



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:34 AM UTC

PDB ID : 2CEX / pdb_00002cex
Title : Structure of a sialic acid binding protein (SiaP) in the presence of the sialic acid analogue Neu5Ac2en
Authors : Muller, A.; Severi, E.; Mulligan, C.; Watts, A.G.; Kelly, D.J.; Wilson, K.S.; Wilkinson, A.J.; Thomas, G.H.
Deposited on : 2006-02-10
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

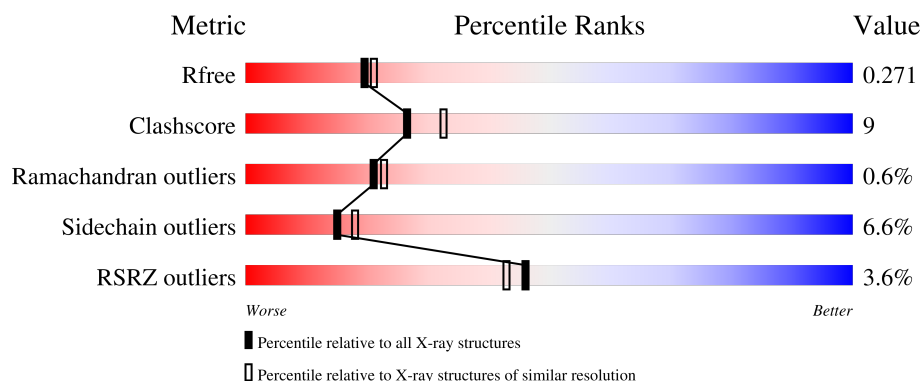
1 Overall quality at a glance

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	306	0% 77% 20% ..
1	B	306	72% 23% .
1	C	306	11% 73% 21% ...
1	D	306	2% 81% 16% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	1308	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10023 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.

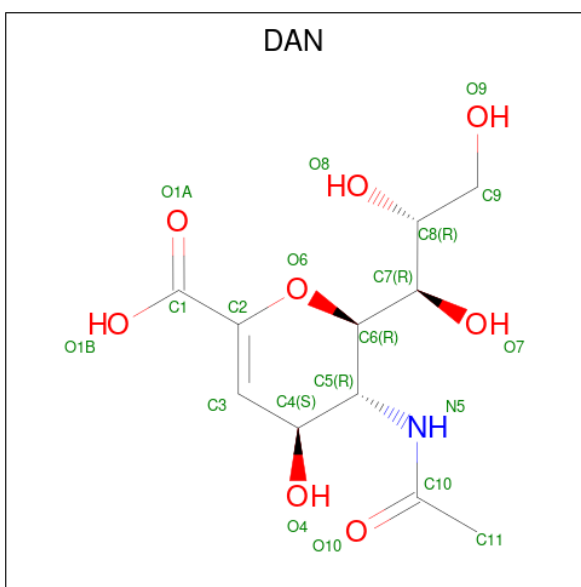
- Molecule 1 is a protein called PROTEIN HI0146.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2362	1516	382	456	8			
1	B	305	Total	C	N	O	S	0	0	0
			2404	1538	391	467	8			
1	C	300	Total	C	N	O	S	0	1	0
			2357	1511	383	455	8			
1	D	305	Total	C	N	O	S	0	0	0
			2401	1536	391	466	8			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

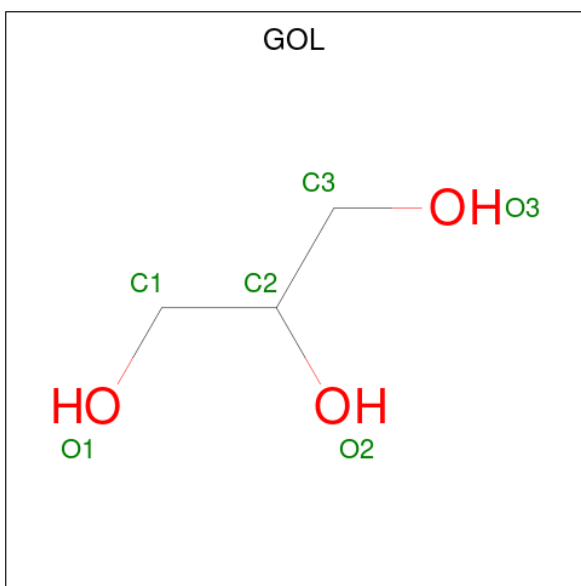
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	1	Total	Zn	0	0
			1	1		

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



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

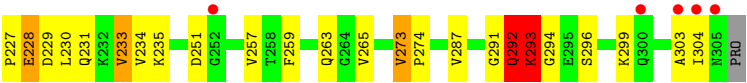
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



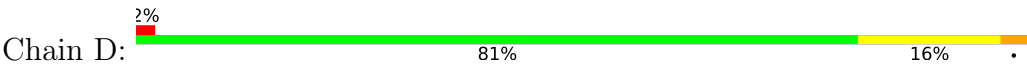
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total 89	O 89	0	0
5	B	147	Total 147	O 147	0	0
5	C	97	Total 97	O 97	0	0
5	D	122	Total 122	O 122	0	0



● Molecule 1: PROTEIN HI0146



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.45Å 88.70Å 115.91Å 90.00° 105.33° 90.00°	Depositor
Resolution (Å)	111.80 – 2.20 111.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	75.6 (111.80-2.20) 60.0 (111.79-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.280 (Not available) , 0.271	Depositor DCC
R_{free} test set	2001 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10023	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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, ZN, DAN

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	0.99	0/2408	1.08	4/3254 (0.1%)
1	B	1.13	4/2451 (0.2%)	1.17	4/3307 (0.1%)
1	C	1.05	5/2402 (0.2%)	1.15	9/3244 (0.3%)
1	D	1.07	1/2447 (0.0%)	1.15	4/3302 (0.1%)
All	All	1.06	10/9708 (0.1%)	1.14	21/13107 (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	C	0	3
1	D	0	3
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	257	VAL	CA-CB	7.03	1.63	1.54
1	B	267	ILE	CA-CB	6.76	1.63	1.54
1	D	233	VAL	CA-CB	6.70	1.62	1.54
1	C	265	VAL	CA-CB	6.21	1.62	1.54
1	C	273	VAL	CA-CB	5.92	1.57	1.54
1	C	218	VAL	CA-CB	5.75	1.62	1.54
1	C	287	VAL	CA-CB	5.27	1.61	1.54
1	B	82	ALA	CA-CB	-5.22	1.44	1.53
1	B	233	VAL	CA-CB	5.11	1.61	1.54
1	B	92	VAL	CA-CB	5.09	1.61	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	LYS	N-CA-C	7.51	122.46	112.25
1	D	290	THR	CA-C-N	-6.39	114.57	122.75
1	D	290	THR	C-N-CA	-6.39	114.57	122.75
1	C	79	ALA	CA-C-N	6.30	129.37	120.42
1	C	79	ALA	C-N-CA	6.30	129.37	120.42
1	A	226	LEU	CA-C-N	6.11	126.12	119.89
1	A	226	LEU	C-N-CA	6.11	126.12	119.89
1	B	112	LYS	N-CA-C	5.74	118.75	111.69
1	C	30	GLU	N-CA-C	-5.73	105.59	112.59
1	B	207	THR	CB-CA-C	5.60	118.11	109.03
1	A	244	TYR	CA-C-N	5.53	129.12	120.82
1	A	244	TYR	C-N-CA	5.53	129.12	120.82
1	B	200	VAL	N-CA-C	5.40	117.40	112.43
1	C	189	LEU	N-CA-C	5.38	117.14	111.28
1	D	243	LYS	N-CA-C	5.32	116.76	111.07
1	D	153	THR	N-CA-C	-5.25	105.62	112.23
1	C	166	THR	CA-C-N	-5.21	115.20	120.31
1	C	166	THR	C-N-CA	-5.21	115.20	120.31
1	B	166	THR	CB-CA-C	5.20	117.41	110.13
1	C	251	ASP	CA-C-N	5.10	125.76	119.99
1	C	251	ASP	C-N-CA	5.10	125.76	119.99

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	292	GLN	Peptide
1	C	293	LYS	Peptide
1	C	30	GLU	Peptide
1	D	1	ALA	Peptide
1	D	186	GLU	Peptide
1	D	291	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	2362	0	2317	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2404	0	2391	58	0
1	C	2357	0	2327	56	0
1	D	2401	0	2392	31	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	B	20	0	16	0	0
4	B	12	0	16	2	0
4	D	6	0	8	0	0
5	A	89	0	0	1	0
5	B	147	0	0	4	0
5	C	97	0	0	10	0
5	D	122	0	0	3	0
All	All	10023	0	9467	176	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 9.

All (176) 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:D:1:ALA:HB1	1:D:2:ASP:HA	1.32	1.08
1:B:289:GLN:HE21	1:C:50:ARG:HH11	1.08	0.95
1:D:1:ALA:CB	1:D:2:ASP:HA	1.96	0.95
1:C:5:LEU:HD22	1:C:36:ILE:HG22	1.54	0.89
1:C:184:GLY:HA2	1:C:201:GLN:HE22	1.38	0.88
1:A:80:VAL:HA	1:A:83:LEU:HD22	1.57	0.87
1:A:151:ALA:HB3	1:A:154:ASN:HD22	1.38	0.87
1:A:186:GLU:HG3	1:A:209:HIS:NE2	1.98	0.78
1:A:71:PHE:CZ	1:A:110:MET:HE3	2.19	0.77
1:A:184:GLY:HA2	1:A:201:GLN:HE22	1.47	0.77
1:B:166:THR:HG21	1:B:182:VAL:HG12	1.67	0.76
1:C:5:LEU:CD2	1:C:36:ILE:HG22	2.18	0.74
1:B:289:GLN:HE21	1:C:50:ARG:NH1	1.85	0.72
1:D:10:ASN:ND2	1:D:44:SER:OG	2.24	0.70
1:B:147:ARG:HD3	1:B:168:MET:HG2	1.75	0.69
1:A:50:ARG:NE	5:A:2014:HOH:O	2.24	0.69
1:A:85:TYR:HB3	1:A:276:LYS:HG3	1.74	0.68
1:D:127:ARG:NE	1:D:186:GLU:OE2	2.21	0.67
1:D:184:GLY:HA2	1:D:201:GLN:HE22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASN:ND2	1:B:44:SER:OG	2.27	0.67
1:B:289:GLN:NE2	1:C:50:ARG:HH11	1.89	0.66
1:C:229:ASP:O	1:C:233:VAL:HG13	1.94	0.66
1:A:147:ARG:NH1	1:A:168:MET:O	2.29	0.66
1:C:291:GLY:O	1:C:293:LYS:N	2.30	0.64
1:B:204:LEU:HG	1:B:206:MET:CE	2.28	0.64
1:B:274:PRO:HG2	4:B:1308:GOL:H32	1.80	0.64
1:B:133:ARG:HD3	5:B:2075:HOH:O	1.98	0.64
1:A:132:ASN:HD22	1:A:180:ASN:HD22	1.47	0.63
1:C:136:ASN:ND2	5:C:2047:HOH:O	2.23	0.61
1:D:1:ALA:HB1	1:D:2:ASP:CA	2.21	0.61
1:B:207:THR:CG2	1:B:209:HIS:ND1	2.65	0.60
1:D:291:GLY:HA3	5:D:2117:HOH:O	2.02	0.59
1:C:293:LYS:HD2	1:C:296:SER:HB3	1.84	0.59
1:B:102:PHE:H	1:B:300:GLN:HE22	1.51	0.58
1:A:283:TYR:O	1:A:287:VAL:HG12	2.04	0.58
1:C:2:ASP:O	1:C:31:LYS:NZ	2.36	0.57
1:B:153:THR:CG2	5:B:2088:HOH:O	2.52	0.56
1:B:129:THR:OG1	1:B:207:THR:HG21	2.05	0.56
1:D:1:ALA:HB3	1:D:35:LYS:HA	1.87	0.55
1:B:84:PRO:HB2	1:B:279:MET:HG3	1.88	0.55
1:D:168:MET:HE1	1:D:176:ALA:HB1	1.89	0.55
1:D:298:LEU:O	1:D:302:GLU:HG3	2.07	0.55
1:A:124:ASN:OD1	1:A:245:HIS:HE1	1.91	0.54
1:B:100:THR:HB	1:B:300:GLN:HE21	1.73	0.54
1:B:133:ARG:NH2	1:B:140:ASP:O	2.41	0.54
1:D:1:ALA:CB	1:D:2:ASP:CA	2.77	0.54
1:A:85:TYR:CB	1:A:276:LYS:HG3	2.38	0.53
1:C:77:GLU:HB3	1:C:293:LYS:HB2	1.89	0.53
1:C:151:ALA:HB3	1:C:154:ASN:HD22	1.73	0.53
1:B:288:LYS:HG2	5:C:2014:HOH:O	2.08	0.53
1:C:30:GLU:C	5:C:2011:HOH:O	2.52	0.53
1:B:288:LYS:HZ2	1:C:50:ARG:NH2	2.07	0.52
1:C:147:ARG:HA	1:C:166:THR:O	2.10	0.52
1:C:221:GLU:O	1:C:225:GLU:HG2	2.10	0.52
1:A:151:ALA:HB3	1:A:154:ASN:ND2	2.16	0.52
1:D:204:LEU:HD23	1:D:267:ILE:HD12	1.92	0.52
1:A:111:ASP:OD1	1:A:220:ASN:ND2	2.41	0.51
1:C:3:TYR:HB2	1:C:36:ILE:HA	1.92	0.51
1:C:69:ALA:O	1:C:72:GLN:HG2	2.09	0.51
1:D:168:MET:HE1	1:D:176:ALA:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:MET:HE1	1:A:215:LEU:HD13	1.93	0.51
1:C:119:LEU:O	1:C:235:LYS:NZ	2.34	0.51
1:A:49:ASP:OD1	1:A:50:ARG:HG3	2.12	0.50
1:C:293:LYS:CD	1:C:296:SER:HB3	2.43	0.49
1:B:184:GLY:HA2	1:B:201:GLN:HE22	1.78	0.49
1:C:31:LYS:N	5:C:2011:HOH:O	2.44	0.49
1:B:230:LEU:O	1:B:233:VAL:HG22	2.12	0.49
1:B:77:GLU:HA	1:B:290:THR:HG21	1.95	0.48
1:D:42:PRO:O	1:D:45:GLN:HG3	2.13	0.48
1:C:293:LYS:HD2	1:C:296:SER:CB	2.42	0.48
1:B:148:VAL:O	1:B:167:PRO:HA	2.13	0.48
1:C:77:GLU:HB2	1:C:293:LYS:HB3	1.95	0.48
1:C:147:ARG:NH1	1:C:168:MET:O	2.46	0.48
1:C:77:GLU:HB2	1:C:293:LYS:CB	2.44	0.48
1:B:133:ARG:NH1	5:B:2076:HOH:O	2.47	0.48
1:C:18:TYR:O	1:C:22:GLU:HB2	2.13	0.48
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.95	0.47
1:C:97:LEU:HD21	1:C:118:LEU:HD21	1.96	0.47
1:C:220:ASN:HB3	1:C:224:LYS:HD2	1.96	0.47
1:C:228:GLU:HA	1:C:231:GLN:HE21	1.79	0.47
1:D:145:LYS:HD2	5:D:2076:HOH:O	2.13	0.47
1:B:278:SER:O	1:B:281:PRO:HD2	2.15	0.47
1:B:128:GLN:O	1:B:186:GLU:HA	2.15	0.47
1:D:301:ILE:HA	1:D:304:ILE:HG12	1.97	0.47
1:C:13:THR:HG23	5:C:2013:HOH:O	2.13	0.47
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.97	0.47
1:D:33:GLN:HG3	1:D:35:LYS:NZ	2.30	0.47
1:C:127:ARG:NE	1:C:186:GLU:OE2	2.36	0.47
1:D:114:LEU:O	1:D:116:VAL:HG13	2.15	0.47
1:B:72:GLN:HA	1:B:75:TYR:O	2.15	0.47
1:A:157:TYR:O	1:A:161:VAL:HG22	2.15	0.46
1:B:288:LYS:NZ	1:C:50:ARG:NH2	2.62	0.46
1:A:16:ASN:HB2	1:A:249:PHE:CE2	2.51	0.46
1:A:91:ASN:HD21	1:A:95:LYS:HE2	1.80	0.46
1:A:280:LYS:N	1:A:281:PRO:HD2	2.30	0.46
1:C:14:SER:HB2	5:C:2005:HOH:O	2.14	0.46
1:B:26:LYS:N	1:B:26:LYS:HD3	2.30	0.46
1:B:66:ALA:HB3	1:B:217:LEU:HD11	1.98	0.46
1:B:177:LEU:HD23	1:B:182:VAL:HG23	1.96	0.46
1:B:97:LEU:HD21	1:B:118:LEU:HD21	1.98	0.46
1:A:280:LYS:N	1:A:281:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLN:NE2	1:C:50:ARG:NH1	2.58	0.46
1:D:2:ASP:HB3	5:D:2015:HOH:O	2.16	0.46
1:D:86:VAL:HG23	1:D:283:TYR:CE1	2.51	0.45
1:A:72:GLN:HA	1:A:75:TYR:O	2.16	0.45
1:B:274:PRO:HG2	4:B:1308:GOL:C3	2.46	0.45
1:B:141:MET:HB3	1:B:161:VAL:HG13	1.99	0.45
1:D:204:LEU:O	1:D:267:ILE:HA	2.16	0.45
1:D:296:SER:O	1:D:300:GLN:HG3	2.17	0.45
1:C:10:ASN:ND2	5:C:2003:HOH:O	2.27	0.45
1:D:290:THR:OG1	1:D:294:GLY:HA3	2.17	0.45
1:A:97:LEU:HD21	1:A:118:LEU:HD21	1.98	0.45
1:C:7:PHE:HB3	1:C:40:LEU:HD23	1.97	0.45
1:B:90:TYR:O	1:B:91:ASN:C	2.59	0.44
1:C:55:GLN:HB3	1:C:61:LEU:HB2	1.99	0.44
1:A:132:ASN:HD22	1:A:180:ASN:ND2	2.12	0.44
1:C:293:LYS:HD3	1:C:296:SER:H	1.82	0.44
1:A:204:LEU:HD23	1:A:267:ILE:HD12	1.99	0.44
1:B:106:LEU:O	1:B:110:MET:HG3	2.18	0.44
1:B:287:VAL:HG13	1:B:295:GLU:HB2	1.99	0.44
1:D:70:ARG:NH1	1:D:73:LEU:HD11	2.32	0.44
1:A:158:ALA:O	1:A:163:ALA:HB3	2.18	0.44
1:A:173:VAL:O	1:A:177:LEU:HG	2.18	0.44
1:B:46:LEU:HD13	1:B:61:LEU:HD13	2.00	0.44
1:B:56:LEU:HD22	1:B:64:THR:HG22	2.00	0.44
1:B:214:GLN:HE21	1:B:214:GLN:HA	1.83	0.43
1:A:49:ASP:OD1	1:A:50:ARG:N	2.51	0.43
1:A:186:GLU:HG2	1:A:187:ASN:N	2.30	0.43
1:D:141:MET:HG3	1:D:161:VAL:HG13	1.99	0.43
1:B:259:PHE:O	1:B:262:LYS:HB2	2.18	0.43
1:A:66:ALA:HB3	1:A:217:LEU:HD11	2.00	0.43
1:C:77:GLU:CB	1:C:293:LYS:CB	2.96	0.43
1:B:227:PRO:HG2	1:B:230:LEU:HB2	1.99	0.43
1:B:296:SER:HA	1:B:299:LYS:HE3	2.01	0.43
1:C:133:ARG:NH1	5:C:2046:HOH:O	2.47	0.43
1:C:151:ALA:HB3	1:C:154:ASN:ND2	2.32	0.43
1:B:141:MET:CB	1:B:161:VAL:HG13	2.48	0.43
1:B:108:LYS:O	1:B:111:ASP:HB3	2.19	0.43
1:B:147:ARG:HA	1:B:166:THR:O	2.19	0.43
1:B:204:LEU:HG	1:B:206:MET:HE3	1.99	0.43
1:C:294:GLY:HA3	5:C:2093:HOH:O	2.18	0.43
1:D:157:TYR:O	1:D:161:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:THR:HG21	1:B:182:VAL:CG1	2.44	0.42
1:D:28:VAL:O	1:D:32:SER:OG	2.33	0.42
1:B:247:LYS:HA	1:B:247:LYS:HD3	1.71	0.42
1:B:289:GLN:NE2	5:B:2133:HOH:O	2.46	0.42
1:B:170:PHE:O	1:B:173:VAL:HG23	2.19	0.42
1:C:31:LYS:HA	5:C:2009:HOH:O	2.19	0.42
1:B:102:PHE:HB3	1:B:300:GLN:NE2	2.34	0.42
1:C:83:LEU:HB2	1:C:86:VAL:HG21	2.02	0.42
1:B:66:ALA:CB	1:B:217:LEU:HD11	2.50	0.42
1:B:178:GLN:HB2	1:B:200:VAL:HG11	2.02	0.41
1:D:52:MET:O	1:D:56:LEU:HD13	2.20	0.41
1:A:96:ALA:O	1:A:100:THR:OG1	2.37	0.41
1:C:259:PHE:O	1:C:263:GLN:HG2	2.20	0.41
1:D:33:GLN:HG3	1:D:35:LYS:HZ1	1.84	0.41
1:C:5:LEU:HA	1:C:62:ASP:OD2	2.21	0.41
1:A:160:TYR:CE1	1:A:281:PRO:HB2	2.56	0.41
1:B:207:THR:HG23	1:B:209:HIS:ND1	2.35	0.41
1:C:69:ALA:HB1	1:C:82:ALA:HB2	2.02	0.41
1:C:148:VAL:CG2	1:C:155:LEU:HD12	2.51	0.41
1:C:227:PRO:HD2	1:C:230:LEU:HD12	2.03	0.40
1:C:230:LEU:O	1:C:234:VAL:HG12	2.21	0.40
1:B:56:LEU:CD2	1:B:64:THR:HG22	2.51	0.40
1:C:30:GLU:OE2	1:C:30:GLU:CA	2.69	0.40
1:C:102:PHE:H	1:C:299:LYS:HE3	1.86	0.40
1:D:10:ASN:HD21	1:D:48:ASP:HA	1.86	0.40
1:A:134:ALA:HB2	1:A:203:PHE:CE1	2.56	0.40
1:A:160:TYR:HB3	1:A:278:SER:O	2.21	0.40
1:A:3:TYR:HB2	1:A:36:ILE:HG12	2.02	0.40
1:A:124:ASN:OD1	1:A:245:HIS:CE1	2.72	0.40
1:A:160:TYR:O	1:A:278:SER:HB2	2.20	0.40
1:C:30:GLU:OE2	1:C:30:GLU:HA	2.21	0.40
1:B:227:PRO:HB2	1:B:229:ASP:OD1	2.21	0.40
1:C:131:SER:OG	1:C:133:ARG:O	2.37	0.40
1:D:91:ASN:HD21	1:D:95:LYS:NZ	2.19	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	294/306 (96%)	287 (98%)	5 (2%)	2 (1%)	18	19
1	B	303/306 (99%)	295 (97%)	8 (3%)	0	100	100
1	C	297/306 (97%)	279 (94%)	14 (5%)	4 (1%)	9	8
1	D	303/306 (99%)	289 (95%)	13 (4%)	1 (0%)	36	42
All	All	1197/1224 (98%)	1150 (96%)	40 (3%)	7 (1%)	21	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	292	GLN
1	C	303	ALA
1	A	187	ASN
1	C	3	TYR
1	C	29	LYS
1	D	292	GLN
1	A	304	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	243/256 (95%)	227 (93%)	16 (7%)	15	18
1	B	256/256 (100%)	233 (91%)	23 (9%)	9	9
1	C	248/256 (97%)	235 (95%)	13 (5%)	21	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	255/256 (100%)	241 (94%)	14 (6%)	19	24
All	All	1002/1024 (98%)	936 (93%)	66 (7%)	15	18

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	26	LYS
1	A	56	LEU
1	A	73	LEU
1	A	83	LEU
1	A	106	LEU
1	A	110	MET
1	A	116	VAL
1	A	147	ARG
1	A	150	ASN
1	A	186	GLU
1	A	187	ASN
1	A	230	LEU
1	A	287	VAL
1	A	296	SER
1	A	298	LEU
1	B	23	MET
1	B	26	LYS
1	B	37	GLU
1	B	101	GLU
1	B	112	LYS
1	B	116	VAL
1	B	133	ARG
1	B	147	ARG
1	B	159	LYS
1	B	161	VAL
1	B	175	LEU
1	B	187	ASN
1	B	207	THR
1	B	214	GLN
1	B	230	LEU
1	B	247	LYS
1	B	248	LEU
1	B	276	LYS
1	B	277	GLU
1	B	288	LYS

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Mol	Chain	Res	Type
1	B	290	THR
1	B	292	GLN
1	B	298	LEU
1	C	5	LEU
1	C	14	SER
1	C	19	LYS
1	C	30	GLU
1	C	36	ILE
1	C	54	LYS
1	C	117	THR
1	C	155	LEU
1	C	214	GLN
1	C	228	GLU
1	C	233	VAL
1	C	292	GLN
1	C	304	ILE
1	D	33	GLN
1	D	39	SER
1	D	88	SER
1	D	108	LYS
1	D	112	LYS
1	D	116	VAL
1	D	147	ARG
1	D	161	VAL
1	D	214	GLN
1	D	230	LEU
1	D	233	VAL
1	D	235	LYS
1	D	288	LYS
1	D	293	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	91	ASN
1	A	136	ASN
1	A	154	ASN
1	A	180	ASN
1	A	187	ASN
1	A	201	GLN
1	A	240	ASN

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Mol	Chain	Res	Type
1	A	245	HIS
1	B	10	ASN
1	B	33	GLN
1	B	136	ASN
1	B	201	GLN
1	B	214	GLN
1	B	289	GLN
1	B	292	GLN
1	B	300	GLN
1	C	132	ASN
1	C	154	ASN
1	C	195	GLN
1	C	201	GLN
1	C	231	GLN
1	C	292	GLN
1	C	305	ASN
1	D	10	ASN
1	D	55	GLN
1	D	91	ASN
1	D	124	ASN
1	D	154	ASN
1	D	201	GLN
1	D	289	GLN
1	D	292	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
4	GOL	B	1309	-	5,5,5	0.52	0	5,5,5	0.22	0
4	GOL	D	1306	-	5,5,5	0.96	0	5,5,5	1.31	1 (20%)
3	DAN	B	1307	-	20,20,20	1.38	3 (15%)	24,28,28	1.29	3 (12%)
4	GOL	B	1308	-	5,5,5	0.86	0	5,5,5	1.49	2 (40%)

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
4	GOL	B	1309	-	-	2/4/4/4	-
4	GOL	D	1306	-	-	2/4/4/4	-
3	DAN	B	1307	-	-	7/18/34/34	0/1/1/1
4	GOL	B	1308	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1307	DAN	C4-C5	3.37	1.57	1.53
3	B	1307	DAN	O1B-C1	-2.39	1.24	1.30
3	B	1307	DAN	O6-C2	2.05	1.44	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1307	DAN	C4-C5-N5	2.76	114.24	111.13
4	B	1308	GOL	O3-C3-C2	2.54	121.80	110.38
3	B	1307	DAN	O1B-C1-O1A	-2.47	118.01	123.90
4	D	1306	GOL	O1-C1-C2	2.32	120.82	110.38
3	B	1307	DAN	O7-C7-C6	2.24	114.28	109.44
4	B	1308	GOL	O2-C2-C3	2.07	117.73	109.18

There are no chirality outliers.

All (15) torsion outliers are listed below:

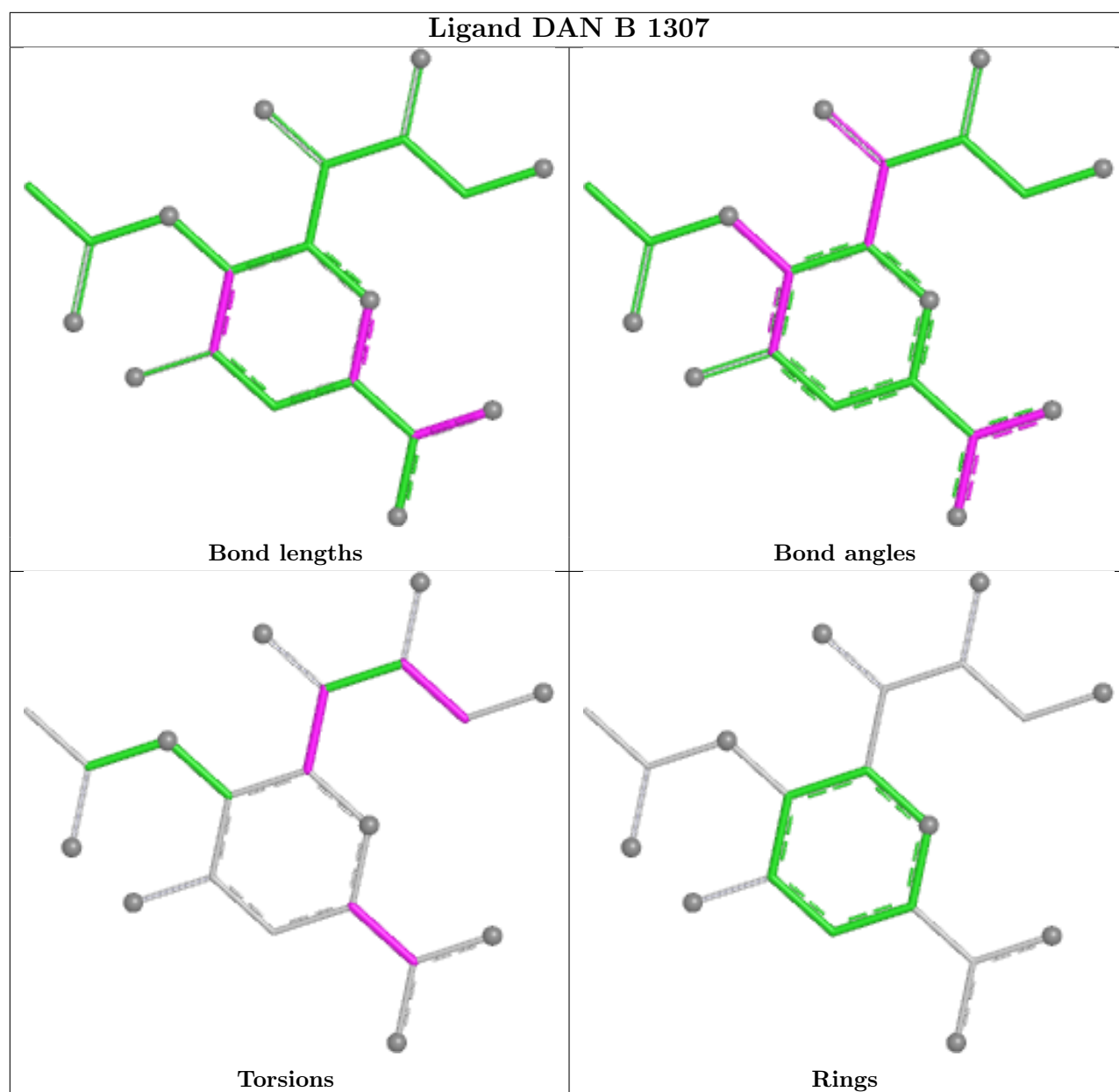
Mol	Chain	Res	Type	Atoms
3	B	1307	DAN	O1A-C1-C2-C3
3	B	1307	DAN	O1A-C1-C2-O6
3	B	1307	DAN	O1B-C1-C2-C3
3	B	1307	DAN	O1B-C1-C2-O6
3	B	1307	DAN	O6-C6-C7-O7
4	B	1308	GOL	O1-C1-C2-O2
4	B	1308	GOL	O1-C1-C2-C3
4	B	1308	GOL	C1-C2-C3-O3
4	B	1309	GOL	O1-C1-C2-C3
4	D	1306	GOL	C1-C2-C3-O3
3	B	1307	DAN	O8-C8-C9-O9
3	B	1307	DAN	C7-C8-C9-O9
4	B	1308	GOL	O2-C2-C3-O3
4	B	1309	GOL	O1-C1-C2-O2
4	D	1306	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1308	GOL	2	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	304/306 (99%)	0.45	4 (1%) 75 73	26, 33, 43, 52	3 (0%)
1	B	305/306 (99%)	0.13	1 (0%) 90 88	22, 33, 37, 48	0
1	C	300/306 (98%)	0.81	34 (11%) 10 8	16, 33, 38, 63	1 (0%)
1	D	305/306 (99%)	0.25	5 (1%) 70 67	24, 32, 38, 49	0
All	All	1214/1224 (99%)	0.41	44 (3%) 46 43	16, 33, 39, 63	4 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	VAL	4.7
1	C	146	LEU	3.5
1	C	36	ILE	3.4
1	C	73	LEU	3.3
1	C	87	ILE	3.2
1	C	88	SER	3.1
1	C	86	VAL	3.1
1	C	304	ILE	3.1
1	D	1	ALA	3.1
1	A	292	GLN	2.9
1	C	252	GLY	2.9
1	C	100	THR	2.9
1	C	99	ASP	2.7
1	A	101	GLU	2.7
1	C	102	PHE	2.7
1	C	3	TYR	2.6
1	C	80	VAL	2.6
1	C	93	ALA	2.6
1	C	83	LEU	2.6
1	D	305	ASN	2.5
1	C	303	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	85	TYR	2.5
1	C	41	TYR	2.4
1	B	255	ASP	2.4
1	C	76	PRO	2.4
1	C	170	PHE	2.4
1	C	82	ALA	2.3
1	C	300	GLN	2.3
1	C	21	ALA	2.3
1	C	97	LEU	2.2
1	D	158	ALA	2.2
1	C	305	ASN	2.1
1	C	39	SER	2.1
1	A	87	ILE	2.1
1	C	95	LYS	2.1
1	C	4	ASP	2.1
1	D	291	GLY	2.1
1	C	84	PRO	2.1
1	C	78	ALA	2.1
1	C	91	ASN	2.1
1	D	138	ILE	2.1
1	A	122	ALA	2.0
1	C	75	TYR	2.0
1	C	205	ALA	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.

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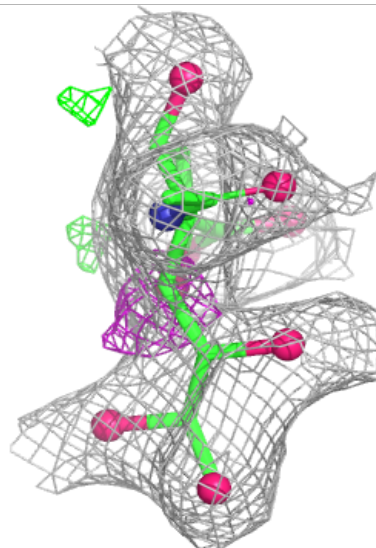
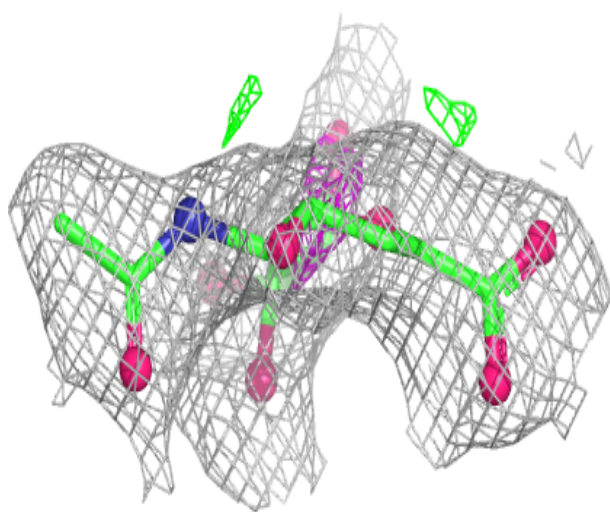
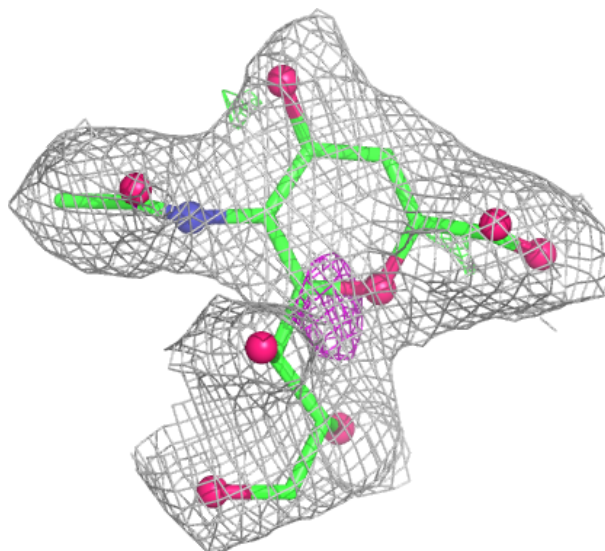
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	1309	6/6	0.76	0.14	52,54,54,54	0
4	GOL	B	1308	6/6	0.86	0.15	36,39,40,41	0
2	ZN	C	1307	1/1	0.89	0.12	53,53,53,53	1
4	GOL	D	1306	6/6	0.91	0.18	33,35,36,37	0
3	DAN	B	1307	20/20	0.92	0.08	23,28,30,30	0
2	ZN	D	1307	1/1	0.93	0.07	21,21,21,21	1
2	ZN	A	1306	1/1	0.95	0.05	39,39,39,39	1
2	ZN	B	1311	1/1	0.98	0.03	32,32,32,32	1
2	ZN	C	1306	1/1	0.98	0.07	30,30,30,30	0
2	ZN	B	1310	1/1	0.99	0.06	30,30,30,30	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 1307:

$2mF_o-DF_c$ (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.