



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:48 AM UTC

PDB ID : 1WCQ / pdb_00001wcq
Title : Mutagenesis of the Nucleophilic Tyrosine in a Bacterial Sialidase to Phenylalanine.
Authors : Newstead, S.; Watson, J.N.; Bennet, A.J.; Taylor, G.
Deposited on : 2004-11-19
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

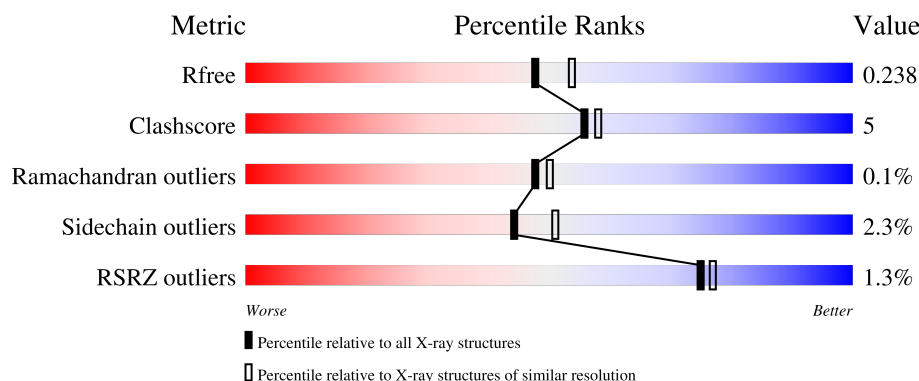
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	601	88% 12% .
1	B	601	89% 10% .
1	C	601	88% 11% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14833 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	6	0
			4556	2822	823	903	8			
1	B	601	Total	C	N	O	S	0	9	0
			4569	2830	824	908	7			
1	C	599	Total	C	N	O	S	0	1	0
			4525	2805	817	895	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	PHE	TYR	engineered mutation	UNP Q02834
B	370	PHE	TYR	engineered mutation	UNP Q02834
C	370	PHE	TYR	engineered mutation	UNP Q02834

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

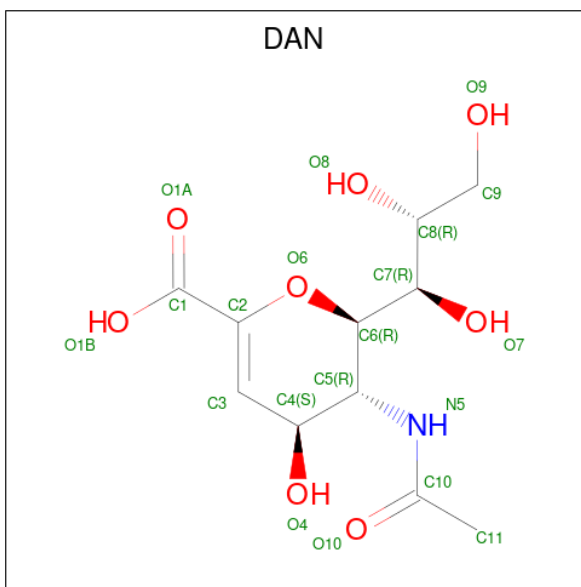
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (CCD ID: DAN) (formula: C₁₁H₁₇NO₈).



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

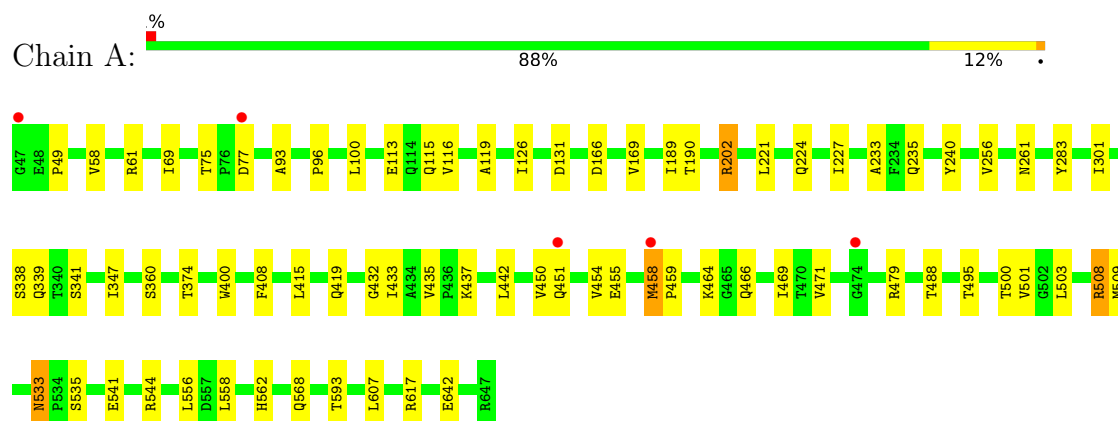
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	320	Total	O	0	0
			320	320		
5	B	399	Total	O	0	0
			399	399		
5	C	359	Total	O	0	0
			359	359		

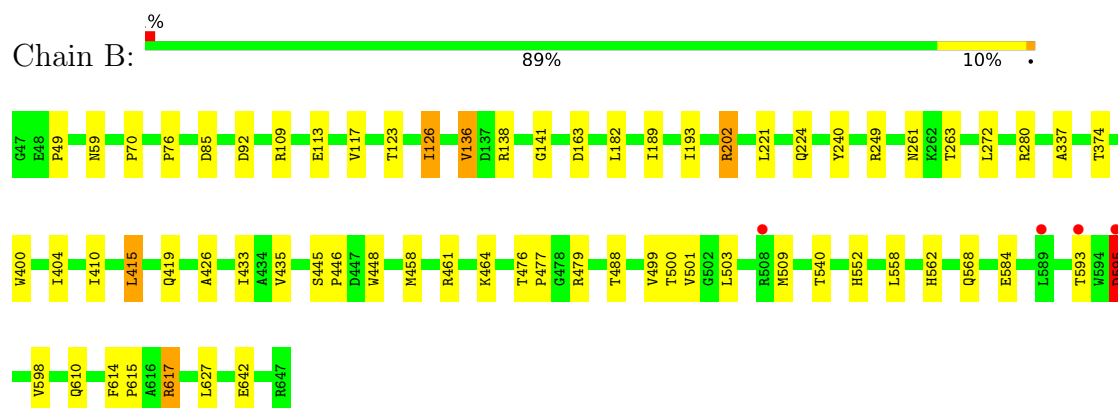
3 Residue-property plots

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.

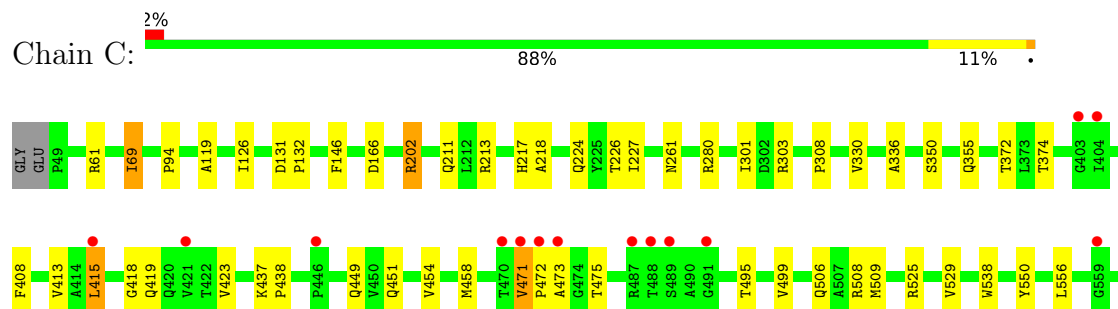
• Molecule 1: SIALIDASE



• Molecule 1: SIALIDASE



• Molecule 1: SIALIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.26Å 143.26Å 160.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	124.03 – 2.10 124.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (124.03-2.10) 99.9 (124.03-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.238 0.177 , 0.238	Depositor DCC
R_{free} test set	5544 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14833	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: GOL, DAN, NA

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	1.22	6/4691 (0.1%)	1.09	7/6403 (0.1%)
1	B	1.29	12/4713 (0.3%)	1.12	10/6433 (0.2%)
1	C	1.22	11/4636 (0.2%)	1.08	3/6329 (0.0%)
All	All	1.24	29/14040 (0.2%)	1.10	20/19165 (0.1%)

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	B	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	595	ASP	CG-OD1	25.48	1.73	1.25
1	A	451	GLN	CD-NE2	20.10	1.75	1.33
1	C	419	GLN	CD-OE1	9.05	1.40	1.23
1	B	126	ILE	CA-CB	7.48	1.61	1.54
1	C	471	VAL	CA-C	7.43	1.59	1.52
1	B	595	ASP	CB-CG	7.10	1.69	1.52
1	A	451	GLN	CD-OE1	-6.92	1.10	1.23
1	C	525	ARG	N-CA	6.78	1.54	1.46
1	C	471	VAL	C-O	6.66	1.31	1.23
1	C	608	ALA	CA-CB	6.42	1.62	1.53
1	B	617[A]	ARG	CZ-NH1	6.24	1.41	1.32
1	B	617[B]	ARG	CZ-NH1	6.24	1.41	1.32
1	C	166	ASP	CA-C	6.12	1.60	1.52
1	B	193	ILE	CA-CB	6.07	1.60	1.54
1	C	419	GLN	CG-CD	6.04	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	ALA	CA-CB	5.94	1.61	1.53
1	B	426	ALA	CA-CB	5.89	1.62	1.53
1	A	93	ALA	CA-CB	5.72	1.61	1.53
1	A	100	LEU	CA-C	-5.66	1.45	1.52
1	B	189	ILE	CA-CB	5.61	1.60	1.54
1	A	451	GLN	CG-CD	5.58	1.66	1.52
1	C	372	THR	CA-CB	5.50	1.63	1.53
1	B	337	ALA	CA-CB	-5.42	1.45	1.52
1	B	136	VAL	CA-CB	5.42	1.60	1.54
1	C	418	GLY	C-O	5.41	1.32	1.24
1	B	70	PRO	CA-C	5.33	1.59	1.52
1	C	529	VAL	CA-CB	5.26	1.60	1.54
1	A	533	ASN	CA-C	5.03	1.58	1.52
1	B	404	ILE	CA-CB	5.01	1.61	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	GLN	CG-CD-NE2	-13.92	95.53	116.40
1	A	451	GLN	OE1-CD-NE2	12.78	135.38	122.60
1	B	595	ASP	CB-CG-OD1	-11.04	93.00	118.40
1	B	595	ASP	CB-CG-OD2	6.37	133.04	118.40
1	C	419	GLN	CB-CG-CD	-6.17	102.11	112.60
1	B	614	PHE	CA-C-N	-5.93	113.83	119.76
1	B	614	PHE	C-N-CA	-5.93	113.83	119.76
1	C	471	VAL	CA-C-N	-5.87	114.71	120.52
1	C	471	VAL	C-N-CA	-5.87	114.71	120.52
1	B	117	VAL	N-CA-C	-5.69	106.16	111.45
1	B	85	ASP	CB-CA-C	-5.68	99.92	109.53
1	B	163	ASP	CA-C-N	5.38	125.71	119.47
1	B	163	ASP	C-N-CA	5.38	125.71	119.47
1	B	410	ILE	CA-C-N	-5.36	114.73	120.03
1	B	410	ILE	C-N-CA	-5.36	114.73	120.03
1	A	419	GLN	N-CA-C	5.13	117.47	110.55
1	A	458[A]	MET	CA-C-N	5.06	125.35	119.93
1	A	458[A]	MET	C-N-CA	5.06	125.35	119.93
1	A	458[B]	MET	CA-C-N	5.06	125.35	119.93
1	A	458[B]	MET	C-N-CA	5.06	125.35	119.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	595	ASP	Sidechain

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	4556	0	4370	47	0
1	B	4569	0	4383	40	0
1	C	4525	0	4350	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	12	0	16	1	0
3	B	18	0	24	1	0
3	C	12	0	16	0	0
4	A	20	0	16	0	0
4	B	20	0	16	0	0
4	C	20	0	16	0	0
5	A	320	0	0	5	0
5	B	399	0	0	15	0
5	C	359	0	0	7	0
All	All	14833	0	13207	128	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 (128) 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:C:413:VAL:HG11	1:C:423:VAL:HG11	1.28	1.13
1:C:640:GLU:HB3	5:C:2355:HOH:O	1.46	1.11
1:C:590:ASN:HD21	1:C:593:THR:HG23	1.16	1.04
1:B:562:HIS:HE1	5:B:2354:HOH:O	1.40	1.02
1:C:413:VAL:HG11	1:C:423:VAL:CG1	1.94	0.96
1:C:355:GLN:HG2	5:C:2228:HOH:O	1.65	0.95
1:C:413:VAL:CG1	1:C:423:VAL:HG11	1.97	0.94
1:C:458:MET:HG2	5:C:2132:HOH:O	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:PRO:HD2	5:B:2295:HOH:O	1.76	0.83
1:C:590:ASN:HD21	1:C:593:THR:CG2	1.89	0.83
1:B:509:MET:HE3	1:B:558:LEU:CD2	2.14	0.78
1:B:182:LEU:HD12	5:B:2122:HOH:O	1.84	0.77
1:B:224:GLN:HE21	1:B:261:ASN:HD21	1.35	0.73
1:C:509[A]:MET:CE	1:C:556:LEU:HD13	2.20	0.72
1:B:202:ARG:HD3	5:B:2136:HOH:O	1.90	0.71
1:B:224:GLN:HE21	1:B:261:ASN:ND2	1.87	0.71
1:C:202:ARG:HD3	5:C:2123:HOH:O	1.90	0.71
1:B:419:GLN:HG2	5:B:2277:HOH:O	1.90	0.71
1:A:224:GLN:HE21	1:A:261:ASN:ND2	1.89	0.71
1:A:509[B]:MET:HE1	1:A:556:LEU:HD13	1.75	0.69
1:A:224:GLN:HE21	1:A:261:ASN:HD21	1.40	0.68
1:C:590:ASN:ND2	1:C:593:THR:HG23	2.00	0.68
1:B:509:MET:CE	1:B:558:LEU:HD23	2.25	0.66
1:A:202:ARG:HD3	5:A:2094:HOH:O	1.95	0.65
1:B:509:MET:CE	1:B:558:LEU:CD2	2.75	0.65
1:B:509:MET:HE3	1:B:558:LEU:HD22	1.79	0.65
1:B:109:ARG:NH2	5:B:2059:HOH:O	2.29	0.64
1:B:479:ARG:HD3	5:B:2312:HOH:O	1.96	0.64
1:C:224:GLN:HE21	1:C:261:ASN:HD21	1.46	0.64
1:A:58:VAL:HB	1:A:61:ARG:HD2	1.81	0.62
1:A:509[B]:MET:HE3	1:A:558:LEU:HD23	1.80	0.61
1:A:455:GLU:HG3	1:A:464:LYS:O	2.01	0.61
1:C:224:GLN:HE21	1:C:261:ASN:ND2	1.99	0.61
1:A:283:TYR:CZ	1:A:339:GLN:NE2	2.68	0.60
1:A:607:LEU:HD11	3:A:1650:GOL:H12	1.83	0.60
1:B:182:LEU:CD1	5:B:2122:HOH:O	2.45	0.59
1:B:509:MET:HE3	1:B:558:LEU:HD23	1.83	0.59
1:A:233:ALA:HB1	1:A:256:VAL:HG12	1.85	0.58
1:A:562:HIS:HE1	5:A:2269:HOH:O	1.86	0.58
1:C:69:ILE:HG21	1:C:131:ASP:HA	1.85	0.58
1:C:562:HIS:HD2	1:C:646:GLN:O	1.86	0.57
1:C:202:ARG:CD	5:C:2123:HOH:O	2.50	0.56
1:B:458:MET:HE3	1:B:461:ARG:HG3	1.86	0.56
1:A:479:ARG:NH1	1:A:642:GLU:OE2	2.39	0.55
1:C:509[A]:MET:HE2	1:C:556:LEU:HD13	1.87	0.55
1:C:473:ALA:HA	5:C:2277:HOH:O	2.07	0.54
1:C:211:GLN:HB3	1:C:213:ARG:HH21	1.72	0.54
1:B:598:VAL:HG12	1:B:617[A]:ARG:NH1	2.23	0.53
1:A:458[B]:MET:HE2	1:A:459:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:HG21	1:A:131:ASP:HA	1.90	0.53
1:C:413:VAL:HG22	1:C:499:VAL:HG22	1.90	0.53
1:B:435:VAL:HG11	1:B:488:THR:HB	1.91	0.52
1:B:500:THR:HG23	1:B:503:LEU:HD12	1.91	0.52
1:A:227:ILE:HD11	1:A:235:GLN:HB2	1.92	0.52
1:A:75:THR:OG1	1:A:77:ASP:HB2	2.09	0.51
1:B:615:PRO:O	1:B:617[B]:ARG:HD2	2.10	0.51
1:C:509[A]:MET:HE1	1:C:556:LEU:HD13	1.92	0.50
1:B:59:ASN:O	5:B:2007:HOH:O	2.19	0.50
1:C:642:GLU:HG2	5:C:2355:HOH:O	2.10	0.50
1:A:509[B]:MET:HE3	1:A:558:LEU:CD2	2.40	0.50
1:C:584:GLU:HB3	1:C:597:PRO:HB3	1.94	0.50
1:B:509:MET:HE2	1:B:558:LEU:HD23	1.95	0.49
1:A:113:GLU:CG	1:A:115:GLN:HG2	2.43	0.49
1:C:415:LEU:HD11	1:C:471:VAL:HG21	1.95	0.49
1:B:464:LYS:HD2	5:B:2300:HOH:O	2.12	0.48
1:A:408:PHE:CE1	1:A:495:THR:HG22	2.48	0.48
1:A:415:LEU:HD11	1:A:501:VAL:HG22	1.94	0.48
1:B:445:SER:HB2	1:B:448:TRP:CD1	2.48	0.48
1:A:500:THR:CG2	1:A:503:LEU:HB2	2.43	0.48
1:C:585:ILE:HD12	1:C:599:ALA:HB3	1.95	0.48
1:B:249:ARG:HG2	5:B:2162:HOH:O	2.13	0.47
1:C:408:PHE:CE1	1:C:495:THR:HG22	2.48	0.47
1:B:540:THR:HG21	1:B:552:HIS:CG	2.50	0.47
1:A:450:VAL:HG22	1:A:469:ILE:HG23	1.96	0.47
1:A:432:GLY:O	1:A:459:PRO:HB3	2.14	0.47
1:A:435:VAL:HG11	1:A:488:THR:HB	1.96	0.47
1:A:442:LEU:HD13	1:A:450:VAL:HG12	1.97	0.47
1:C:631:THR:OG1	1:C:633:HIS:CE1	2.68	0.47
1:C:438:PRO:HG2	1:C:454:VAL:HG13	1.97	0.47
1:C:472:PRO:HD2	1:C:475:THR:OG1	2.15	0.47
1:C:562:HIS:CD2	1:C:646:GLN:O	2.68	0.47
1:C:308:PRO:HD3	1:C:336:ALA:O	2.15	0.46
1:C:506:GLN:HA	1:C:509[A]:MET:SD	2.55	0.46
1:A:533:ASN:OD1	1:A:535:SER:HB2	2.16	0.46
1:B:562:HIS:CE1	5:B:2354:HOH:O	2.31	0.46
1:B:598:VAL:CG1	1:B:617[A]:ARG:NH1	2.79	0.46
1:B:584:GLU:HG3	1:B:627:LEU:HD11	1.97	0.45
1:B:479:ARG:CD	5:B:2312:HOH:O	2.62	0.45
1:B:479:ARG:NE	1:B:642:GLU:OE2	2.48	0.45
1:C:202:ARG:HB3	1:C:227:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:HD11	1:A:471:VAL:HG21	1.98	0.45
1:A:96:PRO:HB3	1:A:126:ILE:HG23	1.98	0.45
1:B:126:ILE:HG12	5:B:2081:HOH:O	2.16	0.45
1:A:221:LEU:O	1:A:240:TYR:HA	2.17	0.44
1:B:49:PRO:HB3	1:B:400:TRP:HA	2.00	0.44
1:C:202:ARG:HA	1:C:226:THR:O	2.17	0.44
1:B:136:VAL:HG12	1:B:138:ARG:HG2	2.00	0.43
1:B:221:LEU:O	1:B:240:TYR:HA	2.19	0.43
1:C:217:HIS:O	1:C:218:ALA:C	2.58	0.43
1:A:415:LEU:CD1	1:A:501:VAL:HG22	2.49	0.43
1:A:479:ARG:NH1	1:A:642:GLU:CD	2.77	0.43
1:A:642:GLU:HG3	5:A:2272:HOH:O	2.18	0.43
1:A:116:VAL:HG11	1:A:119:ALA:HB2	2.01	0.43
1:C:330:VAL:HA	1:C:350:SER:O	2.19	0.43
1:A:227:ILE:CD1	1:A:235:GLN:HB2	2.48	0.43
1:A:541:GLU:OE2	1:A:544:ARG:HD3	2.19	0.43
1:C:550:TYR:CE2	1:C:629:GLU:HB2	2.54	0.42
1:A:508:ARG:CZ	5:A:2240:HOH:O	2.67	0.42
3:B:1650:GOL:H2	5:B:2367:HOH:O	2.19	0.42
1:C:508:ARG:HA	1:C:508:ARG:HD2	1.89	0.42
1:B:477:PRO:HA	1:B:501:VAL:O	2.20	0.42
1:C:538:TRP:O	1:C:637:ALA:HA	2.19	0.42
1:A:509[B]:MET:HE1	1:A:556:LEU:CD1	2.46	0.42
1:A:509[B]:MET:CE	1:A:556:LEU:HD13	2.46	0.42
1:A:166:ASP:CG	1:A:169:VAL:HG23	2.44	0.41
1:A:189:ILE:O	1:A:190:THR:C	2.63	0.41
1:B:263:THR:HA	1:B:272:LEU:O	2.20	0.41
1:B:415:LEU:HD11	1:B:499:VAL:CG1	2.51	0.41
1:A:49:PRO:HB3	1:A:400:TRP:HA	2.02	0.41
1:A:338:SER:HB3	1:A:341:SER:O	2.21	0.41
1:A:617:ARG:HD2	5:A:2304:HOH:O	2.21	0.41
1:B:76:PRO:HG2	1:B:141:GLY:HA2	2.03	0.41
1:A:283:TYR:CE1	1:A:339:GLN:NE2	2.89	0.40
1:A:568:GLN:HB2	1:A:642:GLU:HB2	2.02	0.40
1:B:568:GLN:HA	1:B:610:GLN:O	2.21	0.40
1:A:347:ILE:O	1:A:360:SER:HA	2.20	0.40
1:C:132:PRO:HA	1:C:146:PHE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	605/601 (101%)	588 (97%)	17 (3%)	0	100	100
1	B	608/601 (101%)	590 (97%)	18 (3%)	0	100	100
1	C	598/601 (100%)	583 (98%)	14 (2%)	1 (0%)	43	44
All	All	1811/1803 (100%)	1761 (97%)	49 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	69	ILE

5.3.2 Protein sidechains

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	483/477 (101%)	474 (98%)	9 (2%)	50	58
1	B	486/477 (102%)	474 (98%)	12 (2%)	42	48
1	C	477/477 (100%)	464 (97%)	13 (3%)	39	45
All	All	1446/1431 (101%)	1412 (98%)	34 (2%)	44	49

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ARG
1	A	301	ILE

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Mol	Chain	Res	Type
1	A	374	THR
1	A	433	ILE
1	A	437	LYS
1	A	454	VAL
1	A	466	GLN
1	A	508	ARG
1	A	593	THR
1	B	92	ASP
1	B	113[A]	GLU
1	B	113[B]	GLU
1	B	123	THR
1	B	202	ARG
1	B	280	ARG
1	B	374	THR
1	B	415	LEU
1	B	433	ILE
1	B	476	THR
1	B	593	THR
1	B	595	ASP
1	C	61	ARG
1	C	94	PRO
1	C	126	ILE
1	C	202	ARG
1	C	280	ARG
1	C	301	ILE
1	C	303	ARG
1	C	374	THR
1	C	415	LEU
1	C	437	LYS
1	C	449	GLN
1	C	451	GLN
1	C	593	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	261	ASN
1	A	355	GLN
1	A	420	GLN
1	A	562	HIS
1	B	151	GLN

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Mol	Chain	Res	Type
1	B	173	ASN
1	B	217	HIS
1	B	261	ASN
1	B	395	ASN
1	B	451	GLN
1	B	646	GLN
1	C	54	GLN
1	C	66	ASN
1	C	114	GLN
1	C	173	ASN
1	C	217	HIS
1	C	224	GLN
1	C	261	ASN
1	C	355	GLN
1	C	395	ASN
1	C	420	GLN
1	C	441	GLN
1	C	562	HIS

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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	GOL	B	1649	-	5,5,5	0.84	0	5,5,5	0.52	0
3	GOL	C	1649	-	5,5,5	1.10	0	5,5,5	0.40	0
3	GOL	C	1650	-	5,5,5	0.81	0	5,5,5	0.76	0
3	GOL	A	1650	-	5,5,5	0.85	0	5,5,5	0.77	0
3	GOL	B	1650	-	5,5,5	0.90	0	5,5,5	0.75	0
3	GOL	A	1649	-	5,5,5	0.77	0	5,5,5	0.55	0
4	DAN	C	1651	-	20,20,20	3.10	11 (55%)	24,28,28	2.18	4 (16%)
4	DAN	A	1651	-	20,20,20	2.64	9 (45%)	24,28,28	3.07	12 (50%)
4	DAN	B	1652	-	20,20,20	2.90	5 (25%)	24,28,28	2.40	9 (37%)
3	GOL	B	1651	-	5,5,5	1.09	0	5,5,5	0.39	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	GOL	B	1649	-	-	2/4/4/4	-
3	GOL	C	1649	-	-	4/4/4/4	-
3	GOL	C	1650	-	-	2/4/4/4	-
3	GOL	A	1650	-	-	3/4/4/4	-
3	GOL	B	1650	-	-	2/4/4/4	-
3	GOL	A	1649	-	-	2/4/4/4	-
4	DAN	C	1651	-	-	1/18/34/34	0/1/1/1
4	DAN	A	1651	-	-	1/18/34/34	0/1/1/1
4	DAN	B	1652	-	-	1/18/34/34	0/1/1/1
3	GOL	B	1651	-	-	4/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1651	DAN	O10-C10	7.53	1.40	1.23
4	B	1652	DAN	O6-C6	-7.43	1.33	1.46
4	B	1652	DAN	O10-C10	7.25	1.39	1.23
4	C	1651	DAN	O10-C10	6.86	1.38	1.23
4	C	1651	DAN	C3-C2	6.00	1.43	1.33
4	B	1652	DAN	C3-C2	5.48	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1651	DAN	C4-C3	5.27	1.57	1.50
4	C	1651	DAN	C10-N5	4.31	1.48	1.34
4	A	1651	DAN	C4-C5	-3.91	1.48	1.53
4	A	1651	DAN	C2-C1	3.59	1.57	1.48
4	A	1651	DAN	C3-C2	3.46	1.39	1.33
4	A	1651	DAN	C10-N5	3.22	1.44	1.34
4	C	1651	DAN	C11-C10	3.21	1.57	1.50
4	A	1651	DAN	C4-C3	3.09	1.54	1.50
4	C	1651	DAN	C6-C5	2.91	1.57	1.53
4	C	1651	DAN	O1B-C1	-2.89	1.22	1.30
4	B	1652	DAN	C10-N5	2.78	1.43	1.34
4	C	1651	DAN	C4-C5	2.72	1.56	1.53
4	C	1651	DAN	C8-C7	-2.69	1.48	1.53
4	C	1651	DAN	C2-C1	2.59	1.54	1.48
4	A	1651	DAN	C8-C7	-2.57	1.48	1.53
4	B	1652	DAN	O1B-C1	-2.47	1.23	1.30
4	C	1651	DAN	O7-C7	2.22	1.48	1.43
4	A	1651	DAN	C11-C10	2.15	1.55	1.50
4	A	1651	DAN	O1B-C1	-2.00	1.25	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1651	DAN	O10-C10-N5	-7.97	107.90	121.98
4	B	1652	DAN	O10-C10-C11	-6.37	110.72	122.05
4	B	1652	DAN	O10-C10-N5	-5.96	111.45	121.98
4	A	1651	DAN	O10-C10-C11	-5.70	111.90	122.05
4	C	1651	DAN	O10-C10-C11	-5.57	112.14	122.05
4	C	1651	DAN	O10-C10-N5	-5.55	112.18	121.98
4	C	1651	DAN	C5-N5-C10	-5.02	111.36	123.11
4	A	1651	DAN	O9-C9-C8	-4.88	100.90	111.16
4	A	1651	DAN	C4-C5-N5	-4.87	105.67	111.13
4	A	1651	DAN	O6-C2-C3	-4.75	119.31	124.62
4	B	1652	DAN	C4-C3-C2	-3.73	115.15	121.45
4	A	1651	DAN	O6-C2-C1	3.45	118.91	112.02
4	B	1652	DAN	C9-C8-C7	-2.99	106.08	112.17
4	A	1651	DAN	O7-C7-C6	2.75	115.40	109.44
4	A	1651	DAN	O4-C4-C3	2.73	115.44	109.27
4	B	1652	DAN	C11-C10-N5	-2.51	111.96	116.12
4	A	1651	DAN	C11-C10-N5	-2.49	112.00	116.12
4	C	1651	DAN	C4-C5-N5	-2.38	108.46	111.13
4	B	1652	DAN	C6-C5-N5	-2.35	107.16	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1651	DAN	C4-C3-C2	-2.32	117.52	121.45
4	A	1651	DAN	C6-C5-N5	-2.31	107.22	110.91
4	A	1651	DAN	C5-N5-C10	-2.20	117.97	123.11
4	B	1652	DAN	C5-N5-C10	-2.09	118.20	123.11
4	B	1652	DAN	O8-C8-C9	-2.03	104.40	109.03
4	B	1652	DAN	O6-C6-C7	-2.00	102.45	105.98

There are no chirality outliers.

All (22) torsion outliers are listed below:

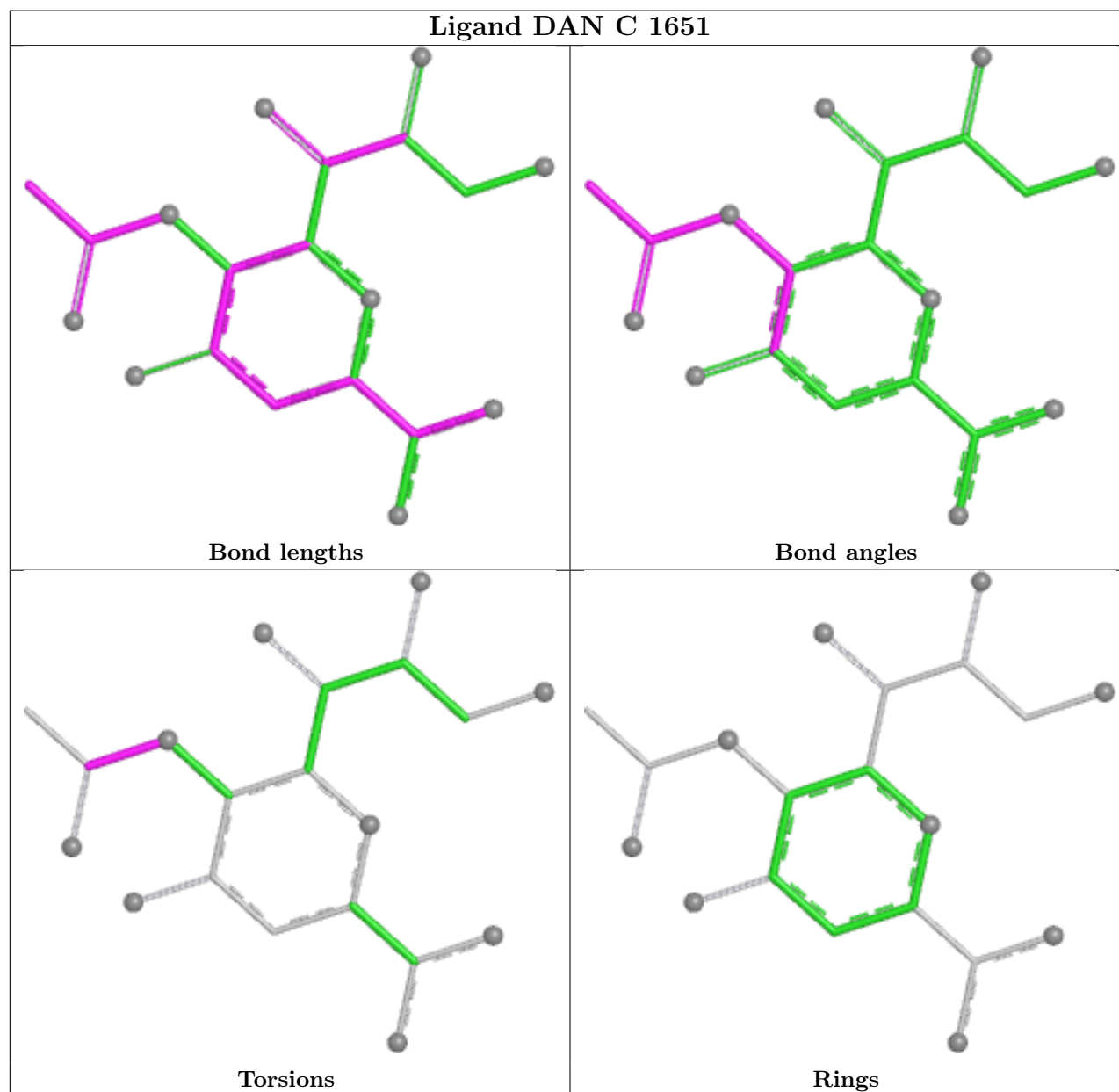
Mol	Chain	Res	Type	Atoms
3	A	1649	GOL	C1-C2-C3-O3
3	A	1650	GOL	C1-C2-C3-O3
3	B	1649	GOL	C1-C2-C3-O3
3	B	1650	GOL	C1-C2-C3-O3
3	B	1651	GOL	O1-C1-C2-O2
3	B	1651	GOL	O1-C1-C2-C3
3	B	1651	GOL	C1-C2-C3-O3
3	B	1651	GOL	O2-C2-C3-O3
3	C	1650	GOL	C1-C2-C3-O3
3	C	1650	GOL	O2-C2-C3-O3
4	B	1652	DAN	O10-C10-N5-C5
4	C	1651	DAN	O10-C10-N5-C5
4	A	1651	DAN	O10-C10-N5-C5
3	C	1649	GOL	O1-C1-C2-C3
3	A	1649	GOL	O2-C2-C3-O3
3	B	1649	GOL	O2-C2-C3-O3
3	B	1650	GOL	O2-C2-C3-O3
3	C	1649	GOL	O1-C1-C2-O2
3	A	1650	GOL	O2-C2-C3-O3
3	C	1649	GOL	C1-C2-C3-O3
3	A	1650	GOL	O1-C1-C2-C3
3	C	1649	GOL	O2-C2-C3-O3

There are no ring outliers.

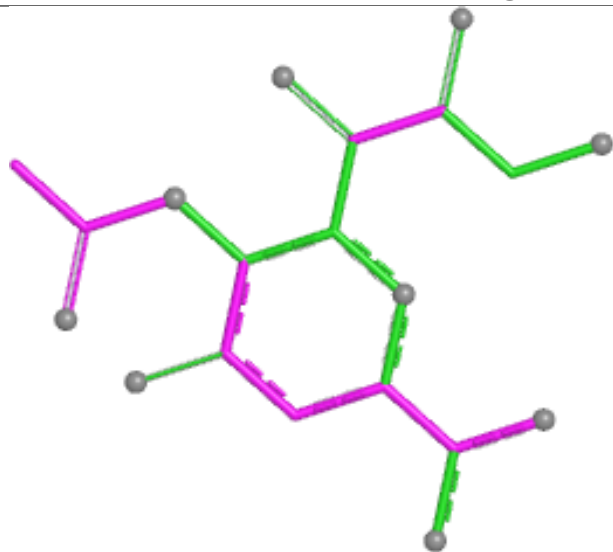
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1650	GOL	1	0
3	B	1650	GOL	1	0

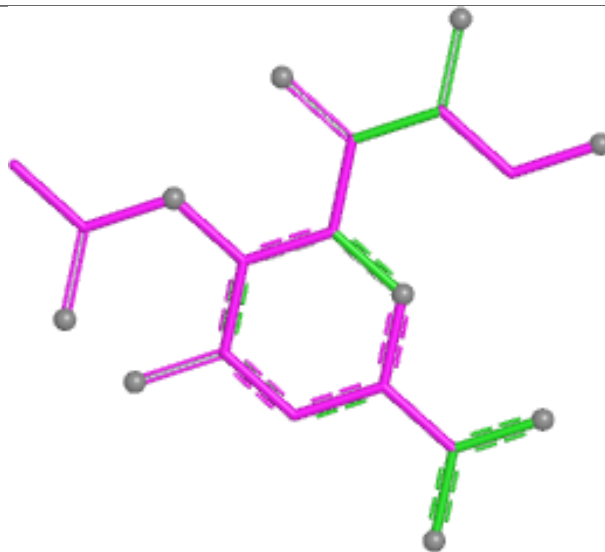
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



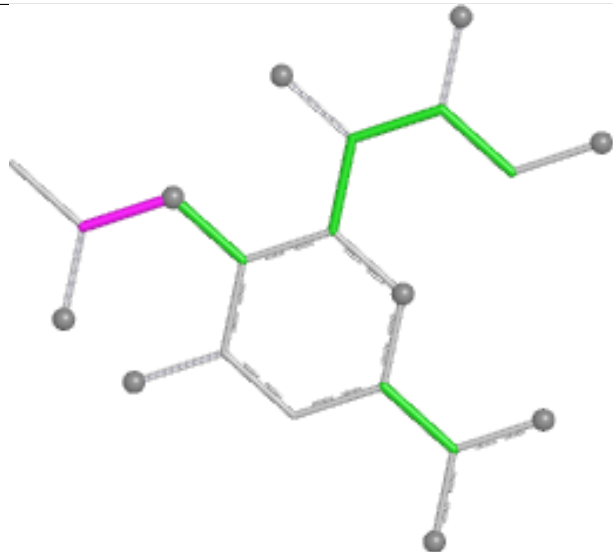
Ligand DAN A 1651



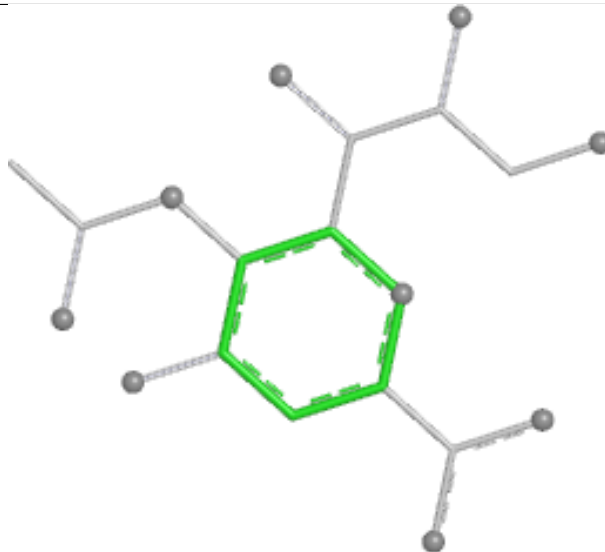
Bond lengths



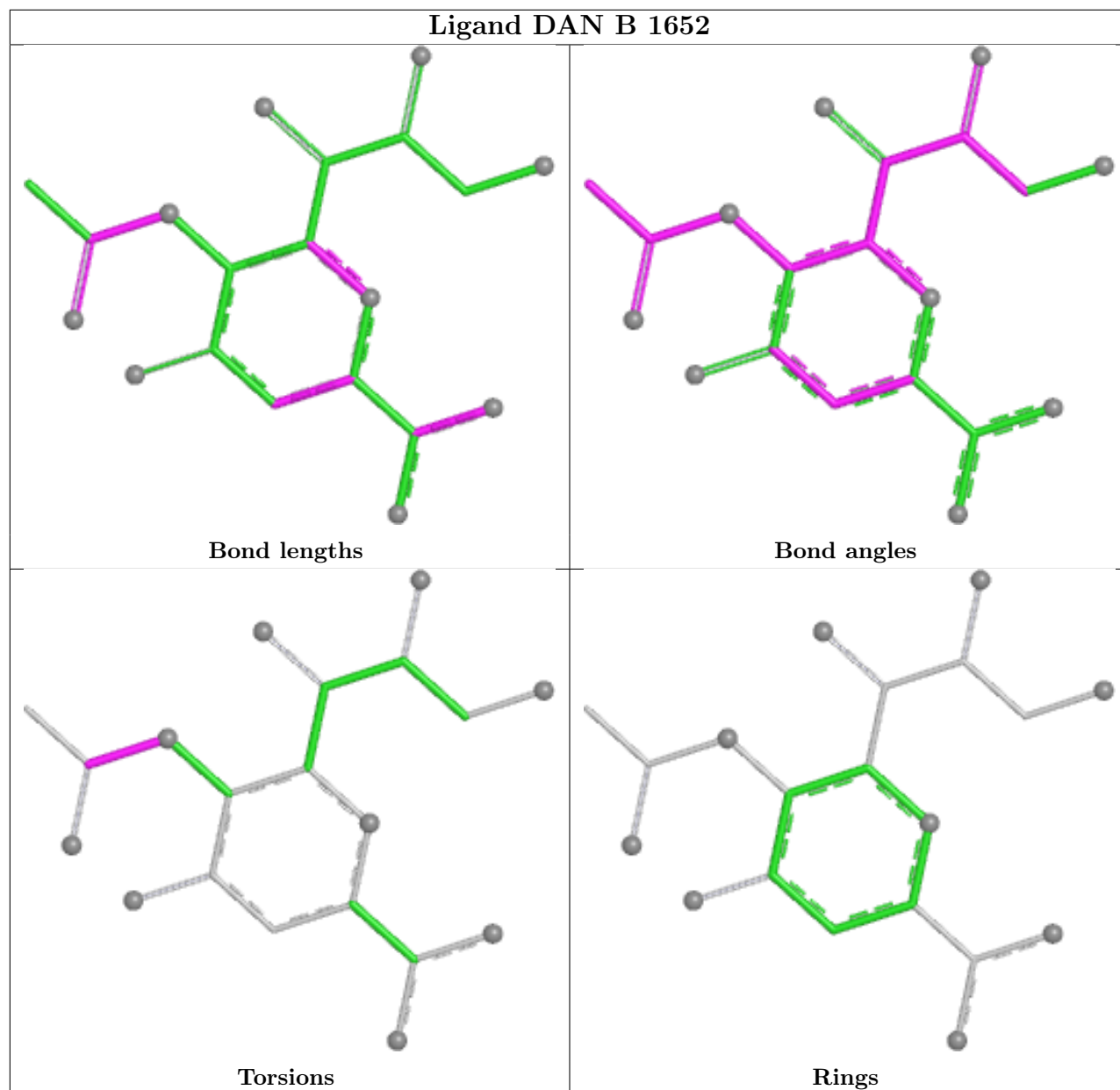
Bond angles



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, 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	601/601 (100%)	0.24	5 (0%) 82 84	15, 29, 45, 54	10 (1%)
1	B	601/601 (100%)	-0.08	4 (0%) 84 86	11, 26, 34, 45	17 (2%)
1	C	599/601 (99%)	0.15	14 (2%) 61 64	19, 27, 41, 54	5 (0%)
All	All	1801/1803 (99%)	0.10	23 (1%) 75 77	11, 28, 42, 54	32 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	GLN	5.1
1	C	471	VAL	4.2
1	C	403	GLY	3.5
1	A	458[A]	MET	2.9
1	C	487	ARG	2.8
1	C	559	GLY	2.8
1	C	415	LEU	2.8
1	B	595	ASP	2.7
1	C	446	PRO	2.5
1	C	473	ALA	2.5
1	B	593	THR	2.4
1	C	472	PRO	2.4
1	C	488	THR	2.4
1	C	404	ILE	2.3
1	B	589	LEU	2.3
1	C	489	SER	2.2
1	C	491	GLY	2.2
1	C	470	THR	2.1
1	A	77	ASP	2.1
1	A	47	GLY	2.1
1	A	474	GLY	2.1
1	B	508	ARG	2.0
1	C	421	VAL	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](#)

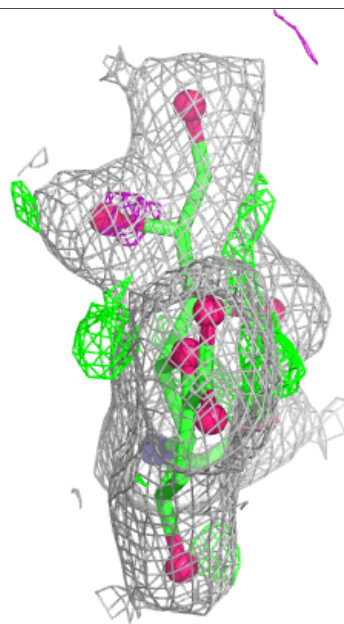
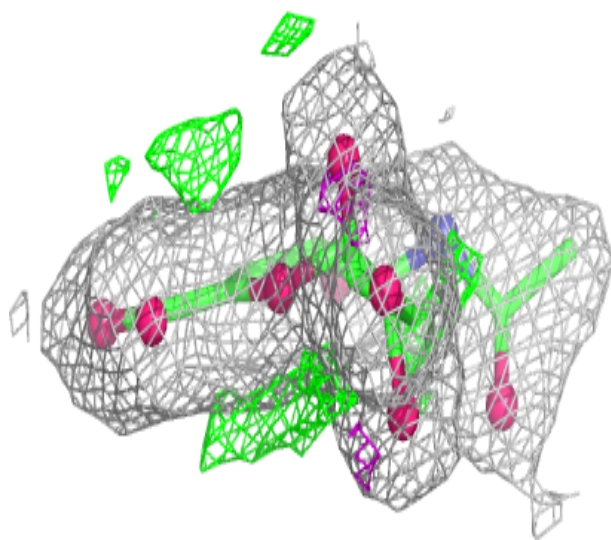
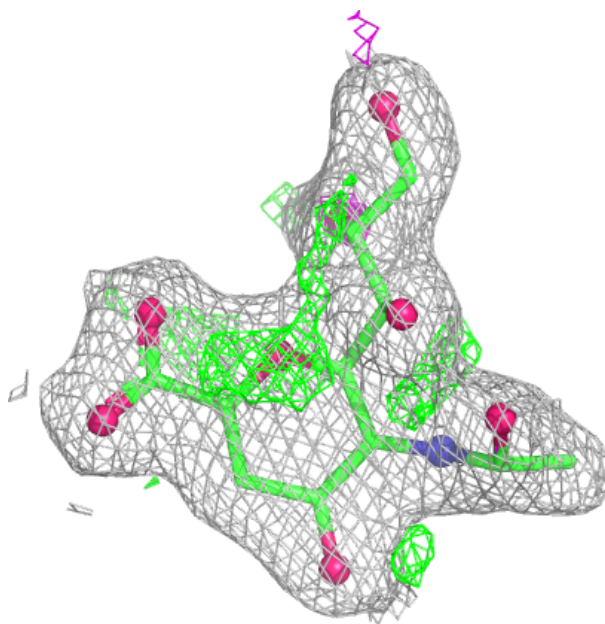
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1649	6/6	0.73	0.14	52,60,63,63	0
3	GOL	B	1649	6/6	0.77	0.17	55,56,57,57	0
3	GOL	C	1649	6/6	0.77	0.15	49,55,55,57	0
3	GOL	A	1650	6/6	0.78	0.14	60,63,64,64	0
3	GOL	C	1650	6/6	0.83	0.14	40,44,47,48	0
3	GOL	B	1651	6/6	0.84	0.17	62,66,67,67	0
4	DAN	B	1652	20/20	0.92	0.08	16,22,27,27	0
4	DAN	C	1651	20/20	0.92	0.08	18,22,28,29	0
3	GOL	B	1650	6/6	0.93	0.12	31,36,39,44	0
4	DAN	A	1651	20/20	0.94	0.07	22,27,31,33	0
2	NA	B	1648	1/1	0.98	0.12	17,17,17,17	0
2	NA	A	1648	1/1	0.99	0.05	19,19,19,19	0
2	NA	C	1648	1/1	0.99	0.06	13,13,13,13	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.

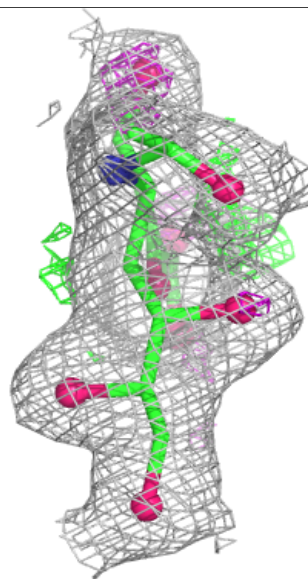
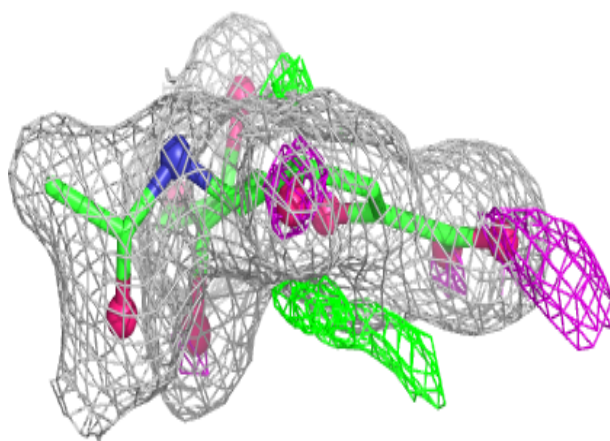
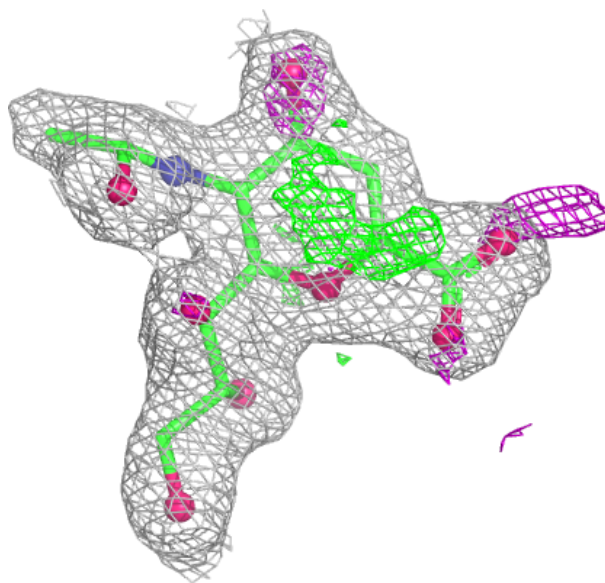
Electron density around DAN B 1652:

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



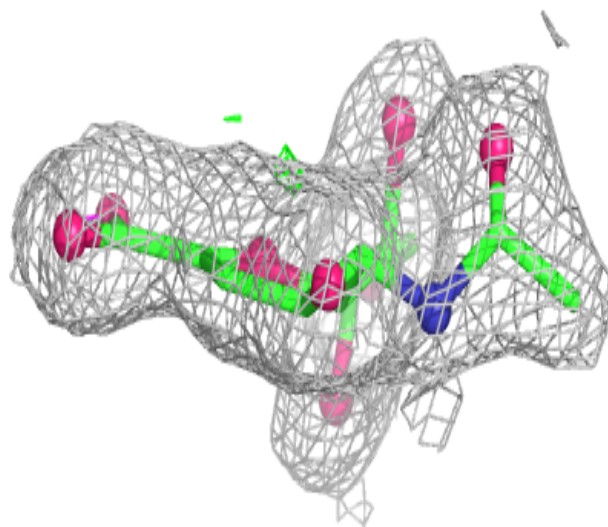
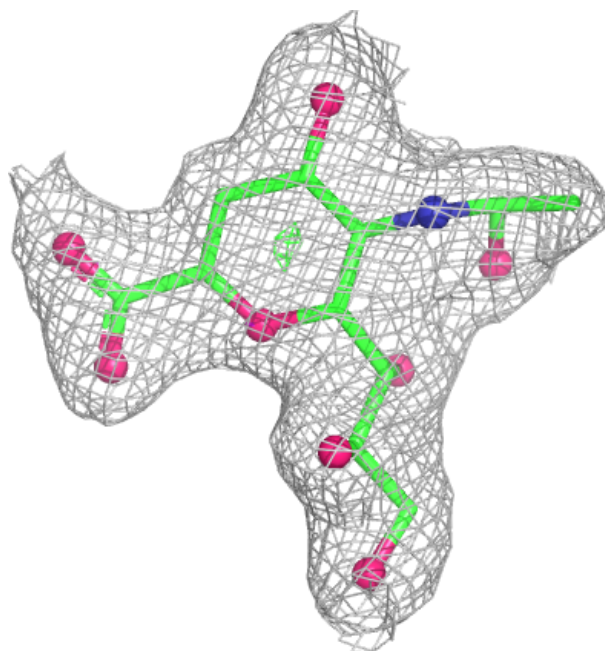
Electron density around DAN C 1651:

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



Electron density around DAN A 1651:

$2mF_o-DF_c$ (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.