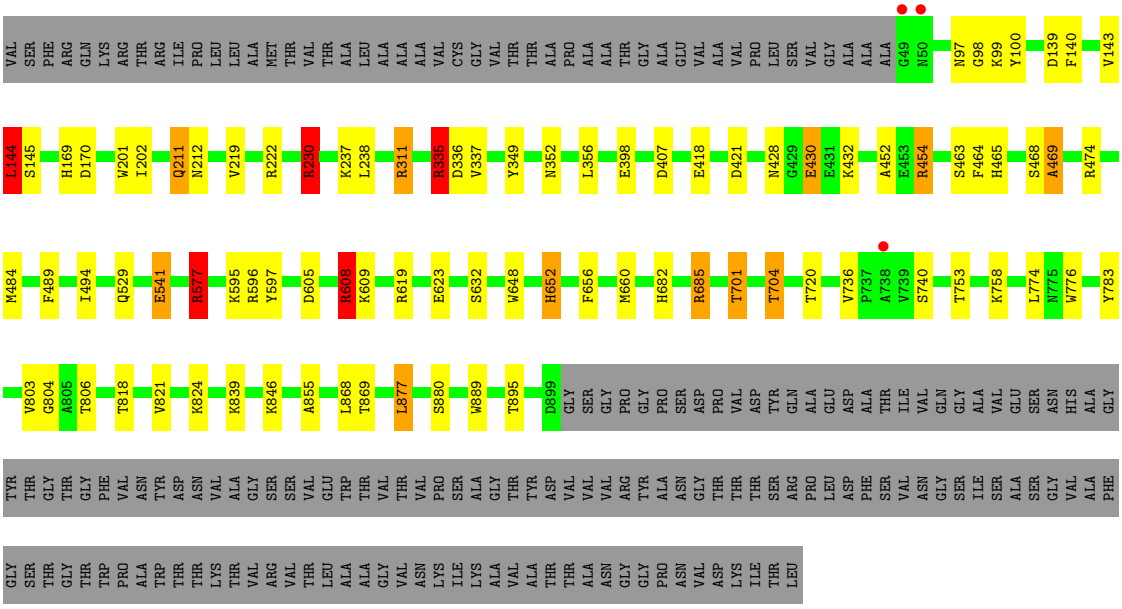
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	451	Total O 451 451	0	0
5	B	428	Total O 428 428	0	0

3 Residue-property plots (i)

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

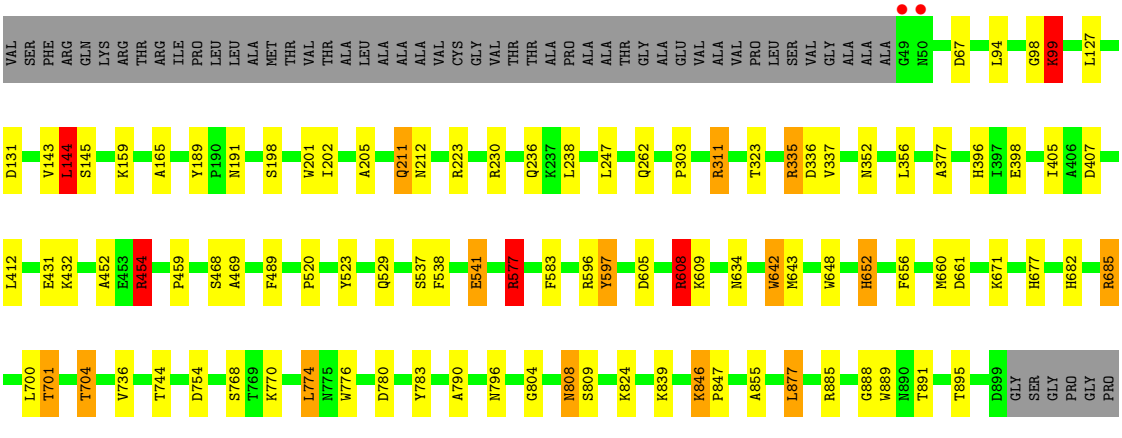
• Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain A:



• Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain B:



SER ASP PRO VAL ASP TYR GLN ALA GLU ASP ALA THR ILE VAL GLN GLY ALA VAL GLU SER ASN HIS ALA GLY TYR THR GLY THR GLY PHE VAL ASN TYR ASP ASN VAL ALA GLY SER SER VAL GLU TRP THR VAL THR VAL PRO SER ALA GLY THR TYR ASP VAL VAL VAL ARG TYR ALA

ASN GLY THR THR THR SER ARG PRO LEU ASP PHE SER VAL ASN GLY SER ILE SER ALA SER GLY VAL ALA PHE GLY SER THR GLY THR TRP PRO ALA TRP THR THR LYS THR VAL ARG VAL THR LEU ALA ALA GLY VAL ASN LYS ILE LYS ALA VAL ALA THR THR ALA ASN GLY GLY PRO

ASN VAL ASP LYS ILE THR LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.60Å 121.96Å 91.81Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.10) 99.7 (40.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.207 0.176 , 0.210	Depositor DCC
R_{free} test set	5546 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13943	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNJ, ACT, CD

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	0.83	1/6669 (0.0%)	0.88	22/9100 (0.2%)
1	B	0.85	0/6669	0.92	27/9100 (0.3%)
All	All	0.84	1/13338 (0.0%)	0.90	49/18200 (0.3%)

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	3
1	B	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	5.41	1.62	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	335	ARG	NE-CZ-NH2	-17.55	111.52	120.30
1	B	454	ARG	NE-CZ-NH2	-17.24	111.68	120.30
1	B	454	ARG	NE-CZ-NH1	16.42	128.51	120.30
1	A	577	ARG	NE-CZ-NH1	12.97	126.78	120.30
1	A	335	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	A	454	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	B	335	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	454	ARG	NE-CZ-NH2	-11.34	114.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	577	ARG	NE-CZ-NH2	-10.99	114.81	120.30
1	A	311	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	B	577	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	B	230	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	B	597	TYR	N-CA-C	8.95	135.15	111.00
1	A	597	TYR	N-CA-C	8.84	134.86	111.00
1	A	335	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	238	LEU	CA-CB-CG	7.86	133.37	115.30
1	A	230	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	608	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	311	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	577	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	774	LEU	CA-CB-CG	-7.10	98.97	115.30
1	B	238	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	230	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	469	ALA	N-CA-C	6.97	129.83	111.00
1	A	577	ARG	CD-NE-CZ	6.89	133.25	123.60
1	B	144	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	474	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	454	ARG	CD-NE-CZ	6.66	132.93	123.60
1	A	311	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	685	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	144	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	469	ALA	N-CA-C	6.14	127.58	111.00
1	B	311	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	230	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	335	ARG	CG-CD-NE	-6.03	99.13	111.80
1	A	430	GLU	CB-CG-CD	6.01	130.42	114.20
1	B	144	LEU	CB-CG-CD2	6.01	121.21	111.00
1	B	99	LYS	N-CA-C	-5.92	95.02	111.00
1	A	474	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	685	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	608	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	127	LEU	CA-CB-CG	5.32	127.54	115.30
1	B	877	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	774	LEU	CA-CB-CG	-5.18	103.38	115.30
1	B	67	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	685	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	97	ASN	C-N-CA	-5.04	111.72	122.30
1	B	454	ARG	CG-CD-NE	-5.03	101.23	111.80
1	B	608	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	SER	Peptide
1	A	596	ARG	Peptide
1	A	98	GLY	Peptide
1	B	468	SER	Peptide
1	B	596	ARG	Peptide
1	B	98	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6506	0	6287	57	0
1	B	6506	0	6287	62	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
3	A	21	0	17	1	0
3	B	21	0	17	1	0
4	B	4	0	3	0	0
5	A	451	0	0	18	0
5	B	428	0	0	15	0
All	All	13943	0	12611	119	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 (119) 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:855:ALA:HB1	5:A:2430:HOH:O	1.19	1.24
1:B:855:ALA:HB1	5:B:2406:HOH:O	1.46	1.14
1:A:821:VAL:HB	5:A:2413:HOH:O	1.46	1.12
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.10	0.97
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.05	0.93
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	2.08	0.87
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HG3	5:A:2074:HOH:O	1.82	0.79
1:B:191:ASN:O	1:B:211:GLN:HG2	1.86	0.76
1:B:656:PHE:CD1	1:B:660:MET:HE1	2.22	0.75
1:A:432:LYS:NZ	5:A:2204:HOH:O	2.19	0.74
1:B:846:LYS:HE2	5:B:2396:HOH:O	1.87	0.73
1:B:94:LEU:O	1:B:99:LYS:HB2	1.87	0.73
1:A:577:ARG:HD3	1:A:652:HIS:CG	2.22	0.73
1:B:577:ARG:HD2	1:B:652:HIS:ND1	2.04	0.73
1:B:577:ARG:HG2	1:B:583:PHE:O	1.87	0.73
1:A:311:ARG:CD	5:A:2130:HOH:O	2.37	0.71
1:B:336:ASP:H	1:B:352:ASN:ND2	1.90	0.69
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.25	0.69
1:B:398:GLU:O	1:B:454:ARG:NH2	2.27	0.67
1:A:577:ARG:HD3	1:A:652:HIS:ND1	2.11	0.66
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.63	0.63
1:A:632:SER:HB2	5:A:2324:HOH:O	1.99	0.62
1:A:311:ARG:HD2	5:A:2130:HOH:O	1.97	0.60
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.87	0.60
1:A:685:ARG:NH1	1:A:736:VAL:O	2.34	0.59
1:A:656:PHE:CD1	1:A:660:MET:HE1	2.38	0.59
1:B:605:ASP:HA	1:B:608:ARG:HD3	1.84	0.59
1:B:885:ARG:HD3	5:B:2420:HOH:O	2.02	0.59
1:B:846:LYS:HE3	1:B:847:PRO:HD2	1.85	0.59
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.68	0.58
1:B:701:THR:CG2	5:B:2338:HOH:O	2.52	0.56
1:B:311:ARG:CD	5:B:2180:HOH:O	2.53	0.56
1:A:143:VAL:HG22	5:A:2050:HOH:O	2.06	0.55
1:B:808:ASN:HD22	1:B:809:SER:H	1.54	0.55
1:A:605:ASP:HA	1:A:608:ARG:HD3	1.89	0.54
1:A:311:ARG:HD3	5:A:2130:HOH:O	2.01	0.54
1:A:701:THR:HB	1:A:720:THR:HA	1.88	0.54
1:A:452:ALA:HB1	1:A:489:PHE:HB2	1.90	0.54
1:A:804:GLY:HA3	1:A:824:LYS:O	2.08	0.54
1:B:577:ARG:HD2	1:B:652:HIS:CG	2.44	0.52
1:B:701:THR:HG22	5:B:2338:HOH:O	2.09	0.52
1:B:704:THR:CG2	5:B:2349:HOH:O	2.57	0.52
1:B:846:LYS:CE	1:B:847:PRO:HD2	2.40	0.52
1:B:520:PRO:HD2	1:B:774:LEU:HD21	1.92	0.51
1:B:311:ARG:HD3	5:B:2180:HOH:O	2.11	0.51
1:B:311:ARG:HD2	1:B:407:ASP:HB3	1.93	0.50
1:B:335:ARG:HD3	1:B:459:PRO:O	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ASP:H	1:B:352:ASN:HD22	1.58	0.50
1:A:704:THR:HG23	5:A:2373:HOH:O	2.10	0.50
1:B:529:GLN:HG3	1:B:776:TRP:CE3	2.47	0.50
1:A:222:ARG:NH2	5:A:2079:HOH:O	2.45	0.49
1:B:609:LYS:NZ	1:B:796:ASN:HD21	2.11	0.49
1:B:529:GLN:HG3	1:B:776:TRP:CD2	2.48	0.48
1:A:336:ASP:H	1:A:352:ASN:ND2	2.11	0.48
1:B:804:GLY:HA3	1:B:824:LYS:O	2.12	0.48
1:A:608:ARG:HG3	1:A:889:TRP:HZ3	1.73	0.48
1:A:704:THR:CG2	5:A:2373:HOH:O	2.61	0.48
1:B:377:ALA:HA	1:B:405:ILE:HG21	1.96	0.48
1:B:656:PHE:CD1	1:B:660:MET:CE	2.96	0.48
1:B:541:GLU:OE2	3:B:1904:PNJ:H1	2.14	0.48
1:B:396:HIS:HB2	5:B:2172:HOH:O	2.12	0.47
1:A:335:ARG:NH2	5:A:2147:HOH:O	2.43	0.47
1:A:660:MET:CE	5:A:2337:HOH:O	2.62	0.47
1:B:537:SER:OG	1:B:538:PHE:N	2.46	0.47
1:A:608:ARG:HG2	1:A:609:LYS:N	2.29	0.47
1:B:671:LYS:O	1:B:677:HIS:CE1	2.68	0.47
1:A:311:ARG:HD2	1:A:407:ASP:HB3	1.95	0.46
1:A:139:ASP:HA	1:A:169:HIS:O	2.14	0.46
1:A:541:GLU:OE2	3:A:1901:PNJ:H1	2.15	0.46
1:B:846:LYS:NZ	5:B:2397:HOH:O	2.47	0.46
1:B:144:LEU:HA	1:B:145:SER:HA	1.71	0.46
1:B:682:HIS:HE1	5:B:2291:HOH:O	1.97	0.46
1:A:398:GLU:O	1:A:454:ARG:NH2	2.44	0.45
1:B:608:ARG:HG2	1:B:609:LYS:N	2.31	0.45
1:B:311:ARG:HD2	5:B:2180:HOH:O	2.14	0.44
1:B:609:LYS:HZ1	1:B:796:ASN:HD21	1.64	0.44
1:B:144:LEU:HD22	1:B:165:ALA:CB	2.48	0.44
1:B:685:ARG:HD2	1:B:736:VAL:O	2.18	0.44
1:B:701:THR:HG23	5:B:2338:HOH:O	2.17	0.44
1:B:770:LYS:O	1:B:790:ALA:HA	2.18	0.44
1:A:99:LYS:HD3	1:A:100:TYR:CE2	2.53	0.43
1:A:144:LEU:HA	1:A:145:SER:HA	1.81	0.43
1:A:619:ARG:O	1:A:623:GLU:HG3	2.18	0.43
1:B:452:ALA:HB1	1:B:489:PHE:HB2	2.00	0.43
1:B:144:LEU:HD22	1:B:165:ALA:HB2	2.00	0.43
1:A:595:LYS:CD	5:A:2302:HOH:O	2.67	0.43
1:A:660:MET:HE2	5:A:2337:HOH:O	2.19	0.43
1:A:577:ARG:HD3	1:A:652:HIS:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ARG:CD	1:A:652:HIS:ND1	2.82	0.43
1:B:888:GLY:HA3	1:B:891:THR:OG1	2.18	0.43
1:B:855:ALA:CB	5:B:2406:HOH:O	2.28	0.42
1:A:349:TYR:OH	1:A:494:ILE:CD1	2.67	0.42
1:A:577:ARG:HD3	1:A:652:HIS:HB3	2.00	0.42
1:A:464:PHE:HB3	1:A:484:MET:HE1	2.01	0.42
1:B:846:LYS:HE3	5:B:2260:HOH:O	2.18	0.42
1:A:418:GLU:OE2	1:A:421:ASP:OD2	2.38	0.42
1:A:463:SER:HB2	1:A:494:ILE:HD12	2.01	0.42
1:B:744:THR:O	1:B:768:SER:HA	2.20	0.42
1:A:682:HIS:HE1	5:A:2313:HOH:O	2.01	0.42
1:B:159:LYS:HD3	1:B:189:TYR:CZ	2.55	0.42
1:A:465:HIS:HD2	5:A:2225:HOH:O	2.03	0.42
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.55	0.41
1:A:803:VAL:HA	1:A:824:LYS:O	2.20	0.41
1:A:656:PHE:CE1	1:A:660:MET:HE1	2.56	0.41
1:B:609:LYS:CE	1:B:796:ASN:HD21	2.34	0.41
1:B:700:LEU:HD23	1:B:754:ASP:HA	2.02	0.41
1:A:140:PHE:HB3	1:A:219:VAL:HA	2.03	0.41
1:A:170:ASP:OD2	1:A:230:ARG:HD2	2.20	0.41
1:A:349:TYR:OH	1:A:494:ILE:HD11	2.21	0.41
1:A:753:THR:HA	1:A:758:LYS:O	2.21	0.41
1:A:818:THR:CG2	1:A:869:THR:HG23	2.50	0.40
1:A:877:LEU:HG	1:A:880:SER:O	2.21	0.40
1:B:303:PRO:HG3	1:B:412:LEU:HD21	2.03	0.40
1:A:821:VAL:CG1	1:A:868:LEU:HB2	2.51	0.40
1:B:431:GLU:HG3	1:B:432:LYS:N	2.36	0.40
1:B:523:TYR:CD2	1:B:523:TYR:C	2.94	0.40
1:B:642:TRP:HA	1:B:643:MET:HA	1.85	0.40
1:B:661:ASP:OD1	1:B:839:LYS:NZ	2.55	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	849/1032 (82%)	833 (98%)	13 (2%)	3 (0%)	30	29
1	B	849/1032 (82%)	825 (97%)	20 (2%)	4 (0%)	25	23
All	All	1698/2064 (82%)	1658 (98%)	33 (2%)	7 (0%)	30	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	ALA
1	B	597	TYR
1	A	202	ILE
1	A	541	GLU
1	B	202	ILE
1	B	541	GLU
1	B	205	ALA

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	697/832 (84%)	675 (97%)	22 (3%)	34	37
1	B	697/832 (84%)	669 (96%)	28 (4%)	27	28
All	All	1394/1664 (84%)	1344 (96%)	50 (4%)	30	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	211	GLN
1	A	230	ARG
1	A	237	LYS
1	A	335	ARG
1	A	337	VAL

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Mol	Chain	Res	Type
1	A	356	LEU
1	A	428	ASN
1	A	430	GLU
1	A	577	ARG
1	A	608	ARG
1	A	648	TRP
1	A	652	HIS
1	A	701	THR
1	A	704	THR
1	A	740	SER
1	A	783	TYR
1	A	806	THR
1	A	839	LYS
1	A	846	LYS
1	A	877	LEU
1	A	895	THR
1	B	99	LYS
1	B	131	ASP
1	B	143	VAL
1	B	144	LEU
1	B	198	SER
1	B	211	GLN
1	B	223	ARG
1	B	236	GLN
1	B	247	LEU
1	B	262	GLN
1	B	323	THR
1	B	337	VAL
1	B	356	LEU
1	B	454	ARG
1	B	577	ARG
1	B	608	ARG
1	B	634	ASN
1	B	642	TRP
1	B	648	TRP
1	B	652	HIS
1	B	701	THR
1	B	704	THR
1	B	780	ASP
1	B	783	TYR
1	B	808	ASN
1	B	846	LYS

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Mol	Chain	Res	Type
1	B	877	LEU
1	B	895	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	128	ASN
1	A	212	ASN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	682	HIS
1	A	796	ASN
1	A	808	ASN
1	B	116	GLN
1	B	176	GLN
1	B	194	ASN
1	B	212	ASN
1	B	299	ASN
1	B	352	ASN
1	B	465	HIS
1	B	682	HIS
1	B	750	ASN
1	B	796	ASN
1	B	808	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 (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	PNJ	B	1904	-	21,22,22	2.66	4 (19%)	29,31,31	1.27	3 (10%)
3	PNJ	A	1901	-	21,22,22	2.82	2 (9%)	29,31,31	1.40	4 (13%)
4	ACT	B	1903	-	3,3,3	1.17	0	3,3,3	1.42	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	PNJ	B	1904	-	-	0/8/30/30	0/2/2/2
3	PNJ	A	1901	-	-	0/8/30/30	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	PNJ	O8-N1	11.47	1.42	1.22
3	B	1904	PNJ	O8-N1	10.15	1.40	1.22
3	B	1904	PNJ	C10-N1	-4.46	1.34	1.45
3	A	1901	PNJ	C10-N1	-4.00	1.35	1.45
3	B	1904	PNJ	C1-C2	2.76	1.57	1.52
3	B	1904	PNJ	O5-C1	2.01	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1901	PNJ	O5-C5-C4	-3.31	103.69	109.69
3	A	1901	PNJ	O1-C1-C2	-3.19	102.75	107.34
3	B	1904	PNJ	C7-O1-C1	3.16	122.42	117.79
3	A	1901	PNJ	C9-C10-N1	2.64	121.36	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1904	PNJ	C11-C10-N1	2.56	121.30	119.38
3	A	1901	PNJ	C3-C2-N2	2.28	115.72	111.05
3	B	1904	PNJ	O1-C1-C2	-2.09	104.33	107.34

There are no chirality outliers.

There are no torsion outliers.

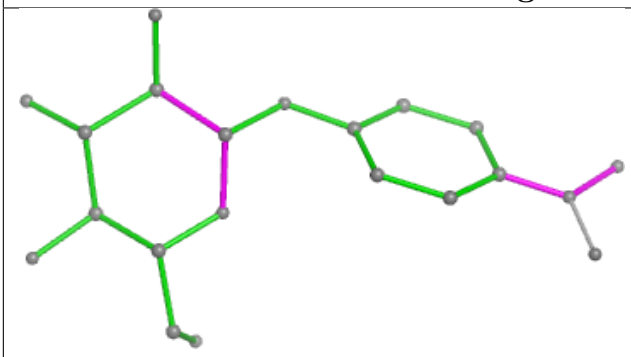
There are no ring outliers.

2 monomers are involved in 2 short contacts:

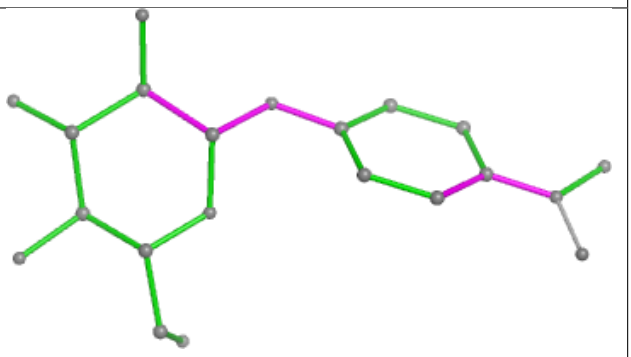
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1904	PNJ	1	0
3	A	1901	PNJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

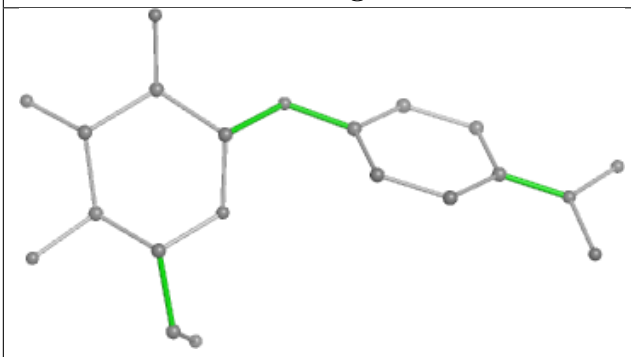
Ligand PNJ B 1904



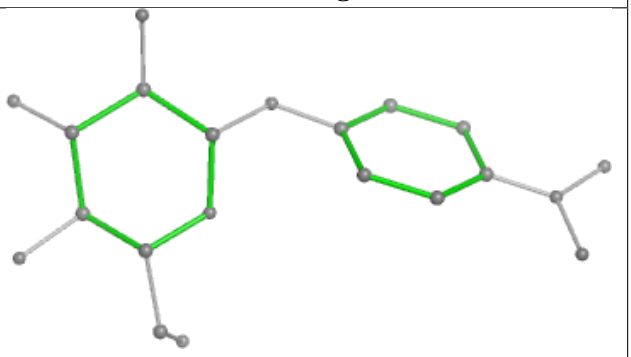
Bond lengths



Bond angles

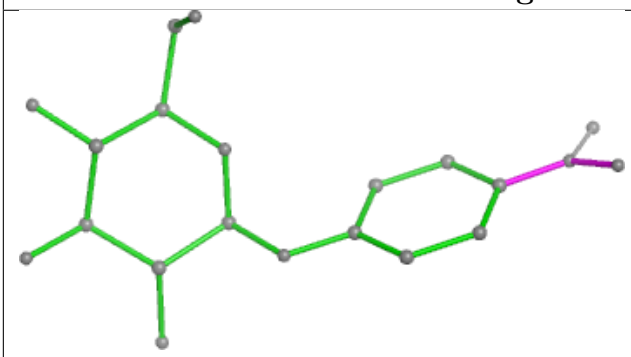


Torsions

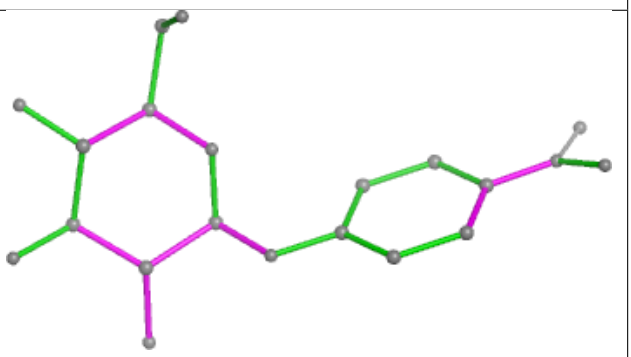


Rings

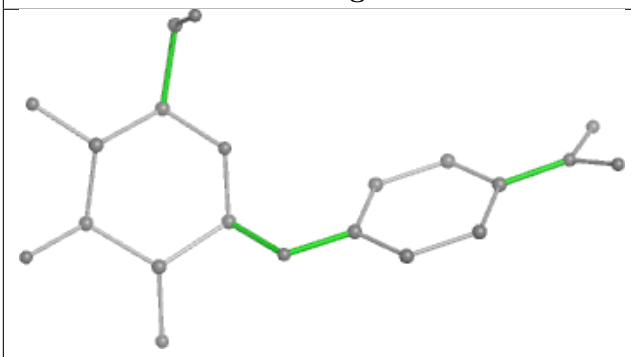
Ligand PNJ A 1901



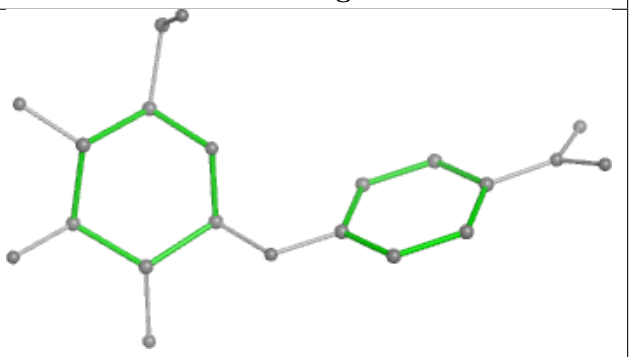
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	851/1032 (82%)	-0.70	3 (0%)	89	90	4, 11, 22, 32	1 (0%)
1	B	851/1032 (82%)	-0.67	2 (0%)	92	92	4, 11, 22, 34	0
All	All	1702/2064 (82%)	-0.69	5 (0%)	90	91	4, 11, 22, 34	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	GLY	3.3
1	B	50	ASN	2.6
1	A	738	ALA	2.5
1	A	50	ASN	2.2
1	B	49	GLY	2.1

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

There are no monosaccharides in this entry.

6.4 Ligands

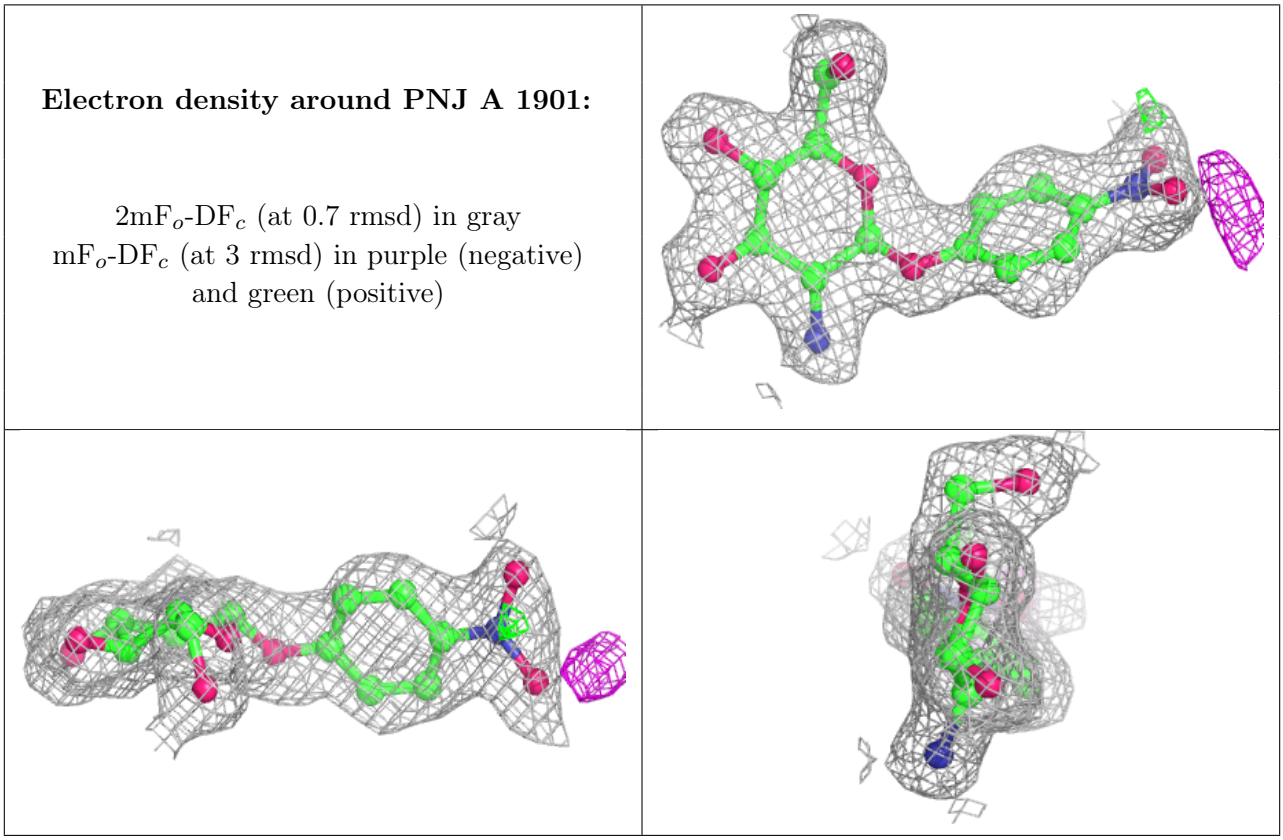
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	B	1903	4/4	0.62	0.20	17,19,20,20	0
2	CD	B	1901	1/1	0.86	0.38	203,203,203,203	0
2	CD	A	1900	1/1	0.88	0.24	117,117,117,117	0
2	CD	B	1902	1/1	0.92	0.20	97,97,97,97	0
2	CD	A	1899	1/1	0.93	0.39	99,99,99,99	0
3	PNJ	A	1901	21/21	0.96	0.06	5,10,26,28	0
3	PNJ	B	1904	21/21	0.97	0.06	5,9,23,25	0
2	CD	B	1900	1/1	1.00	0.01	10,10,10,10	0
2	CD	B	1899	1/1	1.00	0.01	10,10,10,10	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.

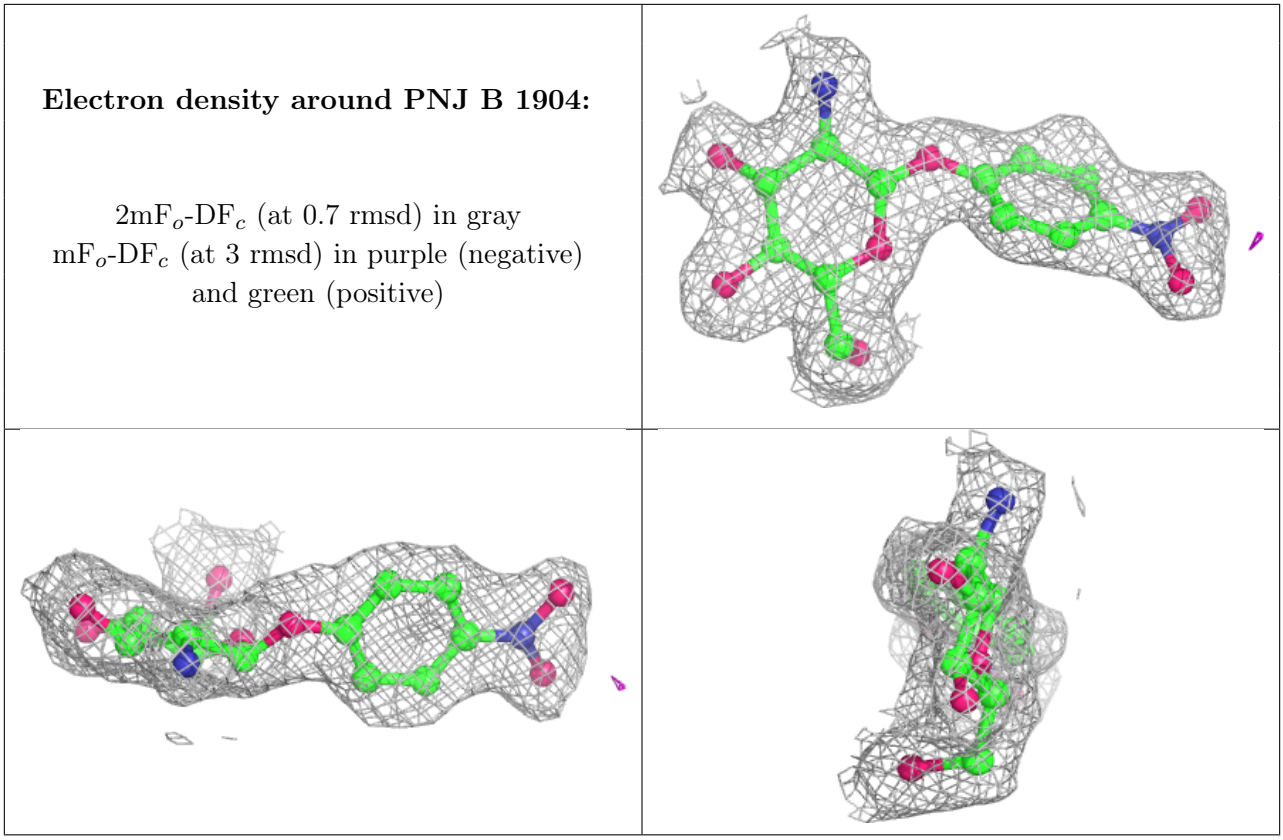
Electron density around PNJ A 1901:

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



Electron density around PNJ B 1904:

$2mF_o$-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.