



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 04:06 pm GMT

PDB ID : 2VVZ
Title : Structure of the catalytic domain of Streptococcus pneumoniae sialidase NanA
Authors : Xu, G.; Li, X.; Andrew, P.W.; Taylor, G.L.
Deposited on : 2008-06-13
Resolution : 2.50 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 : 2.36
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) : 2.36

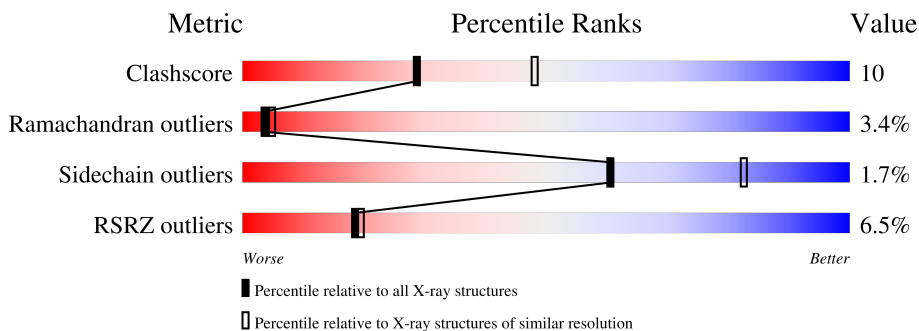
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	504	 3% 75% 15% • 7%
1	B	504	 9% 73% 17% • 7%

2 Entry composition [i](#)

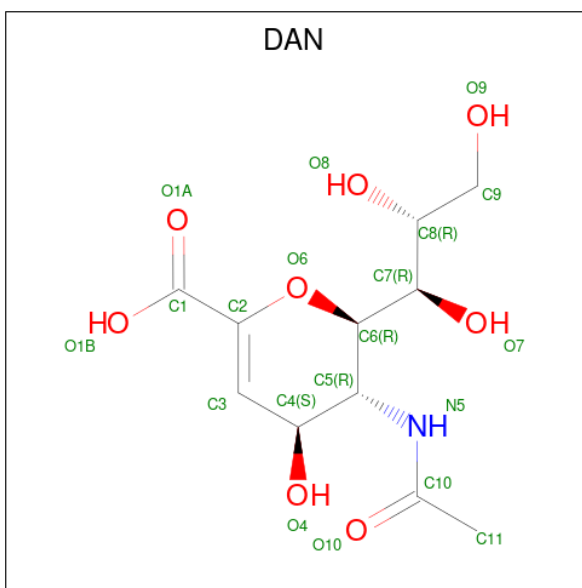
There are 4 unique types of molecules in this entry. The entry contains 7607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIALIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	470	Total 3721	C 2332	N 657	O 720	S 12	0	0	0
1	B	470	Total 3721	C 2332	N 657	O 720	S 12	0	0	0

- Molecule 2 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: DAN) (formula: $C_{11}H_{17}NO_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 20	C 11	N 1	O 8	0	0
2	B	1	Total 20	C 11	N 1	O 8	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

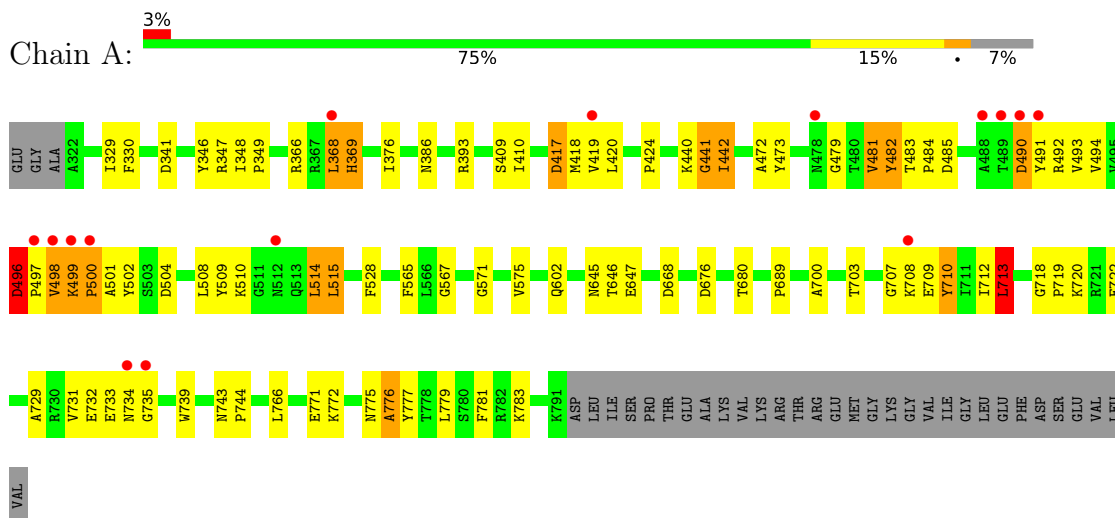
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0
4	B	30	Total O 30 30	0	0

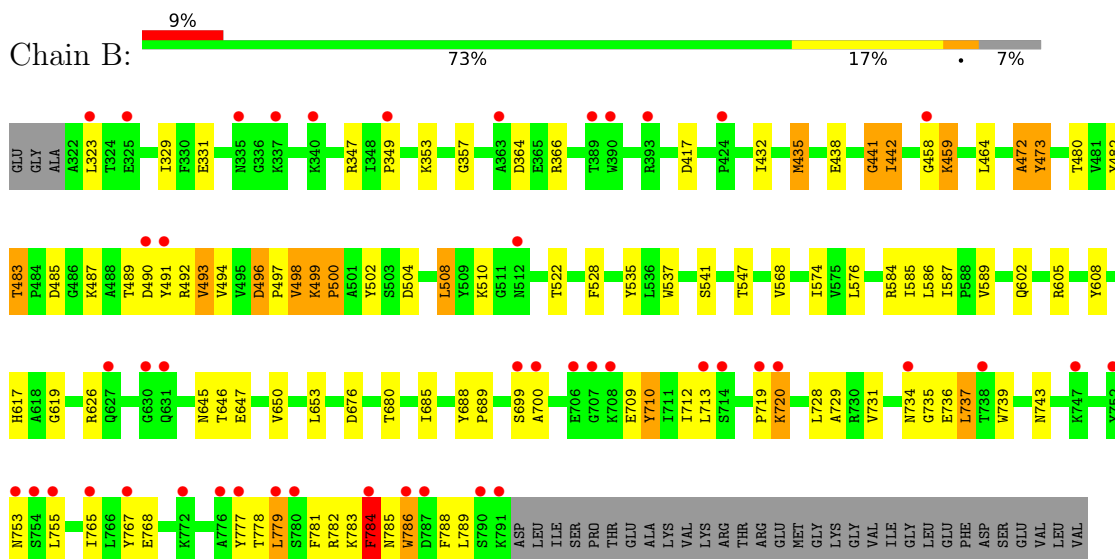
3 Residue-property plots [i](#)

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: SIALIDASE A



• Molecule 1: SIALIDASE A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.21Å 95.63Å 226.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 27.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.50) 93.1 (27.78-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.84 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.298 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: DAN, CL

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	0/3802	0.59	1/5135 (0.0%)
1	B	0.37	0/3802	0.55	0/5135
All	All	0.38	0/7604	0.57	1/10270 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	713	LEU	CA-CB-CG	5.98	129.05	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	LEU	Peptide
1	A	498	VAL	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	3721	0	3641	66	0
1	B	3721	0	3641	78	0
2	A	20	0	16	1	0
2	B	20	0	16	0	0
3	A	1	0	0	0	0
4	A	94	0	0	1	0
4	B	30	0	0	2	0
All	All	7607	0	7314	144	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 (144) 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:785:ASN:HB2	1:B:786:TRP:HB3	1.31	1.10
1:B:709:GLU:HB3	1:B:731:VAL:HB	1.36	1.04
1:B:785:ASN:HB2	1:B:786:TRP:CB	1.87	1.03
1:B:483:THR:HG22	1:B:487:LYS:H	1.39	0.87
1:B:441:GLY:O	1:B:442:ILE:HG22	1.75	0.86
1:A:703:THR:O	1:A:709:GLU:O	1.96	0.82
1:A:481:VAL:O	1:A:482:TYR:HB2	1.79	0.81
1:A:498:VAL:HA	1:A:499:LYS:HB2	1.62	0.79
1:B:783:LYS:O	1:B:784:PHE:HB3	1.84	0.78
1:B:323:LEU:HD11	1:B:782:ARG:HD3	1.67	0.77
1:B:700:ALA:HB2	1:B:713:LEU:HD23	1.68	0.76
1:B:435:MET:HG3	1:B:535:TYR:HB2	1.68	0.76
1:A:500:PRO:HD2	1:A:504:ASP:OD1	1.86	0.75
1:B:676:ASP:OD2	1:B:680:THR:HB	1.88	0.73
1:B:734:ASN:N	1:B:735:GLY:HA2	2.05	0.71
1:B:785:ASN:HB2	1:B:786:TRP:HB2	1.74	0.69
1:B:499:LYS:HB2	1:B:500:PRO:HD3	1.75	0.67
1:B:498:VAL:HG22	1:B:502:TYR:HA	1.76	0.67
1:B:785:ASN:CB	1:B:786:TRP:HB3	2.18	0.66
1:A:499:LYS:HB3	1:A:500:PRO:HD3	1.77	0.66
1:B:489:THR:O	1:B:491:TYR:N	2.28	0.66
1:A:329:ILE:HD11	1:A:781:PHE:HB2	1.78	0.64
1:A:501:ALA:HB3	4:A:2021:HOH:O	1.97	0.64
1:A:719:PRO:O	1:A:720:LYS:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:ASN:N	1:A:735:GLY:HA2	2.15	0.62
1:A:602:GLN:HB3	1:A:646:THR:HG22	1.83	0.61
1:B:458:GLY:HA2	1:B:459:LYS:O	2.00	0.61
1:B:472:ALA:O	1:B:473:TYR:HB2	2.01	0.61
1:B:767:TYR:O	1:B:779:LEU:HA	2.00	0.61
1:B:496:ASP:HB2	1:B:497:PRO:HD3	1.82	0.59
1:A:668:ASP:OD1	1:A:689:PRO:HA	2.02	0.59
1:B:498:VAL:CG2	1:B:502:TYR:HA	2.33	0.59
1:B:785:ASN:CB	1:B:786:TRP:CB	2.74	0.58
1:B:491:TYR:HB3	1:B:510:LYS:HG2	1.86	0.58
1:B:498:VAL:HG23	1:B:504:ASP:OD1	2.02	0.58
1:B:541:SER:HB2	1:B:547:THR:O	2.04	0.58
1:B:719:PRO:O	1:B:720:LYS:HB2	2.04	0.57
1:B:329:ILE:HD11	1:B:781:PHE:HB2	1.85	0.57
1:B:602:GLN:HB3	1:B:646:THR:HG22	1.86	0.56
1:B:480:THR:HA	1:B:493:VAL:HG12	1.88	0.56
1:A:496:ASP:H	1:A:497:PRO:CD	2.20	0.55
1:B:500:PRO:HD2	1:B:504:ASP:OD1	2.07	0.54
1:A:514:LEU:O	1:A:515:LEU:HB2	2.07	0.54
1:B:464:LEU:O	1:B:472:ALA:O	2.26	0.54
1:B:576:LEU:HD22	1:B:584:ARG:HB3	1.90	0.54
1:A:410:ILE:HG21	1:A:440:LYS:HE2	1.90	0.53
1:A:329:ILE:HD12	1:A:766:LEU:HD13	1.90	0.53
1:A:775:ASN:O	1:A:776:ALA:CB	2.56	0.53
1:A:481:VAL:O	1:A:482:TYR:CB	2.55	0.53
1:A:565:PHE:CZ	1:A:567:GLY:HA3	2.43	0.53
1:B:494:VAL:HG12	1:B:508:LEU:HD12	1.91	0.52
1:A:707:GLY:O	1:A:708:LYS:HG2	2.09	0.52
1:B:784:PHE:HE1	1:B:788:PHE:CG	2.28	0.52
1:A:418:MET:CE	1:A:420:LEU:HD21	2.40	0.52
1:B:483:THR:HG23	1:B:485:ASP:H	1.74	0.52
1:B:586:LEU:HD23	1:B:650:VAL:HG21	1.91	0.52
1:A:700:ALA:HB2	1:A:713:LEU:CD2	2.40	0.52
1:A:483:THR:HG23	1:A:485:ASP:HB2	1.91	0.52
1:A:498:VAL:CA	1:A:499:LYS:HB2	2.36	0.51
1:A:718:GLY:HA2	1:A:720:LYS:O	2.11	0.51
1:B:783:LYS:O	1:B:784:PHE:CB	2.57	0.51
1:A:700:ALA:HB2	1:A:713:LEU:HD22	1.91	0.51
1:A:347:ARG:O	1:A:349:PRO:HD3	2.10	0.51
1:A:729:ALA:HB2	1:A:739:TRP:CE3	2.46	0.51
1:A:369:HIS:CD2	1:A:409:SER:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:MET:HG2	1:B:537:TRP:CE2	2.45	0.51
1:B:473:TYR:HA	1:B:482:TYR:O	2.11	0.50
1:B:568:VAL:HA	1:B:589:VAL:HG12	1.93	0.50
1:A:347:ARG:HG2	1:A:366:ARG:CZ	2.42	0.50
1:B:497:PRO:HD2	4:B:2012:HOH:O	2.11	0.49
1:B:755:LEU:HD23	1:B:765:ILE:HB	1.95	0.49
1:A:347:ARG:O	1:A:779:LEU:HD11	2.13	0.49
1:A:330:PHE:HB3	1:A:346:TYR:CG	2.48	0.48
1:A:366:ARG:HG2	1:A:376:ILE:HG12	1.95	0.48
1:A:348:ILE:HG13	1:A:417:ASP:OD1	2.13	0.48
1:A:424:PRO:HD3	1:A:575:VAL:HG21	1.96	0.48
1:A:329:ILE:CD1	1:A:781:PHE:HB2	2.44	0.47
1:A:347:ARG:NH2	2:A:1792:DAN:O1A	2.44	0.47
1:A:719:PRO:O	1:A:722:GLU:OE2	2.32	0.47
1:B:499:LYS:CB	1:B:500:PRO:HD3	2.41	0.47
1:A:771:GLU:HB3	1:A:772:LYS:HG3	1.96	0.47
1:A:498:VAL:HG23	1:A:502:TYR:HD1	1.80	0.47
1:B:646:THR:OG1	1:B:647:GLU:N	2.47	0.47
1:A:441:GLY:O	1:A:442:ILE:HG22	2.13	0.47
1:A:710:TYR:HA	1:A:729:ALA:O	2.14	0.47
1:B:585:ILE:O	1:B:608:TYR:HA	2.15	0.47
1:B:499:LYS:HB2	1:B:500:PRO:CD	2.44	0.47
1:A:490:ASP:O	1:A:491:TYR:HB2	2.15	0.46
1:A:500:PRO:HD2	1:A:504:ASP:CG	2.36	0.46
1:B:438:GLU:OE2	1:B:522:THR:HB	2.15	0.46
1:A:514:LEU:O	1:A:515:LEU:CB	2.64	0.46
1:B:493:VAL:HG21	4:B:2014:HOH:O	2.15	0.46
1:B:736:GLU:HG2	1:B:737:LEU:H	1.80	0.45
1:A:418:MET:HE1	1:A:420:LEU:HD21	1.97	0.45
1:B:432:ILE:HD12	1:B:587:ILE:HG13	1.97	0.45
1:A:646:THR:OG1	1:A:647:GLU:N	2.50	0.45
1:B:349:PRO:HB3	1:B:779:LEU:HD22	1.99	0.45
1:B:458:GLY:HA2	1:B:459:LYS:C	2.37	0.45
1:B:464:LEU:O	1:B:473:TYR:HB2	2.17	0.45
1:B:734:ASN:H	1:B:735:GLY:HA2	1.78	0.45
1:B:626:ARG:CZ	1:B:685:ILE:HD12	2.47	0.45
1:B:784:PHE:HE1	1:B:788:PHE:CD2	2.34	0.44
1:A:775:ASN:O	1:A:776:ALA:HB3	2.16	0.44
1:A:508:LEU:HD13	1:A:528:PHE:HB2	1.99	0.44
1:B:574:ILE:HG12	1:B:650:VAL:HG13	2.00	0.44
1:B:728:LEU:HB2	1:B:789:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:O	1:A:783:LYS:HE3	2.18	0.44
1:A:490:ASP:C	1:A:492:ARG:H	2.22	0.43
1:B:699:SER:HB3	1:B:753:ASN:OD1	2.17	0.43
1:B:441:GLY:O	1:B:442:ILE:CG2	2.56	0.43
1:A:493:VAL:HG23	1:A:509:TYR:HB2	2.01	0.43
1:B:498:VAL:HG23	1:B:504:ASP:CG	2.39	0.43
1:B:729:ALA:HB2	1:B:739:TRP:CE3	2.54	0.43
1:B:347:ARG:HG2	1:B:366:ARG:CZ	2.49	0.43
1:A:733:GLU:CG	1:A:734:ASN:N	2.82	0.42
1:A:347:ARG:HG3	1:A:348:ILE:HD13	2.02	0.42
1:A:676:ASP:OD2	1:A:680:THR:HB	2.20	0.42
1:B:605:ARG:HD3	1:B:619:GLY:O	2.20	0.42
1:A:709:GLU:HB3	1:A:731:VAL:HB	2.02	0.42
1:B:499:LYS:CB	1:B:500:PRO:CD	2.97	0.42
1:A:483:THR:OG1	1:A:484:PRO:HD2	2.19	0.42
1:B:768:GLU:HB3	1:B:777:TYR:CG	2.55	0.42
1:A:491:TYR:HB3	1:A:510:LYS:HG2	2.02	0.41
1:B:492:ARG:HG2	1:B:528:PHE:CE2	2.55	0.41
1:B:653:LEU:HG	1:B:731:VAL:HG11	2.02	0.41
1:A:483:THR:CG2	1:A:485:ASP:HB2	2.50	0.41
1:B:700:ALA:HA	1:B:712:ILE:O	2.20	0.41
1:A:776:ALA:HA	1:A:777:TYR:HA	1.67	0.41
1:A:419:VAL:HA	1:A:571:GLY:O	2.21	0.41
1:B:331:GLU:HA	1:B:778:THR:HG23	2.01	0.41
1:A:479:GLY:HA3	1:A:494:VAL:O	2.21	0.41
1:B:483:THR:HG22	1:B:487:LYS:N	2.20	0.41
1:B:483:THR:HG23	1:B:485:ASP:N	2.34	0.41
1:B:608:TYR:CZ	1:B:617:HIS:HB2	2.56	0.41
1:B:688:TYR:HA	1:B:689:PRO:HD2	1.95	0.41
1:A:490:ASP:HB3	1:A:491:TYR:H	1.65	0.41
1:A:341:ASP:OD2	1:A:393:ARG:NH2	2.55	0.40
1:A:700:ALA:HA	1:A:712:ILE:O	2.21	0.40
1:B:710:TYR:HA	1:B:729:ALA:O	2.21	0.40
1:A:733:GLU:HG2	1:A:734:ASN:H	1.85	0.40
1:B:353:LYS:HE3	1:B:357:GLY:O	2.21	0.40
1:B:329:ILE:CD1	1:B:781:PHE:HB2	2.51	0.40
1:A:743:ASN:HA	1:A:744:PRO:HD3	1.92	0.40
1:B:778:THR:O	1:B:778:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/504 (93%)	420 (90%)	31 (7%)	17 (4%)	3	4
1	B	468/504 (93%)	415 (89%)	38 (8%)	15 (3%)	4	5
All	All	936/1008 (93%)	835 (89%)	69 (7%)	32 (3%)	3	5

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	ILE
1	A	472	ALA
1	A	490	ASP
1	A	499	LYS
1	A	514	LEU
1	A	515	LEU
1	A	776	ALA
1	B	441	GLY
1	B	442	ILE
1	B	472	ALA
1	B	500	PRO
1	A	441	GLY
1	A	481	VAL
1	B	499	LYS
1	B	779	LEU
1	B	784	PHE
1	B	786	TRP
1	A	482	TYR
1	B	417	ASP
1	B	459	LYS
1	A	369	HIS
1	A	417	ASP
1	A	473	TYR
1	A	496	ASP
1	A	500	PRO

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Mol	Chain	Res	Type
1	B	710	TYR
1	A	732	GLU
1	B	473	TYR
1	B	490	ASP
1	B	720	LYS
1	A	710	TYR
1	B	496	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	402/430 (94%)	398 (99%)	4 (1%)	76	90
1	B	402/430 (94%)	392 (98%)	10 (2%)	47	73
All	All	804/860 (94%)	790 (98%)	14 (2%)	60	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	LEU
1	A	496	ASP
1	A	645	ASN
1	A	713	LEU
1	B	364	ASP
1	B	435	MET
1	B	483	THR
1	B	493	VAL
1	B	498	VAL
1	B	508	LEU
1	B	645	ASN
1	B	737	LEU
1	B	743	ASN
1	B	784	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
2	DAN	A	1792	-	20,20,20	0.93	1 (5%)	23,28,28	1.29	4 (17%)
2	DAN	B	1792	-	20,20,20	0.97	1 (5%)	23,28,28	1.14	3 (13%)

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	DAN	A	1792	-	-	3/18/34/34	0/1/1/1
2	DAN	B	1792	-	-	4/18/34/34	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1792	DAN	O6-C2	2.11	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1792	DAN	O6-C6	-2.03	1.42	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1792	DAN	O6-C2-C1	3.13	118.32	112.06
2	A	1792	DAN	O6-C2-C3	-3.01	121.09	124.61
2	B	1792	DAN	O6-C2-C3	-2.75	121.40	124.61
2	A	1792	DAN	O1B-C1-C2	2.45	120.32	114.20
2	A	1792	DAN	O1B-C1-O1A	-2.13	118.74	123.61
2	B	1792	DAN	O1B-C1-C2	2.09	119.43	114.20
2	B	1792	DAN	O6-C2-C1	2.09	116.24	112.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1792	DAN	O1A-C1-C2-C3
2	B	1792	DAN	O1A-C1-C2-O6
2	B	1792	DAN	O1B-C1-C2-C3
2	B	1792	DAN	O1B-C1-C2-O6
2	A	1792	DAN	O1A-C1-C2-C3
2	A	1792	DAN	O1B-C1-C2-C3
2	A	1792	DAN	O1A-C1-C2-O6

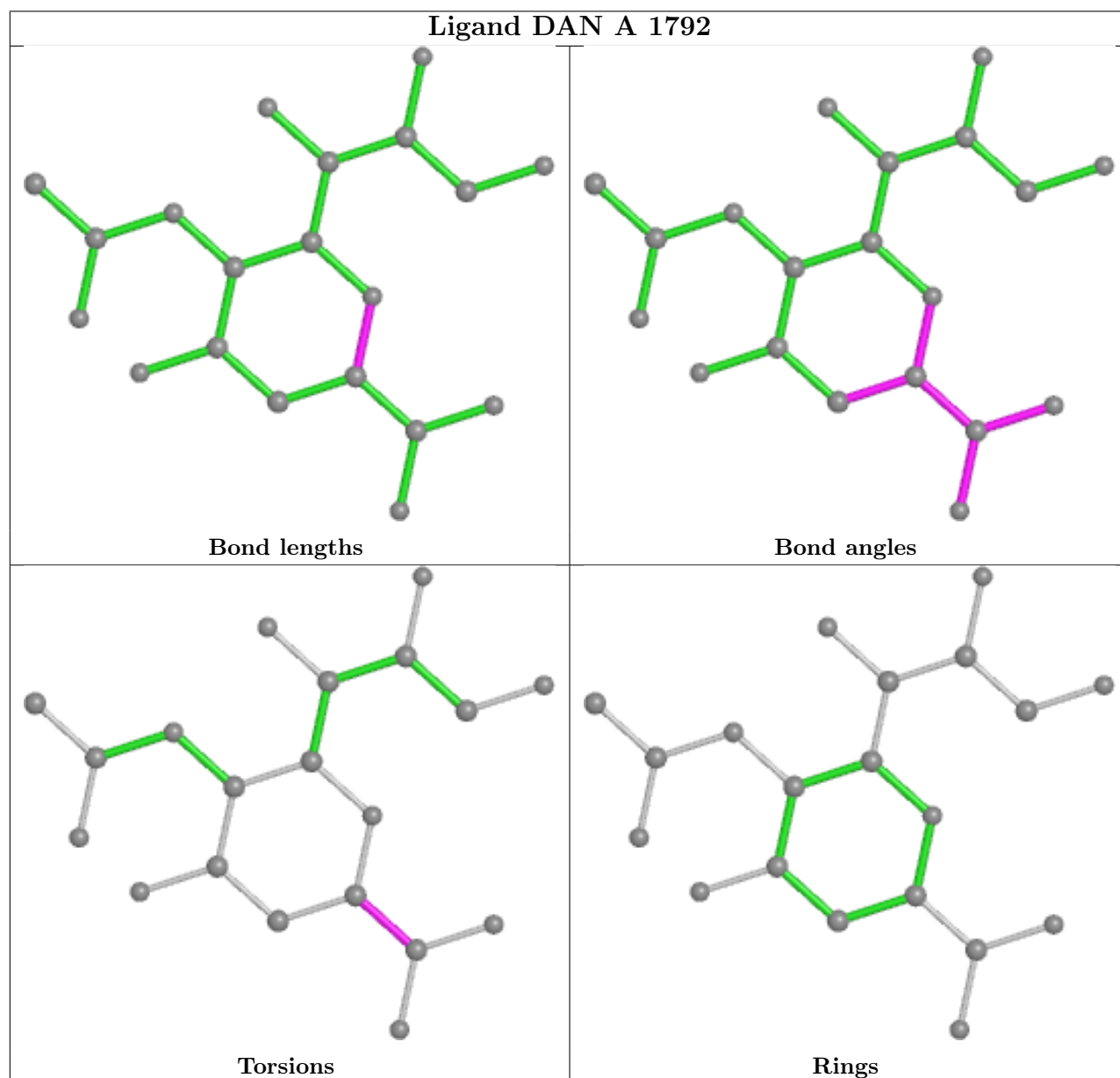
There are no ring outliers.

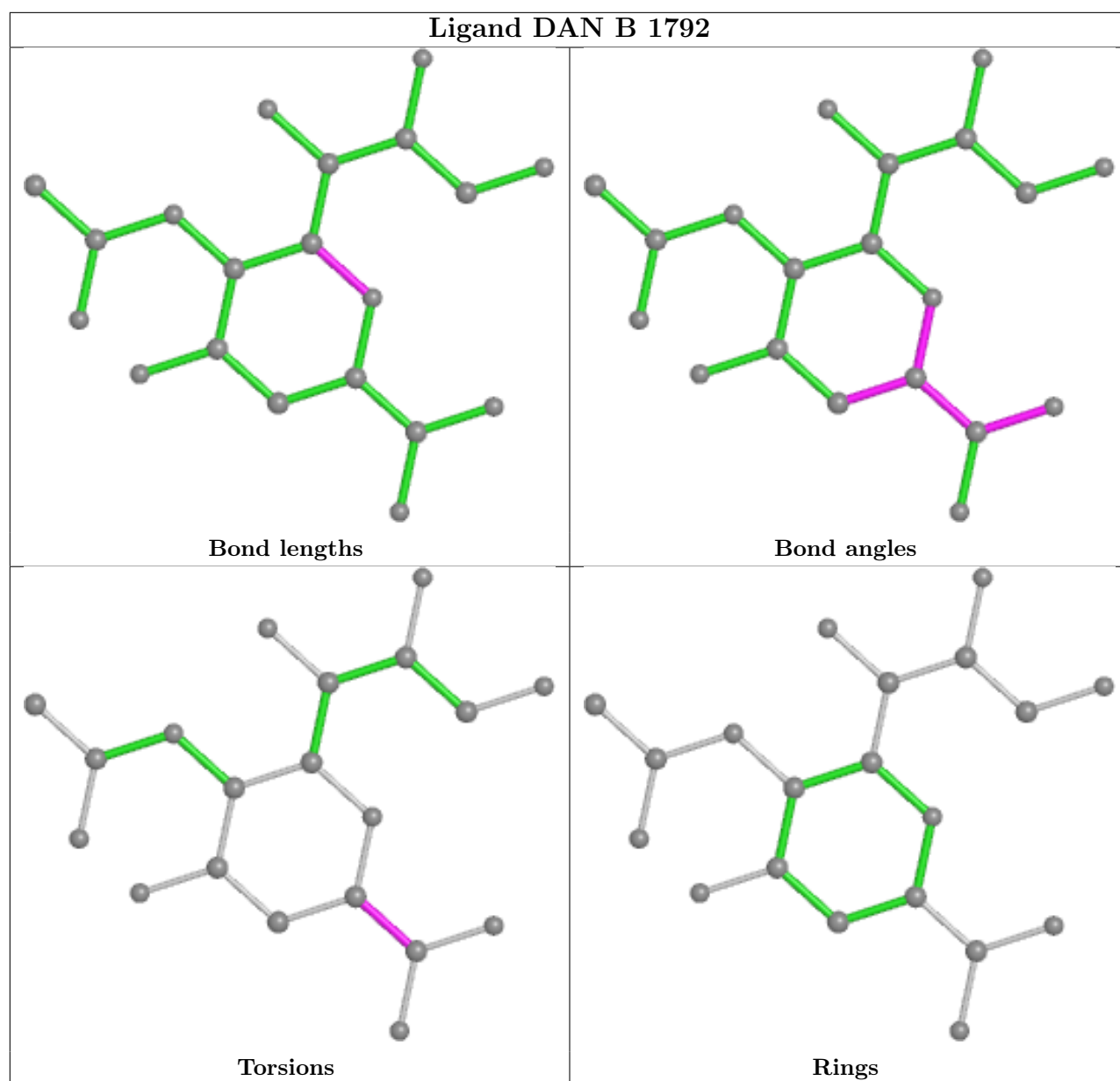
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1792	DAN	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 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	470/504 (93%)	0.12	15 (3%) 47 51	17, 28, 45, 60	0
1	B	470/504 (93%)	0.60	46 (9%) 7 7	24, 42, 67, 82	0
All	All	940/1008 (93%)	0.36	61 (6%) 18 19	17, 34, 63, 82	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	ASP	7.6
1	B	490	ASP	6.4
1	B	719	PRO	5.8
1	A	488	ALA	4.5
1	B	790	SER	4.4
1	A	491	TYR	4.4
1	A	734	ASN	4.3
1	A	499	LYS	4.3
1	B	784	PHE	4.3
1	B	708	LYS	3.9
1	A	500	PRO	3.6
1	B	787	ASP	3.6
1	B	323	LEU	3.5
1	B	335	ASN	3.5
1	B	754	SER	3.4
1	B	325	GLU	3.4
1	B	765	ILE	3.4
1	B	767	TYR	3.3
1	B	753	ASN	3.3
1	B	699	SER	3.3
1	B	772	LYS	3.3
1	A	368	LEU	3.2
1	B	512	ASN	3.1
1	B	630	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	706	GLU	3.1
1	B	393	ARG	3.0
1	B	491	TYR	3.0
1	B	631	GLN	2.9
1	A	478	ASN	2.8
1	B	349	PRO	2.8
1	B	337	LYS	2.8
1	B	791	LYS	2.7
1	B	720	LYS	2.7
1	A	498	VAL	2.7
1	B	738	THR	2.7
1	A	419	VAL	2.6
1	A	735	GLY	2.6
1	B	424	PRO	2.6
1	B	363	ALA	2.6
1	B	777	TYR	2.5
1	A	497	PRO	2.5
1	B	755	LEU	2.5
1	A	708	LYS	2.5
1	B	458	GLY	2.4
1	B	780	SER	2.4
1	B	713	LEU	2.4
1	B	707	GLY	2.4
1	B	700	ALA	2.4
1	B	776	ALA	2.4
1	B	786	TRP	2.4
1	B	734	ASN	2.4
1	A	512	ASN	2.3
1	B	714	SER	2.3
1	B	779	LEU	2.3
1	B	389	THR	2.3
1	B	747	LYS	2.2
1	B	752	TYR	2.2
1	B	340	LYS	2.2
1	B	627	GLN	2.1
1	B	390	TRP	2.1
1	A	489	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

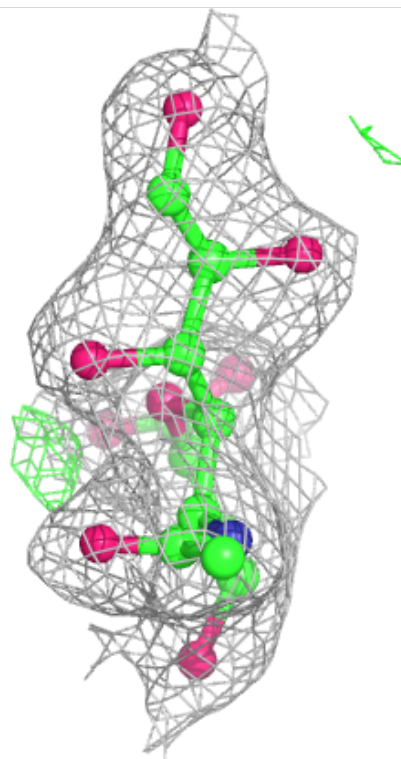
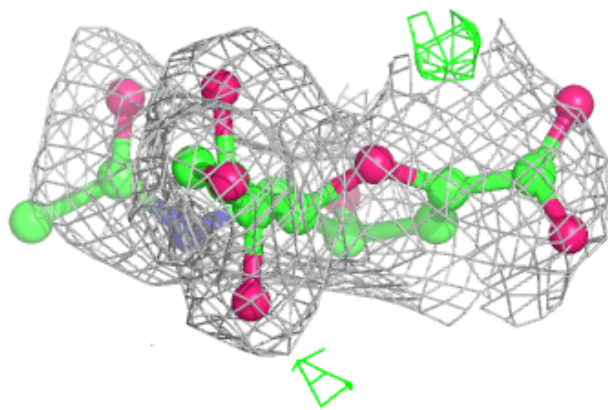
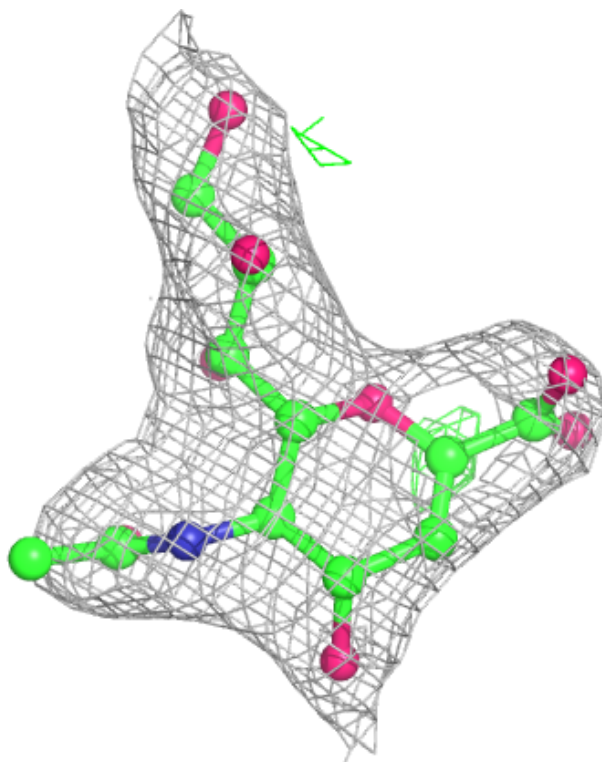
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

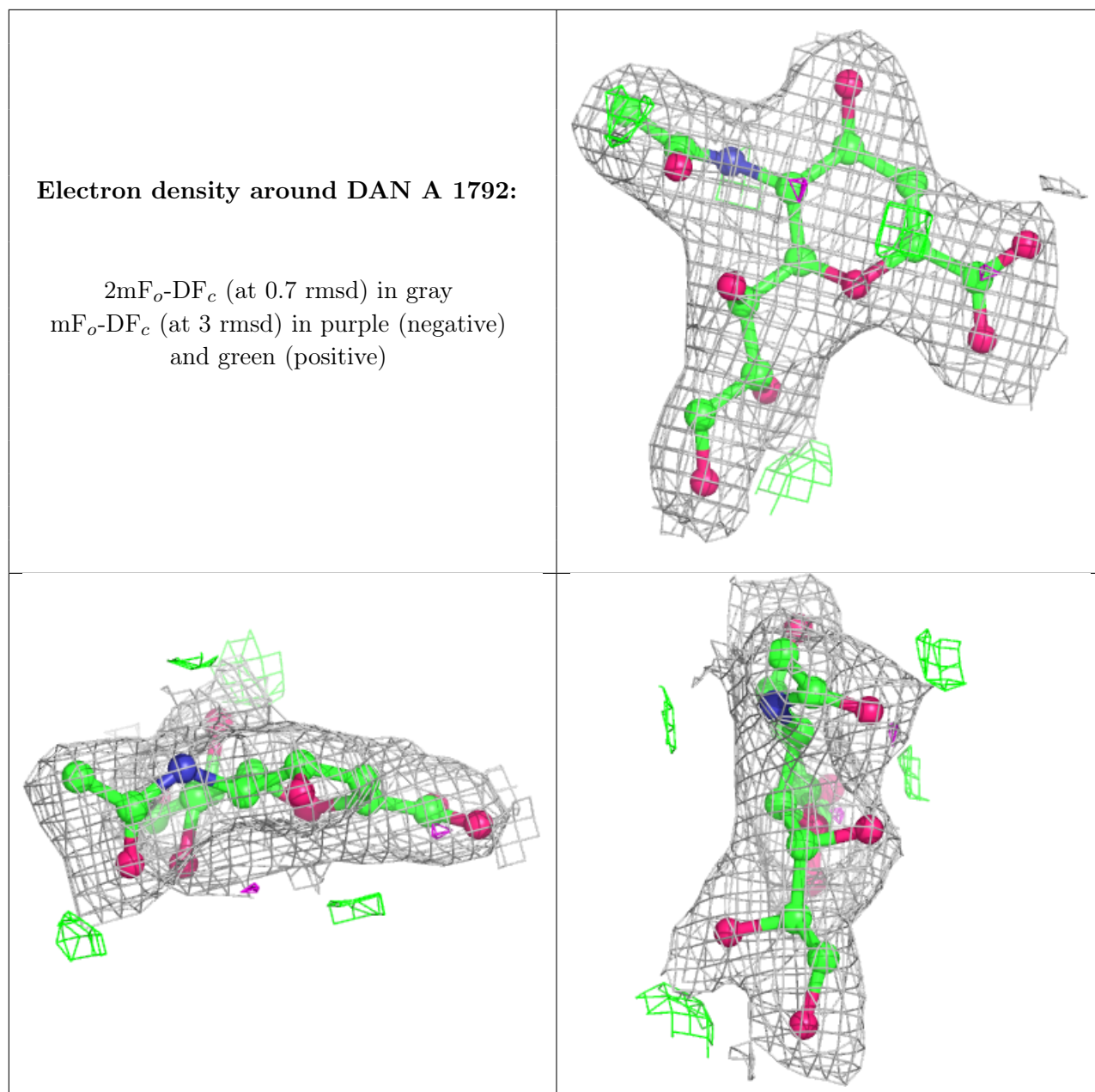
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DAN	B	1792	20/20	0.89	0.18	39,45,47,48	0
2	DAN	A	1792	20/20	0.93	0.15	22,24,26,27	0
3	CL	A	1793	1/1	0.96	0.05	32,32,32,32	0

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 DAN B 1792:

$2mF_o-DF_c$ (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.