



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 2VZT / pdb_00002vzt
Title : Complex of Amycolatopsis orientalis exo-chitosanase CsxA E541A 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 : 2.20 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

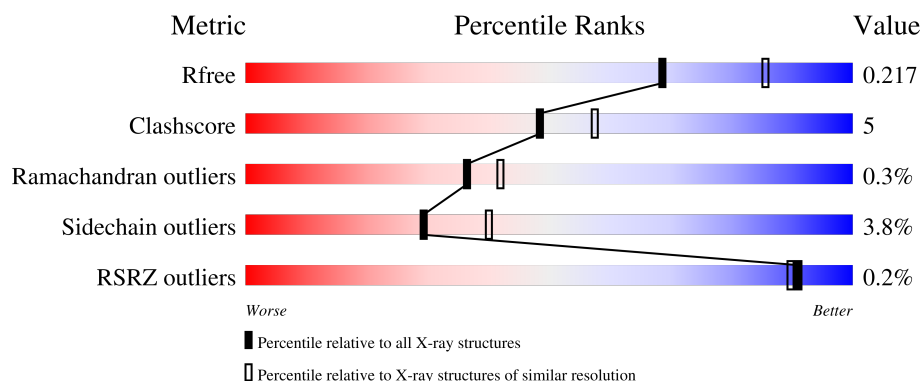
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1032	
1	B	1032	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13888 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
			6505	4087	1126	1275	17			
1	B	851	Total	C	N	O	S	0	0	1
			6505	4087	1126	1275	17			

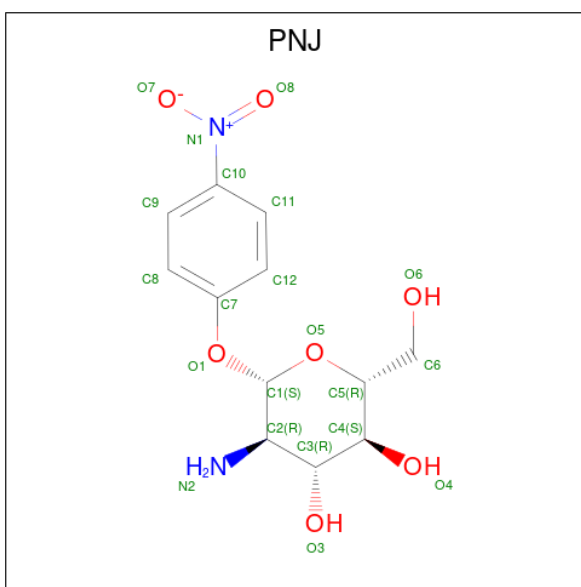
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	ALA	GLU	engineered mutation	UNP Q56F26
A	750	ASN	TRP	conflict	UNP Q56F26
B	541	ALA	GLU	engineered mutation	UNP Q56F26
B	750	ASN	TRP	conflict	UNP Q56F26

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

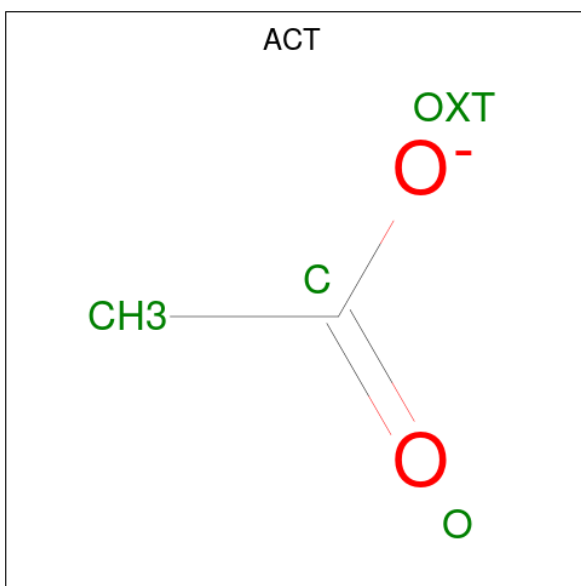
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		
2	B	4	Total	Cd	0	0
			4	4		

- Molecule 3 is 4-nitrophenyl 2-amino-2-deoxy-beta-D-glucopyranoside (CCD ID: PNJ) (formula: C₁₂H₁₆N₂O₇).



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 (CCD ID: 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	420	Total 420	O 420	0	0
5	B	406	Total 406	O 406	0	0

ALA	ASN	S827	D605
TRP	TYR		F606
THR	ASP	K839	F608
THR	ASN		G609
LYS	VAL		A610
THR	ALA	K846	Q611
VAL	GLY	P847	
ARG	SER		Q614
VAL	SER	D855	
THR	VAL		E623
LEU	GLU	K871	
ALA	TRP		N634
ALA	THR	L877	
GLY	VAL		M643
VAL	THR	R885	
ASN	VAL		H652
LYS	PRO	W889	
ILE	SER		F656
LYS	GLY	T895	
ALA	ALA	V896	
VAL	VAL	P897	Y659
ALA	THR	A960	M660
ALA	THR	D899	D661
THR	ASP		
ALA	VAL	GLY	K871
ALA	VAL	SER	
ASN	VAL	PRO	H677
GLY	ARG	GLY	
GLY	THR	TYR	H682
PRO	ALA	PRO	
ASN	ASN	SER	R685
VAL	GLY	ASP	
ASP	THR	PRO	T701
LYS	THR	VAL	
ILE	THR	ASP	T704
THR	SER	TYR	
LEU	ARG	GLN	T720
	PRO	ALA	
	LEU	GLU	
	ASP	ASP	V724
	PHE	ALA	
	SER	THR	V736
	VAL	ILE	
	ASN	VAL	T744
	GLY	GLN	
	ILE	ALA	S768
	SER	ALA	
	SER	VAL	W776
	ALA	GLU	
	SER	ASN	D780
	GLY	ASN	
	VAL	HIS	V803
	ALA	ALA	G804
	PHE	GLY	A805
	GLY	TYR	
	SER	THR	N808
	THR	GLY	S809
	GLY	THR	V810
	THR	GLY	A811
	TRP	PHE	
	PRO	VAL	V821

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 122.23Å 91.86Å 90.00° 90.52° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.00-2.20) 98.9 (40.00-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.218 0.176 , 0.217	Depositor DCC
R_{free} test set	4801 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13888	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: CD, ACT, PNJ

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	0.92	2/6668 (0.0%)	1.03	14/9099 (0.2%)
1	B	0.95	4/6668 (0.1%)	1.02	21/9099 (0.2%)
All	All	0.93	6/13336 (0.0%)	1.03	35/18198 (0.2%)

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	4
1	B	0	3
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	898	ALA	C-N	-6.25	1.24	1.33
1	A	898	ALA	C-N	-5.70	1.25	1.33
1	A	468	SER	CA-C	5.54	1.55	1.52
1	B	811	ALA	CA-CB	-5.51	1.46	1.53
1	B	896	VAL	CA-CB	5.16	1.60	1.54
1	B	803	VAL	CA-CB	5.15	1.62	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	TYR	N-CA-C	19.72	137.00	111.75
1	B	99	LYS	N-CA-C	-15.58	94.72	114.04
1	A	99	LYS	N-CA-C	-12.83	97.76	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	597	TYR	N-CA-C	11.64	135.60	110.80
1	A	432	LYS	N-CA-C	10.09	128.01	111.37
1	A	97	ASN	CA-C-N	-9.31	113.43	123.30
1	A	97	ASN	C-N-CA	-9.31	113.43	123.30
1	A	468	SER	N-CA-C	8.65	122.75	108.48
1	B	469	ASP	N-CA-C	8.55	129.01	110.80
1	A	469	ASP	N-CA-C	8.04	127.93	110.80
1	A	596	ARG	N-CA-C	7.58	122.76	112.68
1	A	430	GLU	CB-CG-CD	6.89	124.31	112.60
1	A	805	ALA	N-CA-C	6.82	120.01	108.90
1	B	596	ARG	N-CA-C	6.66	121.53	112.68
1	A	596	ARG	CA-C-N	6.56	129.96	120.38
1	A	596	ARG	C-N-CA	6.56	129.96	120.38
1	B	219	VAL	N-CA-C	-6.10	98.96	107.80
1	B	335	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	B	262	GLN	N-CA-C	-5.88	99.61	109.07
1	A	98	GLY	N-CA-C	5.68	119.66	113.58
1	B	454	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	B	803	VAL	N-CA-C	-5.53	101.05	108.35
1	B	434	GLU	CA-C-N	5.47	125.48	119.90
1	B	434	GLU	C-N-CA	5.47	125.48	119.90
1	B	803	VAL	CA-C-N	5.38	131.39	121.70
1	B	803	VAL	C-N-CA	5.38	131.39	121.70
1	B	805	ALA	N-CA-C	5.33	117.77	108.76
1	B	335	ARG	CG-CD-NE	-5.24	100.46	112.00
1	A	454	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	B	335	ARG	N-CA-C	-5.22	100.09	108.55
1	B	803	VAL	O-C-N	-5.17	117.10	123.09
1	B	97	ASN	CA-C-N	-5.05	114.65	122.69
1	B	97	ASN	C-N-CA	-5.05	114.65	122.69
1	B	143	VAL	N-CA-CB	5.05	116.75	111.00
1	B	238	LEU	CA-CB-CG	5.04	133.93	116.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	B	98	GLY	Peptide

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	6505	0	6282	62	0
1	B	6505	0	6282	78	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
3	A	21	0	17	0	0
3	B	21	0	17	0	0
4	B	4	0	3	0	0
5	A	420	0	0	10	0
5	B	406	0	0	15	0
All	All	13888	0	12601	140	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 (140) 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:109:MET:HE1	1:B:368:PHE:CE1	1.64	1.31
1:B:109:MET:CE	1:B:368:PHE:CE1	2.18	1.26
1:B:109:MET:CE	1:B:368:PHE:HE1	1.53	1.20
1:B:109:MET:HE1	1:B:368:PHE:HE1	0.93	1.06
1:A:821:VAL:HB	5:A:2385:HOH:O	1.58	1.04
1:A:201:TRP:HE1	1:A:212:ASN:HD21	1.09	0.96
1:B:201:TRP:HE1	1:B:212:ASN:HD21	1.05	0.93
1:A:608:ARG:HG3	1:A:889:TRP:CZ3	2.05	0.92
1:B:608:ARG:HG3	1:B:889:TRP:CZ3	2.06	0.90
1:B:109:MET:CE	1:B:368:PHE:CZ	2.55	0.89
1:B:109:MET:HE3	1:B:368:PHE:CZ	2.08	0.89
1:A:855:ASP:CB	5:A:2402:HOH:O	2.22	0.87
1:B:660:MET:HE3	5:B:2294:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:LYS:HE2	5:B:2378:HOH:O	1.77	0.83
1:A:204:TRP:CD1	1:A:643:MET:HE1	2.13	0.82
1:B:109:MET:HE2	1:B:209:PRO:HD3	1.59	0.82
1:A:642:TRP:NE1	1:A:643:MET:HE2	1.94	0.81
1:B:846:LYS:HE3	1:B:847:PRO:HD2	1.64	0.80
1:B:577:ARG:HG2	1:B:583:PHE:O	1.81	0.80
1:B:109:MET:HE3	1:B:368:PHE:CE1	2.13	0.80
1:A:577:ARG:HD2	1:A:652:HIS:ND1	1.97	0.78
1:B:701:THR:HG22	5:B:2323:HOH:O	1.82	0.78
1:B:191:ASN:O	1:B:211:GLN:HG2	1.85	0.77
1:B:109:MET:HE1	1:B:368:PHE:CZ	2.20	0.76
1:A:660:MET:HE3	5:A:2315:HOH:O	1.85	0.75
1:A:311:ARG:CD	5:A:2121:HOH:O	2.35	0.75
1:B:201:TRP:NE1	1:B:212:ASN:HD21	1.84	0.75
1:A:577:ARG:HG2	1:A:583:PHE:O	1.88	0.73
1:A:311:ARG:HD2	5:A:2121:HOH:O	1.87	0.73
1:B:336:ASP:H	1:B:352:ASN:ND2	1.88	0.72
1:B:94:LEU:O	1:B:99:LYS:HB2	1.90	0.71
1:B:855:ASP:CB	5:B:2304:HOH:O	2.41	0.69
1:B:656:PHE:CE1	1:B:660:MET:HE1	2.29	0.66
1:B:577:ARG:HD2	1:B:652:HIS:ND1	2.12	0.65
1:B:846:LYS:CE	1:B:847:PRO:HD2	2.26	0.65
1:B:398:GLU:O	1:B:454:ARG:NH2	2.30	0.65
1:A:846:LYS:HE3	5:A:2260:HOH:O	1.98	0.64
1:A:143:VAL:HG22	5:A:2047:HOH:O	2.01	0.61
1:A:677:HIS:HD2	1:A:679:GLN:HE21	1.48	0.61
1:A:642:TRP:CE2	1:A:643:MET:HE2	2.35	0.60
1:A:577:ARG:HD2	1:A:652:HIS:CG	2.36	0.60
1:B:808:ASN:HD22	1:B:809:SER:H	1.48	0.60
1:A:335:ARG:NH2	5:A:2132:HOH:O	2.32	0.59
1:A:204:TRP:CG	1:A:643:MET:HE1	2.38	0.58
1:B:463:SER:HB2	1:B:494:ILE:HD12	1.85	0.58
1:A:677:HIS:CD2	1:A:679:GLN:HE21	2.22	0.58
1:B:335:ARG:HA	1:B:352:ASN:HD21	1.68	0.57
1:B:885:ARG:HD3	5:B:2397:HOH:O	2.05	0.56
1:B:204:TRP:CG	1:B:643:MET:HE1	2.40	0.56
1:A:139:ASP:OD2	1:A:222:ARG:NH1	2.38	0.56
1:B:701:THR:CG2	5:B:2323:HOH:O	2.47	0.56
1:A:336:ASP:H	1:A:352:ASN:ND2	2.04	0.55
1:A:349:TYR:OH	1:A:494:ILE:HD11	2.09	0.53
1:B:144:LEU:HD22	1:B:165:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:THR:HB	1:A:720:THR:HA	1.91	0.51
1:A:201:TRP:NE1	1:A:212:ASN:HD21	1.92	0.51
1:A:656:PHE:CE1	1:A:660:MET:HE1	2.45	0.51
1:B:311:ARG:HD2	1:B:407:ASP:HB3	1.92	0.51
1:A:676:LEU:HD23	1:A:760:VAL:HG21	1.93	0.51
1:B:577:ARG:HD2	1:B:652:HIS:CG	2.46	0.51
1:B:704:THR:CG2	5:B:2333:HOH:O	2.58	0.51
1:B:531:ASP:HB2	5:B:2236:HOH:O	2.09	0.51
1:A:335:ARG:HA	1:A:352:ASN:HD21	1.75	0.50
1:B:246:ASP:HB3	1:B:292:LEU:HD11	1.94	0.50
1:A:608:ARG:HG2	1:A:609:LYS:N	2.27	0.50
1:B:605:ASP:HA	1:B:608:ARG:CD	2.41	0.50
1:A:804:GLY:HA3	1:A:824:LYS:O	2.12	0.49
1:B:685:ARG:HD2	1:B:736:VAL:O	2.13	0.49
1:A:398:GLU:O	1:A:454:ARG:NH2	2.40	0.49
1:B:448:MET:SD	1:B:484:MET:HE3	2.53	0.49
1:B:336:ASP:H	1:B:352:ASN:HD22	1.60	0.49
1:B:608:ARG:HG2	1:B:609:LYS:N	2.26	0.48
1:A:687:VAL:HG21	1:A:704:THR:HG21	1.94	0.48
1:B:605:ASP:HA	1:B:608:ARG:HD3	1.96	0.48
1:A:211:GLN:HG3	5:A:2068:HOH:O	2.13	0.48
1:A:155:LYS:HD3	1:A:158:THR:HG22	1.96	0.48
1:A:337:VAL:HG13	1:A:491:LEU:CD2	2.43	0.47
1:A:407:ASP:CG	1:A:459:PRO:HD2	2.39	0.47
1:B:839:LYS:HE3	5:B:2376:HOH:O	2.15	0.47
1:A:193:PRO:HD3	1:A:211:GLN:HG2	1.96	0.47
1:A:465:HIS:HD2	5:A:2209:HOH:O	1.98	0.47
1:A:773:THR:OG1	1:A:787:SER:OG	2.33	0.46
1:B:659:TYR:O	1:B:660:MET:HB2	2.15	0.46
1:B:682:HIS:HE1	5:B:2275:HOH:O	1.97	0.46
1:B:465:HIS:HD2	5:B:2207:HOH:O	1.98	0.46
1:B:660:MET:HA	1:B:660:MET:HE2	1.97	0.46
1:B:72:SER:O	1:B:183:SER:HB2	2.17	0.45
1:B:144:LEU:HD22	1:B:165:ALA:CB	2.46	0.45
1:A:72:SER:O	1:A:183:SER:HB2	2.16	0.45
1:B:452:ALA:HB1	1:B:489:PHE:HB2	1.98	0.45
1:B:529:GLN:HG3	1:B:776:TRP:CD2	2.52	0.45
1:A:660:MET:HE2	1:A:660:MET:HA	1.98	0.45
1:B:311:ARG:HD3	5:B:2169:HOH:O	2.16	0.45
1:B:656:PHE:CD1	1:B:660:MET:CE	3.01	0.44
1:A:468:SER:O	1:A:497:ALA:N	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.52	0.44
1:A:137:TYR:OH	1:A:256:ASP:OD2	2.30	0.44
1:A:349:TYR:OH	1:A:494:ILE:CD1	2.65	0.44
1:A:659:TYR:O	1:A:660:MET:HB2	2.16	0.44
1:B:250:LYS:HA	1:B:288:VAL:O	2.17	0.44
1:B:605:ASP:OD1	1:B:608:ARG:HD3	2.18	0.43
1:B:50:ASN:HD22	1:B:50:ASN:N	2.15	0.43
1:B:339:ALA:HB1	1:B:347:ARG:HD2	2.00	0.43
1:A:685:ARG:NH1	1:A:736:VAL:O	2.51	0.43
1:A:874:THR:O	1:A:877:LEU:HB2	2.19	0.43
1:B:377:ALA:HA	1:B:405:ILE:HG21	2.00	0.43
1:B:661:ASP:OD1	1:B:839:LYS:NZ	2.51	0.43
1:B:846:LYS:NZ	5:B:2244:HOH:O	2.52	0.43
1:A:139:ASP:HA	1:A:169:HIS:O	2.17	0.43
1:B:701:THR:HB	1:B:720:THR:HA	1.99	0.43
1:A:362:GLY:O	1:A:643:MET:HB3	2.18	0.43
1:A:377:ALA:HA	1:A:405:ILE:HG21	2.00	0.43
1:B:311:ARG:CD	5:B:2169:HOH:O	2.66	0.43
1:A:511:LYS:HE2	1:A:536:TRP:O	2.19	0.42
1:B:69:SER:HA	1:B:150:TRP:CZ3	2.53	0.42
1:B:537:SER:OG	1:B:538:PHE:N	2.47	0.42
1:B:201:TRP:HE1	1:B:212:ASN:ND2	1.90	0.42
1:A:804:GLY:O	1:A:823:LEU:HA	2.19	0.42
1:A:144:LEU:HD22	1:A:165:ALA:CB	2.49	0.42
1:A:452:ALA:HB1	1:A:489:PHE:HB2	2.02	0.42
1:B:448:MET:HE3	1:B:448:MET:HA	2.01	0.42
1:B:846:LYS:HE3	5:B:2243:HOH:O	2.17	0.42
1:B:656:PHE:CD1	1:B:660:MET:HE2	2.55	0.42
1:A:464:PHE:HB3	1:A:484:MET:HE1	2.02	0.42
1:B:548:ILE:H	1:B:614:GLN:NE2	2.18	0.42
1:B:109:MET:HE2	1:B:209:PRO:CD	2.40	0.41
1:B:335:ARG:HD3	1:B:459:PRO:O	2.19	0.41
1:B:671:LYS:O	1:B:677:HIS:CE1	2.73	0.41
1:A:577:ARG:HD3	1:A:652:HIS:HB3	2.02	0.41
1:B:303:PRO:HG3	1:B:412:LEU:HD21	2.02	0.41
1:A:700:LEU:HD23	1:A:754:ASP:HA	2.02	0.41
1:B:623:GLU:OE2	1:B:677:HIS:NE2	2.54	0.41
1:B:607:VAL:O	1:B:611:GLN:HG2	2.21	0.41
1:A:201:TRP:HE1	1:A:212:ASN:ND2	1.93	0.41
1:B:744:THR:O	1:B:768:SER:HA	2.21	0.41
1:A:753:THR:HA	1:A:758:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:LEU:HD13	1:A:776:TRP:CZ2	2.56	0.40
1:A:106:SER:OG	1:A:562:GLU:OE2	2.36	0.40
1:B:223:ARG:HH11	1:B:223:ARG:HD3	1.65	0.40
1:A:255:ASN:HB2	1:A:280:LEU:HD13	2.03	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%)	827 (97%)	19 (2%)	3 (0%)	30	34
1	B	849/1032 (82%)	824 (97%)	23 (3%)	2 (0%)	43	51
All	All	1698/2064 (82%)	1651 (97%)	42 (2%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	B	469	ASP
1	A	202	ILE
1	A	541	ALA
1	B	202	ILE

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	697/833 (84%)	674 (97%)	23 (3%)	33	45
1	B	697/833 (84%)	667 (96%)	30 (4%)	26	35
All	All	1394/1666 (84%)	1341 (96%)	53 (4%)	29	40

All (53) 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
1	A	356	LEU
1	A	428	ASN
1	A	430	GLU
1	A	431	GLU
1	A	577	ARG
1	A	608	ARG
1	A	685	ARG
1	A	698	SER
1	A	701	THR
1	A	704	THR
1	A	740	SER
1	A	773	THR
1	A	783	TYR
1	A	806	THR
1	A	839	LYS
1	A	877	LEU
1	A	895	THR
1	B	50	ASN
1	B	85	SER
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	230	ARG
1	B	236	GLN
1	B	240	SER

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Mol	Chain	Res	Type
1	B	247	LEU
1	B	262	GLN
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	701	THR
1	B	704	THR
1	B	724	VAL
1	B	780	ASP
1	B	821	VAL
1	B	827	SER
1	B	846	LYS
1	B	871	LYS
1	B	877	LEU
1	B	895	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	64	GLN
1	A	176	GLN
1	A	194	ASN
1	A	211	GLN
1	A	212	ASN
1	A	348	GLN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	679	GLN
1	A	796	ASN
1	A	808	ASN
1	B	50	ASN
1	B	110	GLN
1	B	176	GLN
1	B	194	ASN
1	B	212	ASN
1	B	276	GLN
1	B	299	ASN

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	465	HIS
1	B	614	GLN
1	B	682	HIS
1	B	750	ASN
1	B	796	ASN
1	B	800	GLN
1	B	808	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 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	-	22,22,22	2.32	3 (13%)	29,31,31	1.11	3 (10%)
3	PNJ	A	1901	-	22,22,22	2.17	2 (9%)	29,31,31	1.69	5 (17%)
4	ACT	B	1903	-	3,3,3	1.09	0	3,3,3	1.16	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1904	PNJ	O8-N1	9.01	1.38	1.22
3	A	1901	PNJ	O8-N1	8.81	1.38	1.22
3	A	1901	PNJ	C10-N1	-4.28	1.35	1.45
3	B	1904	PNJ	C10-N1	-4.10	1.35	1.45
3	B	1904	PNJ	O1-C1	3.18	1.46	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	PNJ	C11-C10-N1	4.06	122.88	119.34
3	A	1901	PNJ	O1-C1-C2	-3.66	102.13	107.35
3	B	1904	PNJ	O1-C1-C2	-3.09	102.94	107.35
3	A	1901	PNJ	C7-O1-C1	-2.74	113.95	117.82
3	A	1901	PNJ	C9-C10-N1	-2.68	117.00	119.34
3	A	1901	PNJ	C3-C2-N2	2.37	115.92	111.05
3	B	1904	PNJ	O3-C3-C4	-2.09	105.44	110.38
3	B	1904	PNJ	O3-C3-C2	2.02	113.85	110.22

There are no chirality outliers.

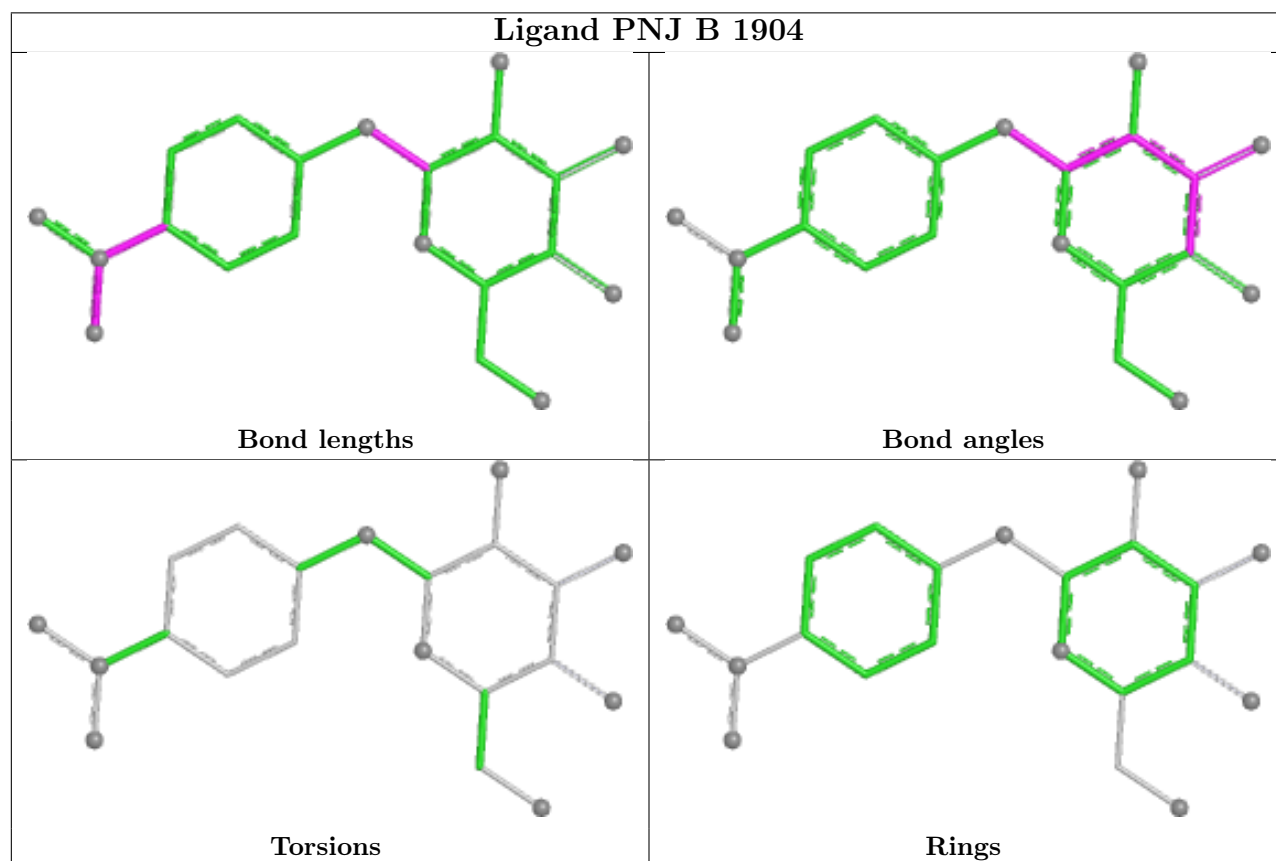
There are no torsion outliers.

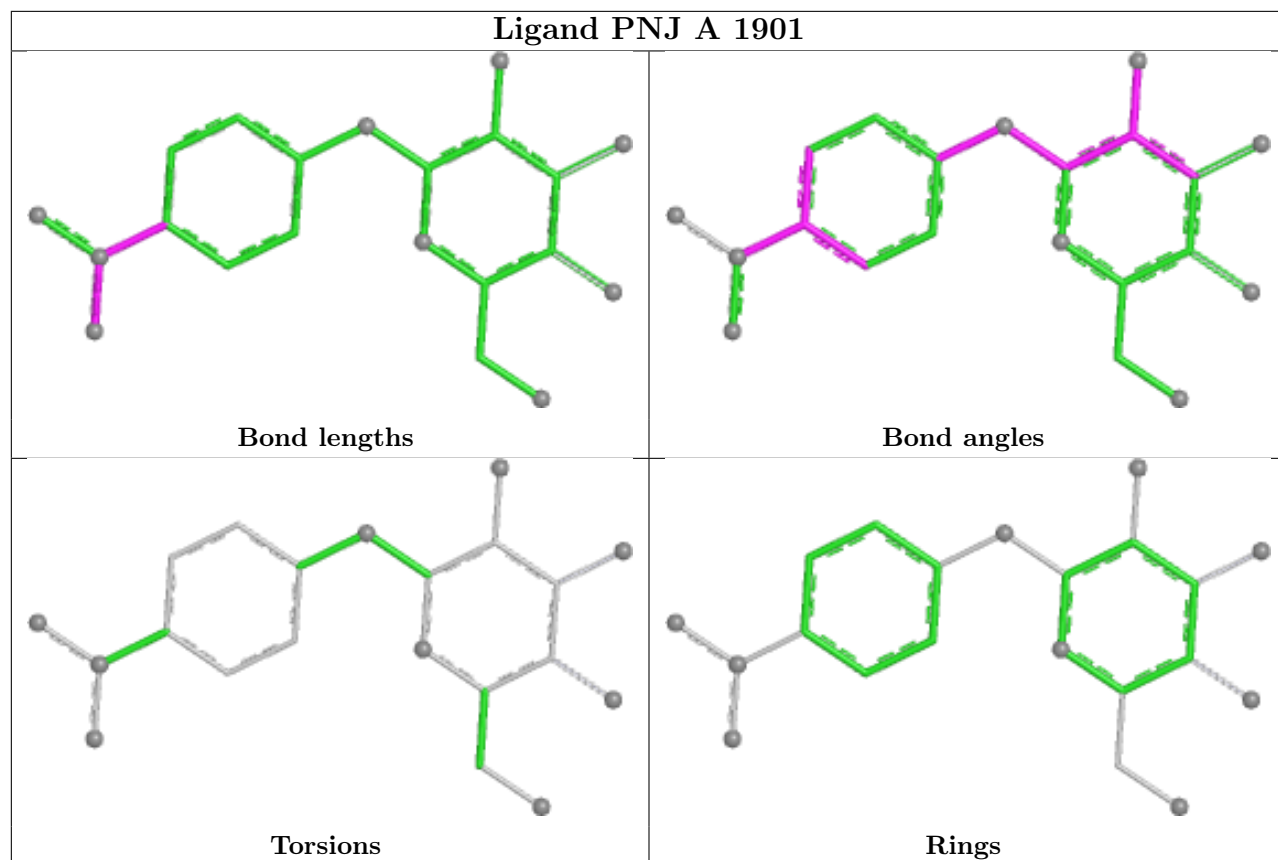
There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	851/1032 (82%)	-0.63	1 (0%) 92 90	3, 11, 21, 32	1 (0%)
1	B	851/1032 (82%)	-0.62	2 (0%) 91 90	2, 10, 21, 32	0
All	All	1702/2064 (82%)	-0.62	3 (0%) 91 90	2, 11, 21, 32	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	GLY	2.4
1	A	432	LYS	2.1
1	B	50	ASN	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(Å ²)	Q<0.9
4	ACT	B	1903	4/4	0.64	0.19	14,16,17,17	0
2	CD	B	1901	1/1	0.87	0.29	137,137,137,137	0

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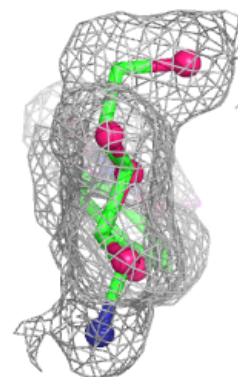
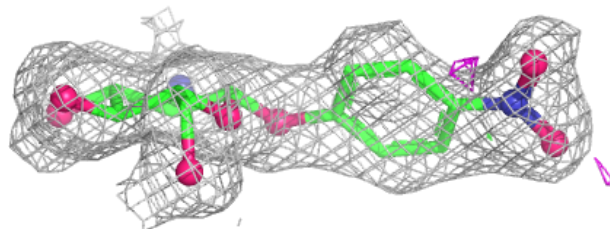
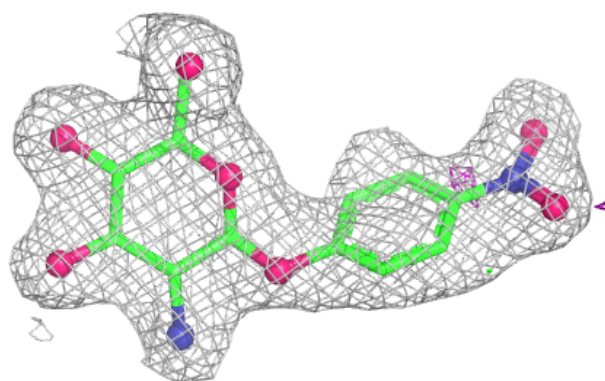
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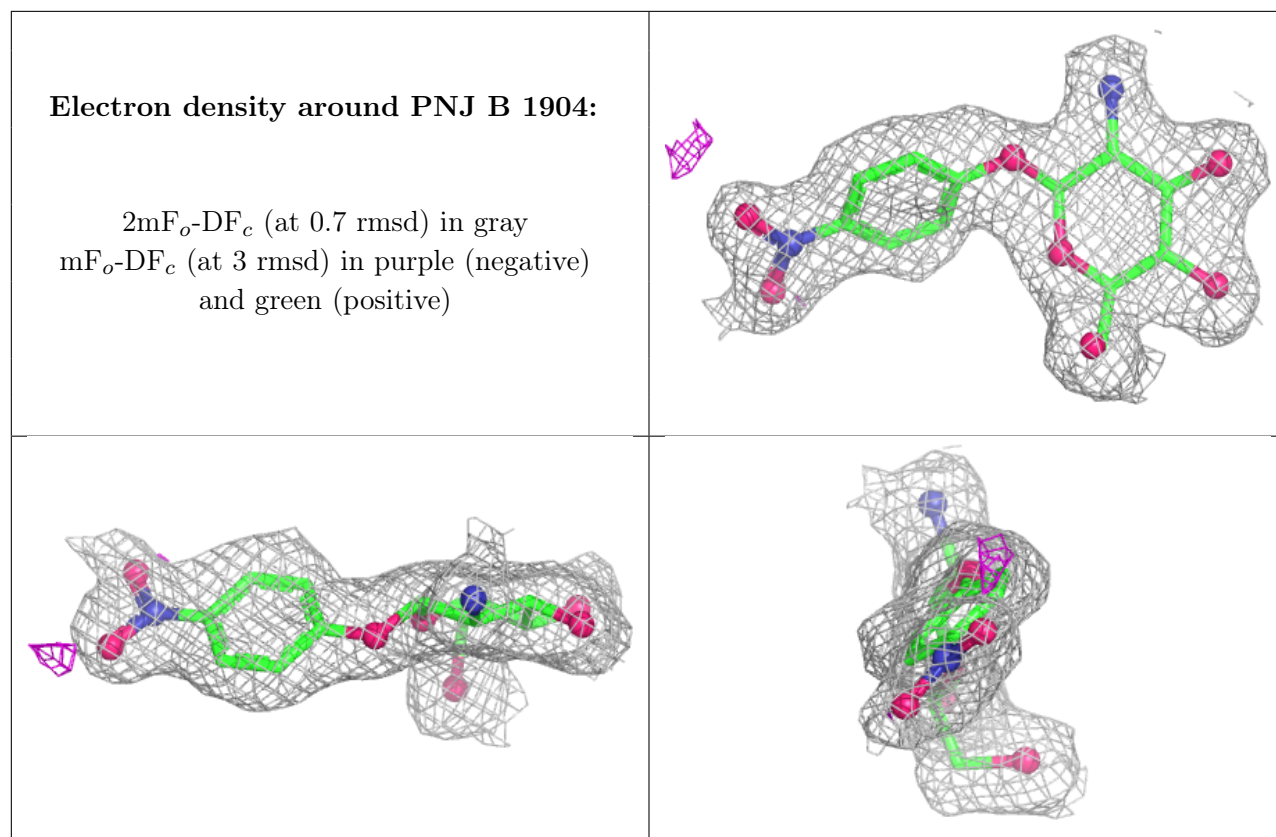
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	A	1900	1/1	0.88	0.21	104,104,104,104	0
2	CD	A	1899	1/1	0.91	0.36	80,80,80,80	0
2	CD	B	1902	1/1	0.92	0.14	87,87,87,87	0
3	PNJ	A	1901	21/21	0.96	0.05	2,8,13,14	0
3	PNJ	B	1904	21/21	0.97	0.05	2,7,12,16	0
2	CD	B	1900	1/1	1.00	0.01	9,9,9,9	0
2	CD	B	1899	1/1	1.00	0.01	9,9,9,9	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)





6.5 Other polymers [i](#)

There are no such residues in this entry.