Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:48 PM BST

PDB ID	:	2VZT
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 following versions of software and data (see references ⓘ) were used in the production of this report:

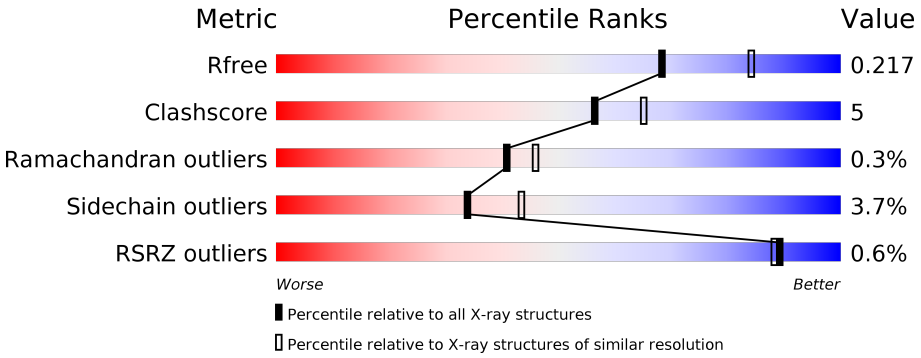
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	73% 8% • 18%
1	B	1032	% 72% 9% • 18%

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			

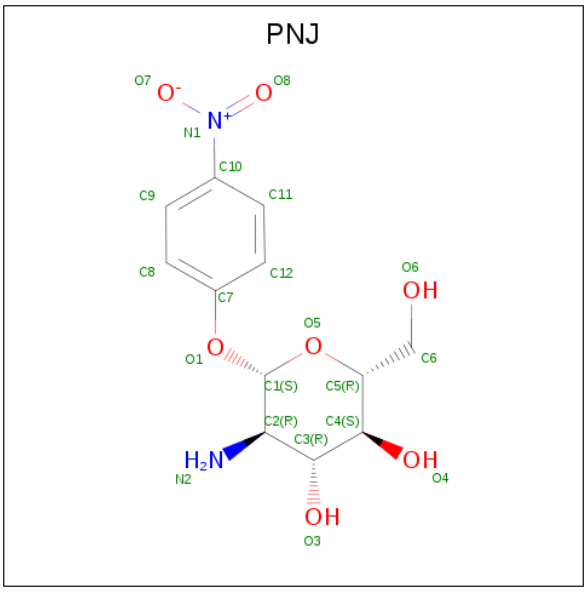
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: CD) (formula: Cd).

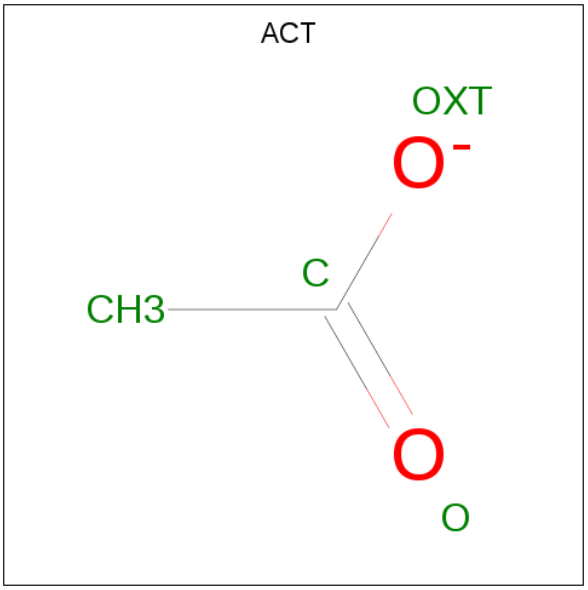
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cd	0	0
			4	4		
2	A	2	Total	Cd	0	0
			2	2		

- 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.

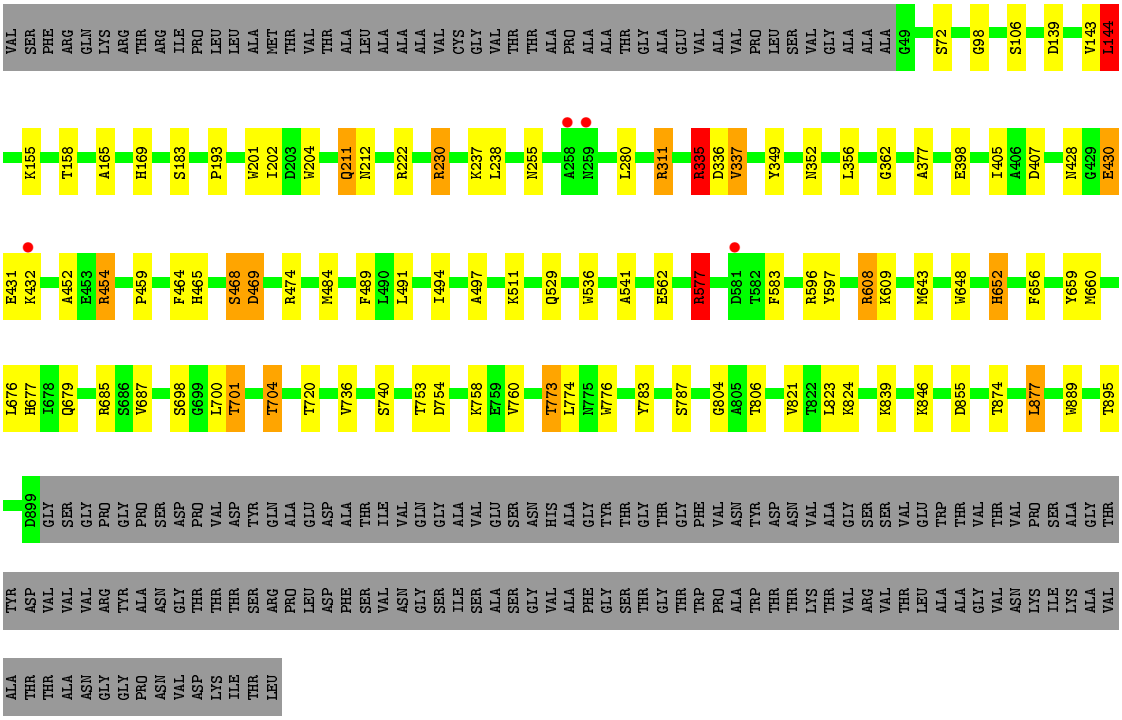
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	420	Total 420	O 420	0	0
5	B	406	Total 406	O 406	0	0

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.

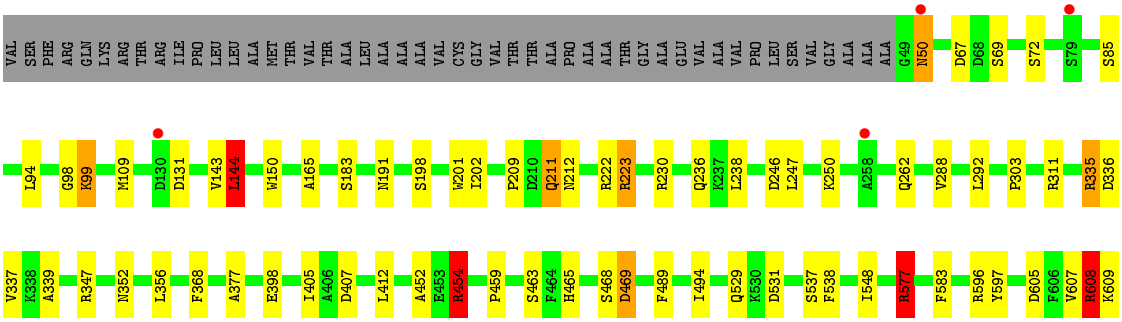
- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

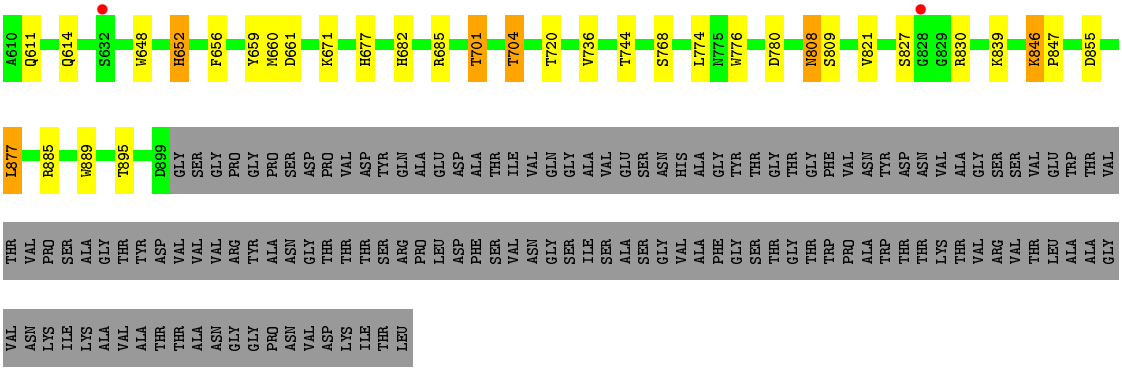
Chain A:



- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain B:




A610 Q611 Q614 S632 W648 H652 F656 Y659 M660 D661 K671 H677 H682 R685 T701 T704 T720 V736 T744 S768 L774 N775 W776 D780 N808 S809 V821 S827 G828 G829 R830 K839 K846 P847 D855
L877 R885 W889 T895 D899 GLY SER GLY PRO GLY PRO 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	86.69Å 122.23Å 91.86Å 90.00° 90.52° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.00-2.20) 99.1 (19.97-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.00%)	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)	0.37 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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: CD, PNJ, ACT

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	0.75	1/6668 (0.0%)	0.83	15/9099 (0.2%)
1	B	0.77	0/6668	0.84	19/9099 (0.2%)
All	All	0.76	1/13336 (0.0%)	0.84	34/18198 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CB-CG	7.95	1.67	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	335	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	B	454	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	454	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	B	454	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	A	454	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	335	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	311	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	597	TYR	N-CA-C	9.63	137.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	577	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	B	597	TYR	N-CA-C	9.11	135.60	111.00
1	B	238	LEU	CA-CB-CG	8.10	133.93	115.30
1	B	144	LEU	CA-CB-CG	8.02	133.75	115.30
1	A	238	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	230	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	335	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	230	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	577	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	469	ASP	N-CA-C	6.67	129.01	111.00
1	B	774	LEU	CA-CB-CG	-6.42	100.54	115.30
1	B	230	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	432	LYS	N-CA-C	6.30	128.01	111.00
1	A	469	ASP	N-CA-C	6.27	127.93	111.00
1	A	144	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	99	LYS	N-CA-C	-6.03	94.72	111.00
1	B	608	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	335	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	577	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	67	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	608	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	335	ARG	CG-CD-NE	-5.40	100.46	111.80
1	B	222	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	877	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	144	LEU	CB-CG-CD2	5.19	119.83	111.00
1	A	474	ARG	NE-CZ-NH1	5.02	122.81	120.30

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
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	6505	0	6282	56	0
1	B	6505	0	6282	73	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	9	0
5	B	406	0	0	16	0
All	All	13888	0	12601	129	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 (129) 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	1.65	1.29
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	0.92	1.08
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:B:109:MET:HE3	1:B:368:PHE:CZ	2.04	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:A:855:ASP:CB	5:A:2402:HOH:O	2.22	0.87
1:B:846:LYS:HE2	5:B:2378:HOH:O	1.77	0.83
1:B:109:MET:HE2	1:B:209:PRO:HD3	1.59	0.82
1:B:109:MET:HE3	1:B:368:PHE:CE1	2.11	0.80
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:656:PHE:CD1	1:B:660:MET:HE1	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:311:ARG:CD	5:A:2121:HOH:O	2.35	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: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:109:MET:HE1	1:B:368:PHE:CZ	2.24	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: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:B:656:PHE:CE1	1:B:660:MET:HE1	2.39	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:A:656:PHE:CD1	1:A:660:MET:HE1	2.39	0.57
1:B:885:ARG:HD3	5:B:2397:HOH:O	2.05	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
1:A:701:THR:HB	1:A:720:THR:HA	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ARG:HD2	1:B:736:VAL:O	2.13	0.49
1:B:109:MET:HE3	1:B:368:PHE:HZ	1.74	0.49
1:A:398:GLU:O	1:A:454:ARG:NH2	2.40	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: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:537:SER:OG	1:B:538:PHE:N	2.47	0.46
1:B:72:SER:O	1:B:183:SER:HB2	2.17	0.45
1:B:660:MET:HE3	5:B:2294:HOH:O	2.16	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:B:311:ARG:HD3	5:B:2169:HOH:O	2.16	0.45
1:A:468:SER:O	1:A:497:ALA:N	2.39	0.44
1:A:529:GLN:HG3	1:A:776:TRP:CE3	2.52	0.44
1:A:349:TYR:OH	1:A:494:ILE:CD1	2.65	0.44
1:A:464:PHE:HB3	1:A:484:MET:HE1	1.98	0.44
1:A:656:PHE:CE1	1:A:660:MET:HE1	2.53	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:339:ALA:HB1	1:B:347:ARG:HD2	2.00	0.43
1:B:50:ASN:HD22	1:B:50:ASN:N	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:846:LYS:HE3	5:B:2243:HOH:O	2.17	0.42
1:A:407:ASP:CG	1:A:459:PRO:HD2	2.39	0.42
1:B:109:MET:HE2	1:B:209:PRO:CD	2.40	0.42
1:B:548:ILE:H	1:B:614:GLN:NE2	2.18	0.42
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:204:TRP:CD1	1:A:643:MET:HE1	2.56	0.41
1:A:700:LEU:HD23	1:A:754:ASP:HA	2.02	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
1:A:774:LEU:HD13	1:A:776:TRP:CZ2	2.56	0.40
1:B:660:MET:CE	5:B:2294:HOH:O	2.69	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%)	34 37
1	B	849/1032 (82%)	824 (97%)	23 (3%)	2 (0%)	47 55
All	All	1698/2064 (82%)	1651 (97%)	42 (2%)	5 (0%)	41 46

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%)	673 (97%)	24 (3%)	37 47
1	B	697/833 (84%)	669 (96%)	28 (4%)	31 40
All	All	1394/1666 (84%)	1342 (96%)	52 (4%)	34 43

All (52) 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

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Mol	Chain	Res	Type
1	A	608	ARG
1	A	648	TRP
1	A	652	HIS
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	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	337	VAL
1	B	356	LEU
1	B	454	ARG
1	B	577	ARG
1	B	608	ARG
1	B	648	TRP
1	B	652	HIS
1	B	701	THR
1	B	704	THR
1	B	780	ASP
1	B	808	ASN
1	B	821	VAL
1	B	827	SER
1	B	830	ARG
1	B	846	LYS
1	B	877	LEU
1	B	895	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	128	ASN
1	A	194	ASN
1	A	212	ASN
1	A	352	ASN
1	A	428	ASN
1	A	465	HIS
1	A	679	GLN
1	A	682	HIS
1	A	750	ASN
1	A	796	ASN
1	A	808	ASN
1	B	50	ASN
1	B	176	GLN
1	B	194	ASN
1	B	212	ASN
1	B	348	GLN
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	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 monosaccharides 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	A	1901	-	21,22,22	2.24	2 (9%)	29,31,31	1.76	5 (17%)
3	PNJ	B	1904	-	21,22,22	2.39	3 (14%)	29,31,31	1.12	4 (13%)
4	ACT	B	1903	-	1,3,3	4.18	1 (100%)	0,3,3	0.00	-

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	A	1901	-	-	0/8/30/30	0/2/2/2
3	PNJ	B	1904	-	-	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	B	1904	PNJ	O8-N1	9.15	1.38	1.22
3	A	1901	PNJ	O8-N1	8.95	1.38	1.22
3	A	1901	PNJ	C10-N1	-4.22	1.35	1.45
4	B	1903	ACT	CH3-C	4.18	1.54	1.48
3	B	1904	PNJ	C10-N1	-4.04	1.35	1.45
3	B	1904	PNJ	O1-C1	3.19	1.46	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1901	PNJ	C11-C10-N1	4.66	122.88	119.38
3	A	1901	PNJ	O1-C1-C2	-3.61	102.13	107.34
3	A	1901	PNJ	C9-C10-N1	-3.16	117.00	119.38
3	B	1904	PNJ	O1-C1-C2	-3.05	102.94	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1901	PNJ	C7-O1-C1	-2.62	113.95	117.79
3	A	1901	PNJ	C3-C2-N2	2.37	115.92	111.05
3	B	1904	PNJ	C11-C10-N1	2.26	121.08	119.38
3	B	1904	PNJ	O3-C3-C4	-2.12	105.44	110.35
3	B	1904	PNJ	O3-C3-C2	2.02	113.85	110.22

There are no chirality outliers.

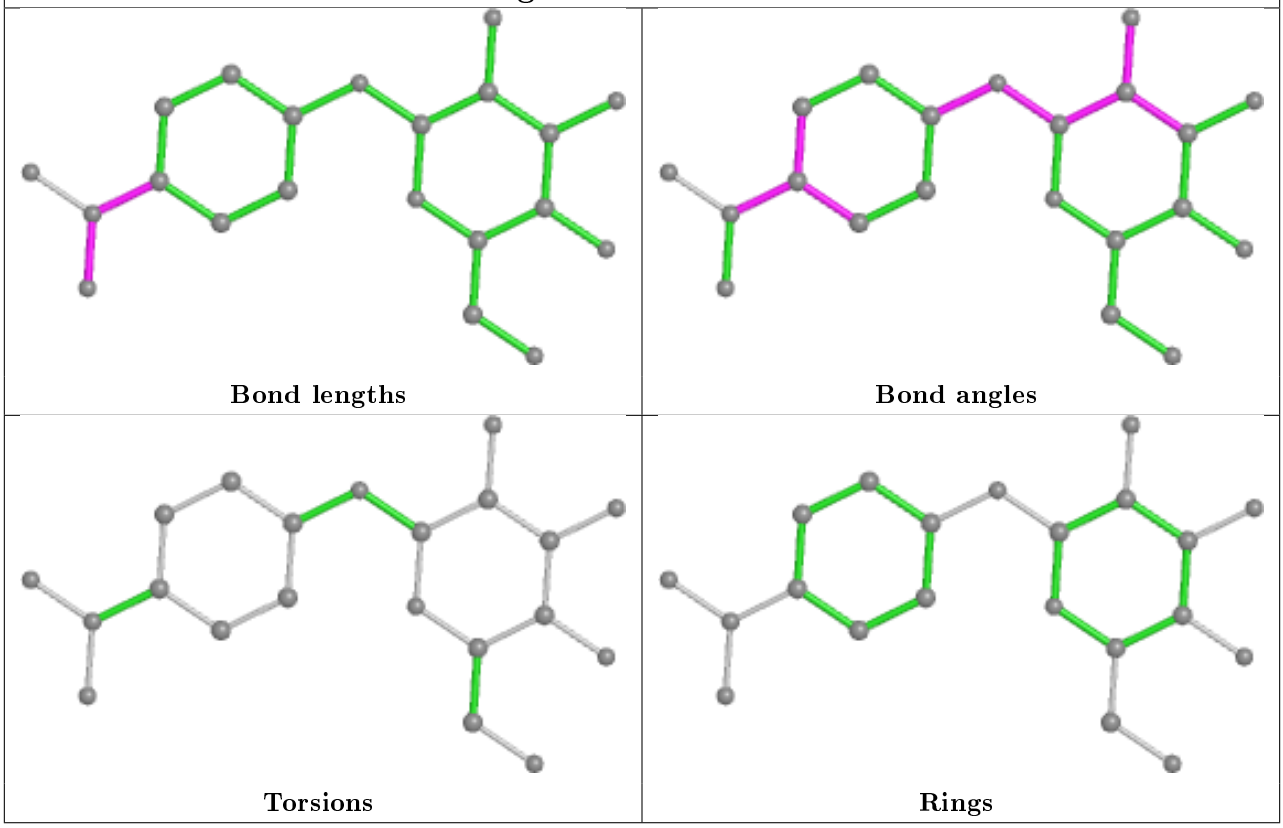
There are no torsion outliers.

There are no ring outliers.

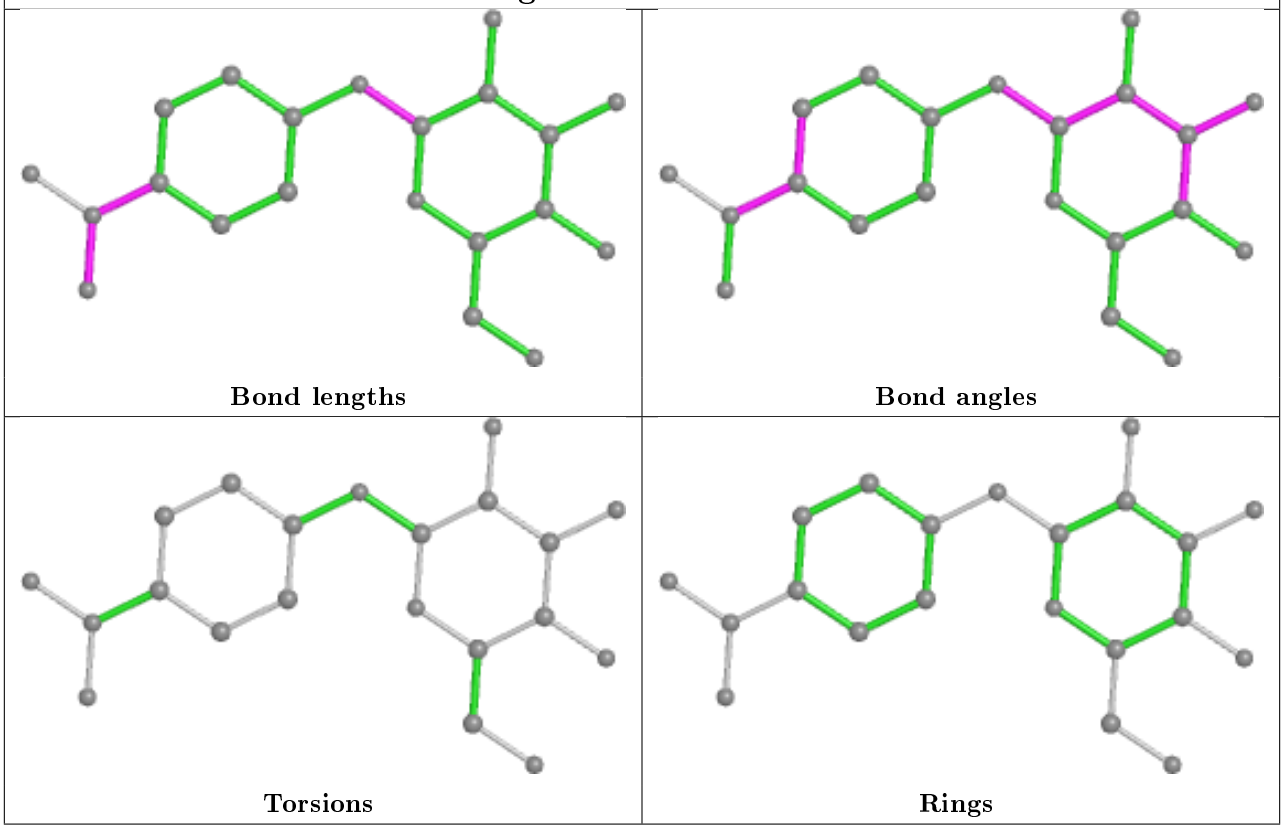
No monomer is involved in short contacts.

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 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 A 1901



Ligand PNJ B 1904



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.60	4 (0%)	91	90	3, 11, 21, 32	1 (0%)
1	B	851/1032 (82%)	-0.58	6 (0%)	87	86	2, 10, 21, 32	0
All	All	1702/2064 (82%)	-0.59	10 (0%)	89	88	2, 11, 21, 32	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	SER	2.7
1	B	50	ASN	2.7
1	B	258	ALA	2.5
1	B	130	ASP	2.4
1	B	632	SER	2.2
1	A	259	ASN	2.1
1	A	581	ASP	2.1
1	A	432	LYS	2.1
1	B	828	GLY	2.1
1	A	258	ALA	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

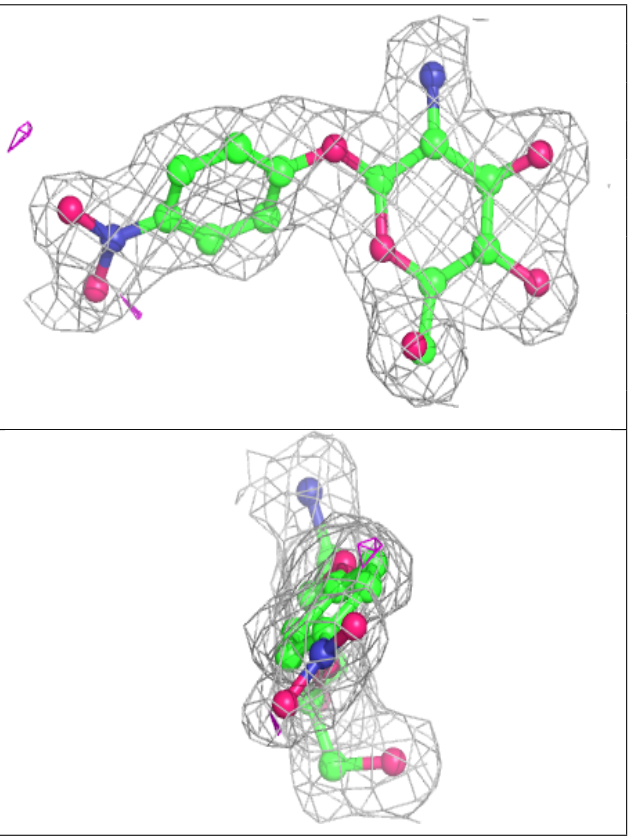
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

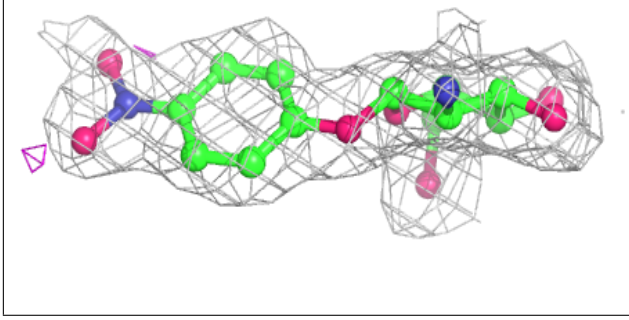
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	B	1903	4/4	0.59	0.27	14,16,17,17	0
2	CD	B	1901	1/1	0.83	0.17	137,137,137,137	0
2	CD	A	1900	1/1	0.86	0.14	104,104,104,104	0
2	CD	A	1899	1/1	0.91	0.35	80,80,80,80	0
2	CD	B	1902	1/1	0.91	0.08	87,87,87,87	0
3	PNJ	B	1904	21/21	0.96	0.09	2,7,12,16	0
3	PNJ	A	1901	21/21	0.97	0.08	2,8,13,14	0
2	CD	B	1899	1/1	1.00	0.03	9,9,9,9	0
2	CD	B	1900	1/1	1.00	0.04	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 B 1904:

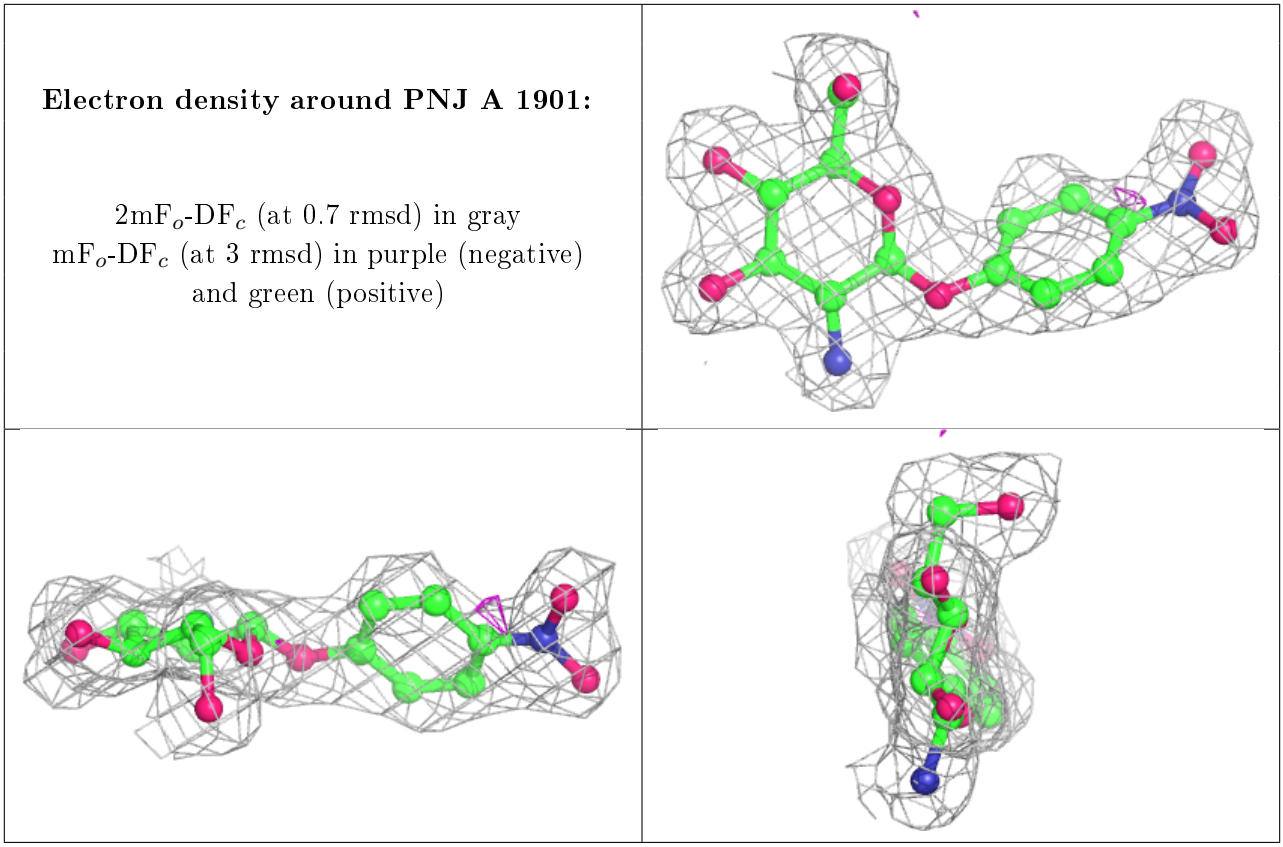
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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

There are no such residues in this entry.