



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:51 AM UTC

PDB ID : 9DB6 / pdb_00009db6
Title : Sialidase682 co-crystallized with inhibitor DANA
Authors : Young, M.A.; Rees, S.D.; Chang, G.
Deposited on : 2024-08-23
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

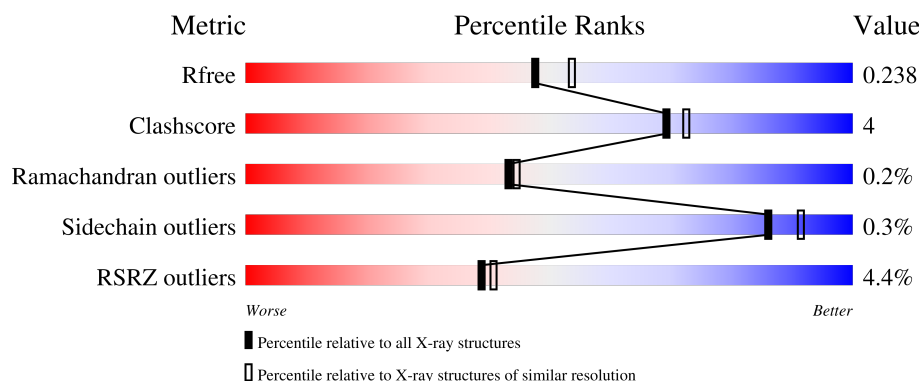
1 Overall quality at a glance

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	540	5% 89% 8% .
1	B	540	3% 89% 7% .
1	C	540	4% 90% 6% .
1	D	540	5% 86% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33822 atoms, of which 16362 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 BNR/Asp-box repeat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	521	Total	C	H	N	O	S	0	0	0
			8152	2584	4067	707	771	23			
1	B	521	Total	C	H	N	O	S	0	0	0
			8173	2584	4088	707	771	23			
1	C	521	Total	C	H	N	O	S	0	0	0
			8155	2584	4070	707	771	23			
1	D	521	Total	C	H	N	O	S	0	0	0
			8166	2584	4081	707	771	23			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C9KXU6
A	4	ALA	THR	conflict	UNP C9KXU6
A	18	THR	ILE	conflict	UNP C9KXU6
A	37	LYS	GLU	conflict	UNP C9KXU6
A	38	ASP	GLU	conflict	UNP C9KXU6
A	41	LEU	PHE	conflict	UNP C9KXU6
A	55	LEU	GLN	conflict	UNP C9KXU6
A	75	ASP	ASN	conflict	UNP C9KXU6
A	78	ARG	CYS	conflict	UNP C9KXU6
A	87	GLY	SER	conflict	UNP C9KXU6
A	157	LYS	ARG	conflict	UNP C9KXU6
A	158	VAL	ASP	conflict	UNP C9KXU6
A	160	ASP	THR	conflict	UNP C9KXU6
A	231	GLU	LYS	conflict	UNP C9KXU6
A	368	ARG	GLN	conflict	UNP C9KXU6
A	444	GLN	LEU	conflict	UNP C9KXU6
A	491	PRO	SER	conflict	UNP C9KXU6
A	527	LEU	ILE	conflict	UNP C9KXU6
A	531	HIS	-	expression tag	UNP C9KXU6
A	532	HIS	-	expression tag	UNP C9KXU6
A	533	HIS	-	expression tag	UNP C9KXU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	HIS	-	expression tag	UNP C9KXU6
A	535	HIS	-	expression tag	UNP C9KXU6
A	536	HIS	-	expression tag	UNP C9KXU6
A	537	HIS	-	expression tag	UNP C9KXU6
A	538	HIS	-	expression tag	UNP C9KXU6
A	539	HIS	-	expression tag	UNP C9KXU6
A	540	HIS	-	expression tag	UNP C9KXU6
B	1	MET	-	initiating methionine	UNP C9KXU6
B	4	ALA	THR	conflict	UNP C9KXU6
B	18	THR	ILE	conflict	UNP C9KXU6
B	37	LYS	GLU	conflict	UNP C9KXU6
B	38	ASP	GLU	conflict	UNP C9KXU6
B	41	LEU	PHE	conflict	UNP C9KXU6
B	55	LEU	GLN	conflict	UNP C9KXU6
B	75	ASP	ASN	conflict	UNP C9KXU6
B	78	ARG	CYS	conflict	UNP C9KXU6
B	87	GLY	SER	conflict	UNP C9KXU6
B	157	LYS	ARG	conflict	UNP C9KXU6
B	158	VAL	ASP	conflict	UNP C9KXU6
B	160	ASP	THR	conflict	UNP C9KXU6
B	231	GLU	LYS	conflict	UNP C9KXU6
B	368	ARG	GLN	conflict	UNP C9KXU6
B	444	GLN	LEU	conflict	UNP C9KXU6
B	491	PRO	SER	conflict	UNP C9KXU6
B	527	LEU	ILE	conflict	UNP C9KXU6
B	531	HIS	-	expression tag	UNP C9KXU6
B	532	HIS	-	expression tag	UNP C9KXU6
B	533	HIS	-	expression tag	UNP C9KXU6
B	534	HIS	-	expression tag	UNP C9KXU6
B	535	HIS	-	expression tag	UNP C9KXU6
B	536	HIS	-	expression tag	UNP C9KXU6
B	537	HIS	-	expression tag	UNP C9KXU6
B	538	HIS	-	expression tag	UNP C9KXU6
B	539	HIS	-	expression tag	UNP C9KXU6
B	540	HIS	-	expression tag	UNP C9KXU6
C	1	MET	-	initiating methionine	UNP C9KXU6
C	4	ALA	THR	conflict	UNP C9KXU6
C	18	THR	ILE	conflict	UNP C9KXU6
C	37	LYS	GLU	conflict	UNP C9KXU6
C	38	ASP	GLU	conflict	UNP C9KXU6
C	41	LEU	PHE	conflict	UNP C9KXU6
C	55	LEU	GLN	conflict	UNP C9KXU6

Continued on next page...

Continued from previous page...

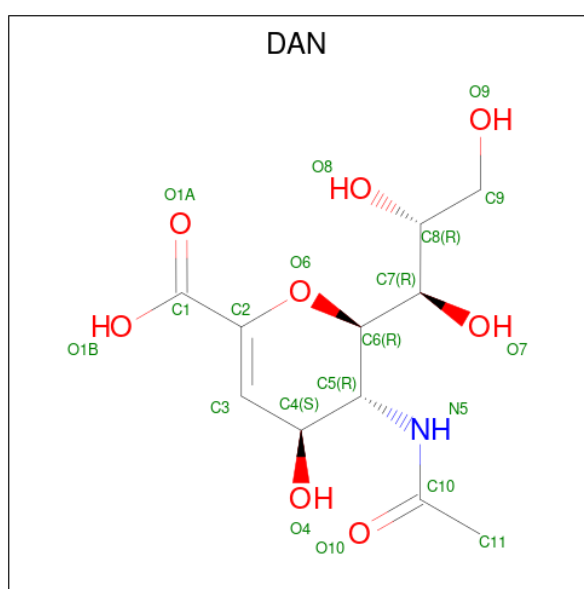
Chain	Residue	Modelled	Actual	Comment	Reference
C	75	ASP	ASN	conflict	UNP C9KXU6
C	78	ARG	CYS	conflict	UNP C9KXU6
C	87	GLY	SER	conflict	UNP C9KXU6
C	157	LYS	ARG	conflict	UNP C9KXU6
C	158	VAL	ASP	conflict	UNP C9KXU6
C	160	ASP	THR	conflict	UNP C9KXU6
C	231	GLU	LYS	conflict	UNP C9KXU6
C	368	ARG	GLN	conflict	UNP C9KXU6
C	444	GLN	LEU	conflict	UNP C9KXU6
C	491	PRO	SER	conflict	UNP C9KXU6
C	527	LEU	ILE	conflict	UNP C9KXU6
C	531	HIS	-	expression tag	UNP C9KXU6
C	532	HIS	-	expression tag	UNP C9KXU6
C	533	HIS	-	expression tag	UNP C9KXU6
C	534	HIS	-	expression tag	UNP C9KXU6
C	535	HIS	-	expression tag	UNP C9KXU6
C	536	HIS	-	expression tag	UNP C9KXU6
C	537	HIS	-	expression tag	UNP C9KXU6
C	538	HIS	-	expression tag	UNP C9KXU6
C	539	HIS	-	expression tag	UNP C9KXU6
C	540	HIS	-	expression tag	UNP C9KXU6
D	1	MET	-	initiating methionine	UNP C9KXU6
D	4	ALA	THR	conflict	UNP C9KXU6
D	18	THR	ILE	conflict	UNP C9KXU6
D	37	LYS	GLU	conflict	UNP C9KXU6
D	38	ASP	GLU	conflict	UNP C9KXU6
D	41	LEU	PHE	conflict	UNP C9KXU6
D	55	LEU	GLN	conflict	UNP C9KXU6
D	75	ASP	ASN	conflict	UNP C9KXU6
D	78	ARG	CYS	conflict	UNP C9KXU6
D	87	GLY	SER	conflict	UNP C9KXU6
D	157	LYS	ARG	conflict	UNP C9KXU6
D	158	VAL	ASP	conflict	UNP C9KXU6
D	160	ASP	THR	conflict	UNP C9KXU6
D	231	GLU	LYS	conflict	UNP C9KXU6
D	368	ARG	GLN	conflict	UNP C9KXU6
D	444	GLN	LEU	conflict	UNP C9KXU6
D	491	PRO	SER	conflict	UNP C9KXU6
D	527	LEU	ILE	conflict	UNP C9KXU6
D	531	HIS	-	expression tag	UNP C9KXU6
D	532	HIS	-	expression tag	UNP C9KXU6
D	533	HIS	-	expression tag	UNP C9KXU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	534	HIS	-	expression tag	UNP C9KXU6
D	535	HIS	-	expression tag	UNP C9KXU6
D	536	HIS	-	expression tag	UNP C9KXU6
D	537	HIS	-	expression tag	UNP C9KXU6
D	538	HIS	-	expression tag	UNP C9KXU6
D	539	HIS	-	expression tag	UNP C9KXU6
D	540	HIS	-	expression tag	UNP C9KXU6

- Molecule 2 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (CCD ID: DAN) (formula: C₁₁H₁₇NO₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 34	C 11	H 14	N 1	O 8	10	0
2	B	1	Total 34	C 11	H 14	N 1	O 8	10	0
2	C	1	Total 34	C 11	H 14	N 1	O 8	10	0
2	D	1	Total 34	C 11	H 14	N 1	O 8	10	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	285	Total	O	0	0
			285	285		

Continued on next page...

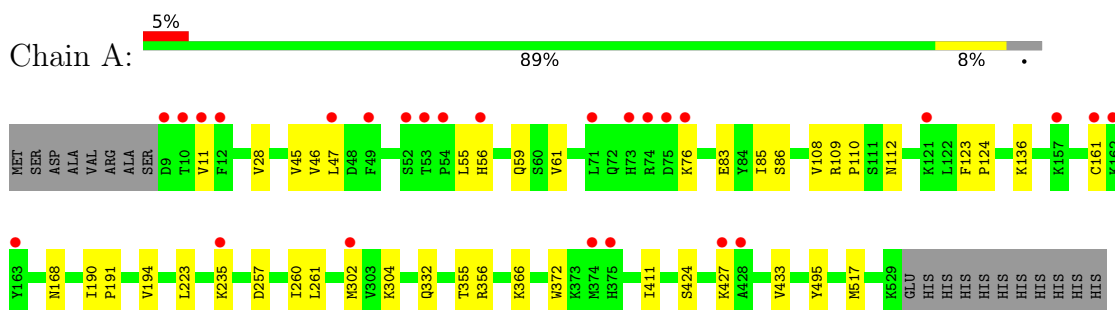
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	311	Total 311	O 311	0	0
3	C	236	Total 236	O 236	0	0
3	D	208	Total 208	O 208	0	0

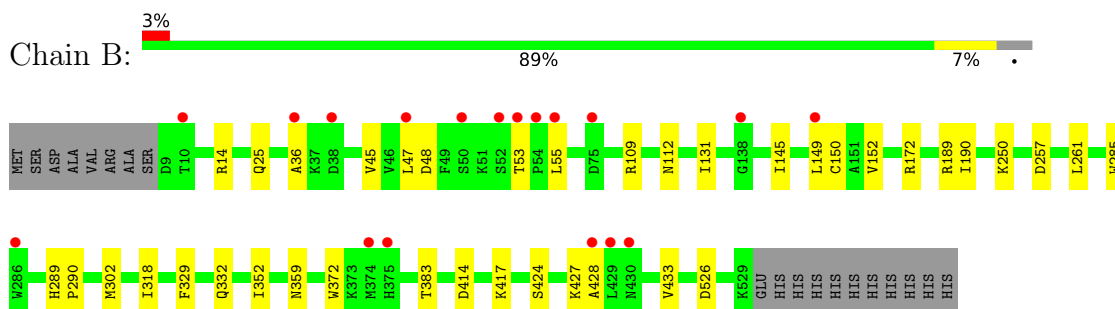
3 Residue-property plots [i](#)

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.

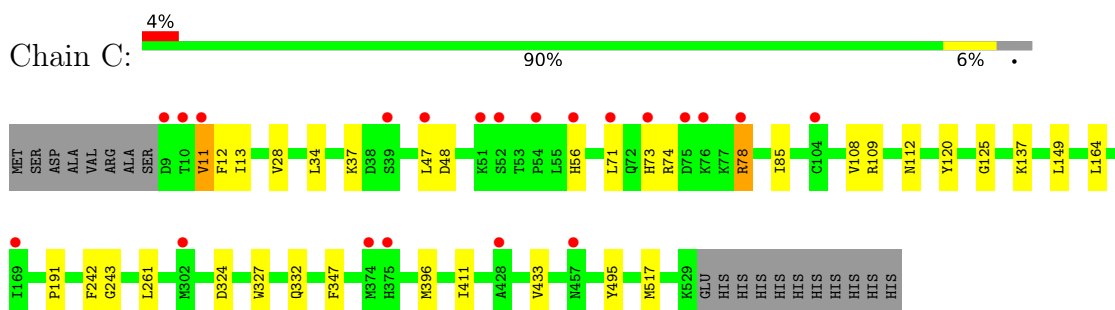
- Molecule 1: BNR/Asp-box repeat protein



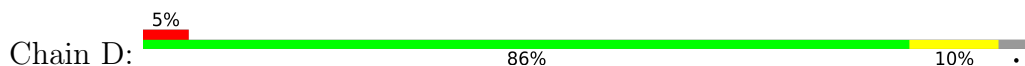
- Molecule 1: BNR/Asp-box repeat protein

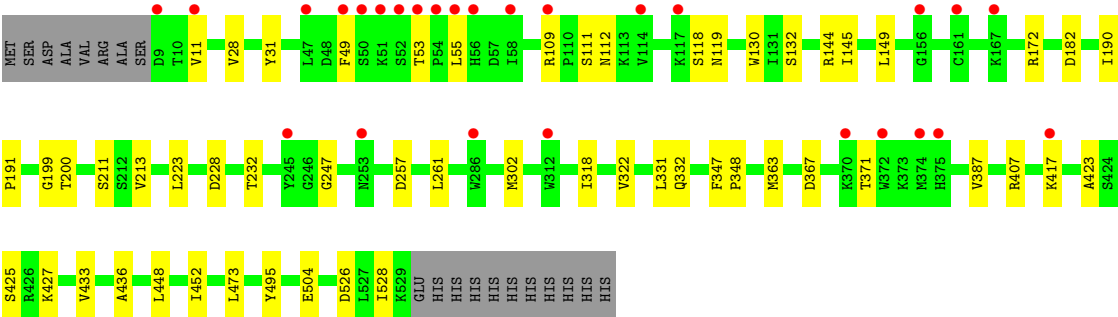


- Molecule 1: BNR/Asp-box repeat protein



- Molecule 1: BNR/Asp-box repeat protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.25Å 149.52Å 100.44Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	78.51 – 2.10 78.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.51-2.10) 99.8 (78.51-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.207 , 0.238 0.207 , 0.238	Depositor DCC
R_{free} test set	6320 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33822	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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: 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	0.31	0/4174	0.48	0/5658
1	B	0.31	0/4174	0.48	0/5658
1	C	0.31	1/4174 (0.0%)	0.47	0/5658
1	D	0.33	3/4174 (0.1%)	0.47	0/5658
All	All	0.31	4/16696 (0.0%)	0.47	0/22632

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	ARG	C-O	-7.59	1.20	1.23
1	D	11	VAL	CA-C	7.05	1.61	1.52
1	D	11	VAL	C-O	-5.70	1.18	1.24
1	C	11	VAL	C-N	5.13	1.40	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4085	4067	4086	27	0
1	B	4085	4088	4086	27	1
1	C	4085	4070	4086	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4085	4081	4086	36	1
2	A	20	14	16	2	0
2	B	20	14	16	3	0
2	C	20	14	16	1	0
2	D	20	14	16	0	0
3	A	285	0	0	5	1
3	B	311	0	0	6	0
3	C	236	0	0	1	1
3	D	208	0	0	4	0
All	All	17460	16362	16408	116	2

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 4.

All (116) 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:A:168:ASN:OD1	3:A:701:HOH:O	2.00	0.77
1:D:144:ARG:NH1	1:D:526:ASP:OD2	2.21	0.74
1:D:473:LEU:HD21	1:D:528:ILE:HD13	1.68	0.74
1:D:367:ASP:OD2	1:D:371:THR:OG1	2.08	0.71
1:B:36:ALA:O	3:B:701:HOH:O	2.07	0.71
1:A:366:LYS:NZ	3:A:705:HOH:O	2.27	0.67
1:A:304:LYS:NZ	3:A:704:HOH:O	2.27	0.67
1:D:228:ASP:O	3:D:702:HOH:O	2.14	0.66
1:B:302:MET:HE1	1:B:372:TRP:CE2	2.31	0.65
1:D:199:GLY:O	3:D:701:HOH:O	2.12	0.65
1:D:448:LEU:HD12	1:D:452:ILE:HD11	1.79	0.65
1:B:55:LEU:HD11	1:B:112:ASN:CG	2.25	0.62
1:D:322:VAL:HG11	1:D:363:MET:HE2	1.80	0.62
1:A:46:VAL:C	1:A:47:LEU:HD12	2.25	0.61
1:C:37:LYS:HG2	1:C:125:GLY:HA2	1.83	0.61
1:B:250:LYS:NZ	3:B:704:HOH:O	2.26	0.60
1:B:14:ARG:NE	3:B:702:HOH:O	2.17	0.59
1:C:11:VAL:O	1:C:11:VAL:HG13	2.00	0.59
1:B:53:THR:HG23	1:B:145:ILE:HD13	1.86	0.58
1:D:182:ASP:OD1	3:D:703:HOH:O	2.17	0.58
1:D:172:ARG:NH2	1:D:526:ASP:OD2	2.37	0.58
1:A:45:VAL:HG12	1:A:47:LEU:CD1	2.35	0.57
1:C:108:VAL:HG12	1:C:109:ARG:HG3	1.86	0.56
1:B:190:ILE:HG21	1:B:257:ASP:HA	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:C	1:B:261:LEU:HD12	2.30	0.55
1:D:302:MET:CE	1:D:318:ILE:HD13	2.36	0.55
1:D:55:LEU:HD21	1:D:111:SER:C	2.32	0.54
1:D:473:LEU:HD21	1:D:528:ILE:CD1	2.35	0.54
1:D:200:THR:OG1	3:D:704:HOH:O	2.18	0.54
1:B:302:MET:HE3	1:B:318:ILE:HD13	1.91	0.53
1:D:49:PHE:O	1:D:112:ASN:ND2	2.42	0.53
1:D:191:PRO:HD2	1:D:495:TYR:HB3	1.90	0.53
1:C:120:TYR:OH	1:D:247:GLY:O	2.28	0.52
1:A:356:ARG:NH1	3:A:710:HOH:O	2.41	0.52
1:C:261:LEU:HD23	1:C:347:PHE:CZ	2.45	0.52
1:C:137:LYS:H	1:C:137:LYS:HE2	1.75	0.52
1:C:73:HIS:HE1	1:C:78:ARG:CZ	2.23	0.52
1:B:45:VAL:HG11	1:B:131:ILE:HD11	1.92	0.51
1:C:13:ILE:HD12	1:C:149:LEU:CD2	2.41	0.51
1:A:194:VAL:HG13	1:A:260:ILE:HG23	1.94	0.50
1:B:285:TRP:HE3	2:B:601:DAN:H112	1.76	0.50
1:A:11:VAL:HG13	1:A:11:VAL:O	2.12	0.49
2:A:601:DAN:O10	2:A:601:DAN:O4	2.30	0.49
1:A:83:GLU:OE2	1:A:86:SER:HA	2.12	0.49
1:A:302:MET:HE1	1:A:372:TRP:CE2	2.47	0.49
1:D:223:LEU:C	1:D:223:LEU:HD23	2.38	0.49
1:A:55:LEU:HD11	1:A:112:ASN:CG	2.38	0.48
1:A:332:GLN:H	1:A:332:GLN:CD	2.21	0.48
1:C:28:VAL:HG23	1:C:85:ILE:HD12	1.95	0.48
1:A:28:VAL:HG23	1:A:85:ILE:HD12	1.95	0.48
2:C:601:DAN:H91	3:C:788:HOH:O	2.13	0.48
1:A:190:ILE:HG21	1:A:257:ASP:HA	1.95	0.48
1:C:12:PHE:HD1	1:C:164:LEU:HD11	1.79	0.48
1:C:324:ASP:HB3	1:C:327:TRP:CE2	2.49	0.48
1:A:223:LEU:C	1:A:223:LEU:HD23	2.38	0.48
1:B:424:SER:HB2	1:B:428:ALA:HB3	1.96	0.47
1:C:47:LEU:HD13	1:C:149:LEU:HD12	1.94	0.47
1:C:396:MET:HA	1:C:411:ILE:HD13	1.97	0.47
1:D:425:SER:O	1:D:427:LYS:HG3	2.15	0.47
1:D:211:SER:OG	1:D:213:VAL:HG12	2.15	0.47
1:B:526:ASP:OD2	3:B:703:HOH:O	2.21	0.46
1:D:448:LEU:HD12	1:D:452:ILE:CD1	2.45	0.46
1:A:11:VAL:CG1	1:A:161:CYS:SG	3.04	0.46
1:A:56:HIS:O	1:A:136:LYS:NZ	2.48	0.46
1:B:383:THR:HG21	2:B:601:DAN:H91	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ILE:HG21	1:D:257:ASP:HA	1.96	0.45
1:B:149:LEU:HD11	1:B:152:VAL:HG23	1.98	0.45
1:B:172:ARG:NH1	3:B:710:HOH:O	2.38	0.45
1:B:329:PHE:HB3	1:B:352:ILE:HD12	1.98	0.45
1:D:55:LEU:HD21	1:D:112:ASN:N	2.31	0.45
1:A:59:GLN:HB2	1:A:136:LYS:HG3	1.99	0.45
1:A:261:LEU:C	1:A:261:LEU:HD12	2.41	0.45
1:C:332:GLN:CD	1:C:332:GLN:H	2.24	0.45
1:B:285:TRP:CE3	2:B:601:DAN:H112	2.52	0.45
1:C:11:VAL:HG23	1:C:34:LEU:HD23	1.99	0.44
1:D:331:LEU:HD23	1:D:331:LEU:N	2.33	0.44
1:B:55:LEU:HD11	1:B:112:ASN:ND2	2.32	0.44
1:C:191:PRO:HD2	1:C:495:TYR:HB3	2.00	0.44
1:A:61:VAL:HG23	1:A:110:PRO:HG3	1.99	0.44
1:D:423:ALA:O	1:D:427:LYS:CE	2.66	0.43
1:B:47:LEU:HD21	1:B:131:ILE:HG21	2.00	0.43
2:A:601:DAN:H91	3:A:822:HOH:O	2.17	0.43
1:C:47:LEU:HD11	1:C:149:LEU:HD13	2.00	0.43
1:A:191:PRO:HB3	1:A:517:MET:SD	2.59	0.42
1:B:332:GLN:H	1:B:332:GLN:CD	2.27	0.42
1:B:414:ASP:CG	1:B:417:LYS:HB2	2.44	0.42
1:D:322:VAL:HG21	1:D:363:MET:HE1	2.01	0.42
1:C:48:ASP:HA	1:C:112:ASN:O	2.18	0.42
1:D:28:VAL:HG11	1:D:31:TYR:CZ	2.54	0.42
1:D:118:SER:O	1:D:119:ASN:C	2.61	0.42
1:D:332:GLN:H	1:D:332:GLN:CD	2.28	0.42
1:D:423:ALA:O	1:D:427:LYS:HE2	2.19	0.42
1:B:25:GLN:NE2	3:B:723:HOH:O	2.53	0.42
1:C:56:HIS:H	1:C:56:HIS:CD2	2.37	0.42
1:D:261:LEU:HD23	1:D:347:PHE:CZ	2.54	0.42
1:D:53:THR:HG23	1:D:145:ILE:HD13	2.02	0.42
1:D:348:PRO:HD3	1:D:387:VAL:HG12	2.01	0.42
1:A:424:SER:O	1:A:427:LYS:O	2.38	0.42
1:B:289:HIS:HB3	1:B:290:PRO:HD2	2.02	0.42
1:D:149:LEU:HD13	1:D:149:LEU:C	2.46	0.41
1:C:13:ILE:HD12	1:C:149:LEU:HD21	2.02	0.41
1:C:73:HIS:CE1	1:C:78:ARG:NE	2.89	0.41
1:C:191:PRO:HB3	1:C:517:MET:SD	2.60	0.41
1:C:71:LEU:HA	1:C:74:ARG:HH11	1.85	0.41
1:A:191:PRO:HD2	1:A:495:TYR:HB3	2.03	0.41
1:A:108:VAL:HG12	1:A:109:ARG:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:C	1:B:190:ILE:HG12	2.46	0.41
1:D:228:ASP:OD2	1:D:232:THR:OG1	2.28	0.41
1:D:407:ARG:CZ	1:D:436:ALA:HB3	2.50	0.41
1:B:53:THR:HG23	1:B:145:ILE:CD1	2.50	0.41
1:A:123:PHE:CD1	1:A:124:PRO:HD2	2.57	0.40
1:A:76:LYS:HA	1:A:76:LYS:HD2	1.88	0.40
1:B:48:ASP:HB2	1:B:150:CYS:SG	2.61	0.40
1:D:130:TRP:CZ3	1:D:132:SER:HB2	2.57	0.40
1:A:355:THR:O	1:A:356:ARG:HB2	2.22	0.40
1:C:242:PHE:O	1:C:243:GLY:C	2.63	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:836:HOH:O	3:C:777:HOH:O[2_545]	2.11	0.09
1:B:109:ARG:NH2	1:D:504:GLU:OE2[2_545]	2.14	0.06

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	519/540 (96%)	499 (96%)	19 (4%)	1 (0%)	43	44
1	B	519/540 (96%)	493 (95%)	25 (5%)	1 (0%)	43	44
1	C	519/540 (96%)	496 (96%)	22 (4%)	1 (0%)	43	44
1	D	519/540 (96%)	494 (95%)	24 (5%)	1 (0%)	43	44
All	All	2076/2160 (96%)	1982 (96%)	90 (4%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	VAL
1	D	433	VAL
1	B	433	VAL
1	C	433	VAL

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	455/472 (96%)	453 (100%)	2 (0%)	84	89
1	B	455/472 (96%)	453 (100%)	2 (0%)	84	89
1	C	455/472 (96%)	454 (100%)	1 (0%)	87	93
1	D	455/472 (96%)	454 (100%)	1 (0%)	87	93
All	All	1820/1888 (96%)	1814 (100%)	6 (0%)	86	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LYS
1	A	411	ILE
1	B	359	ASN
1	B	427	LYS
1	C	78	ARG
1	D	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	B	27	ASN
1	B	89	HIS
1	B	134	GLN
1	B	430	ASN
1	C	56	HIS
1	C	73	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	134	GLN
1	C	440	ASN
1	C	484	GLN
1	D	27	ASN
1	D	197	ASN
1	D	277	HIS
1	D	295	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	601	-	20,20,20	2.30	7 (35%)	24,28,28	2.70	10 (41%)
2	DAN	C	601	-	20,20,20	2.00	6 (30%)	24,28,28	2.42	10 (41%)
2	DAN	D	601	-	20,20,20	1.71	6 (30%)	24,28,28	2.17	9 (37%)
2	DAN	B	601	-	20,20,20	1.41	3 (15%)	24,28,28	1.90	7 (29%)

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	601	-	-	1/18/34/34	0/1/1/1
2	DAN	C	601	-	-	2/18/34/34	0/1/1/1
2	DAN	D	601	-	-	8/18/34/34	0/1/1/1
2	DAN	B	601	-	-	2/18/34/34	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	DAN	C4-C5	5.78	1.59	1.53
2	C	601	DAN	C4-C5	4.58	1.58	1.53
2	A	601	DAN	C6-C5	4.51	1.60	1.53
2	C	601	DAN	C6-C5	3.84	1.59	1.53
2	A	601	DAN	C2-C1	3.83	1.57	1.48
2	C	601	DAN	C2-C1	3.59	1.57	1.48
2	B	601	DAN	O1B-C1	-3.42	1.21	1.30
2	A	601	DAN	C5-N5	-3.31	1.40	1.45
2	D	601	DAN	O1B-C1	-3.24	1.21	1.30
2	D	601	DAN	C4-C5	3.01	1.56	1.53
2	A	601	DAN	C4-C3	3.01	1.54	1.50
2	D	601	DAN	C2-C1	2.99	1.55	1.48
2	C	601	DAN	C5-N5	-2.92	1.41	1.45
2	C	601	DAN	C4-C3	2.88	1.54	1.50
2	B	601	DAN	C2-C1	2.69	1.54	1.48
2	C	601	DAN	O1B-C1	-2.68	1.23	1.30
2	D	601	DAN	C6-C5	2.55	1.57	1.53
2	D	601	DAN	C5-N5	-2.51	1.41	1.45
2	D	601	DAN	C4-C3	2.49	1.53	1.50
2	B	601	DAN	C5-N5	-2.29	1.42	1.45
2	A	601	DAN	O1B-C1	-2.11	1.24	1.30
2	A	601	DAN	O6-C6	-2.07	1.42	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	DAN	O6-C2-C3	-7.05	116.73	124.62
2	C	601	DAN	O6-C2-C3	-5.80	118.13	124.62
2	D	601	DAN	C4-C5-N5	5.79	117.64	111.13
2	C	601	DAN	C4-C5-N5	5.26	117.04	111.13
2	A	601	DAN	C4-C5-N5	4.63	116.33	111.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	DAN	C4-C5-N5	4.41	116.08	111.13
2	A	601	DAN	O1B-C1-C2	4.25	123.70	114.06
2	D	601	DAN	C8-C7-C6	4.12	120.80	113.05
2	D	601	DAN	O6-C2-C3	-3.66	120.52	124.62
2	A	601	DAN	C3-C2-C1	3.59	131.34	123.56
2	A	601	DAN	C6-C5-N5	3.51	116.51	110.91
2	C	601	DAN	O4-C4-C5	3.48	118.91	112.66
2	A	601	DAN	O4-C4-C5	3.48	118.90	112.66
2	A	601	DAN	O1A-C1-C2	-3.43	112.17	120.57
2	C	601	DAN	C4-C3-C2	3.22	126.91	121.45
2	C	601	DAN	O1B-C1-C2	3.20	121.32	114.06
2	A	601	DAN	C8-C7-C6	3.20	119.06	113.05
2	B	601	DAN	O1A-C1-C2	-3.19	112.76	120.57
2	C	601	DAN	C3-C2-C1	3.09	130.25	123.56
2	D	601	DAN	C9-C8-C7	-3.04	105.97	112.17
2	B	601	DAN	O1B-C1-C2	3.01	120.87	114.06
2	D	601	DAN	C4-C3-C2	2.99	126.51	121.45
2	B	601	DAN	O6-C6-C7	2.77	110.85	105.98
2	C	601	DAN	C6-C5-N5	2.67	115.16	110.91
2	B	601	DAN	C4-C3-C2	2.62	125.89	121.45
2	B	601	DAN	O6-C2-C3	-2.50	121.82	124.62
2	B	601	DAN	O8-C8-C7	-2.39	103.66	109.25
2	D	601	DAN	O7-C7-C6	-2.38	104.30	109.44
2	C	601	DAN	C8-C7-C6	2.38	117.52	113.05
2	D	601	DAN	O4-C4-C5	2.31	116.80	112.66
2	C	601	DAN	O1A-C1-C2	-2.29	114.97	120.57
2	A	601	DAN	C4-C3-C2	2.27	125.31	121.45
2	A	601	DAN	O10-C10-N5	-2.23	118.04	121.98
2	D	601	DAN	C6-C5-N5	2.06	114.19	110.91
2	D	601	DAN	C3-C2-C1	2.02	127.94	123.56
2	C	601	DAN	C5-N5-C10	-2.02	118.39	123.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	DAN	O1A-C1-C2-C3
2	D	601	DAN	O1A-C1-C2-O6
2	D	601	DAN	O1B-C1-C2-C3
2	D	601	DAN	O1B-C1-C2-O6
2	D	601	DAN	C7-C8-C9-O9
2	D	601	DAN	O8-C8-C9-O9

Continued on next page...

Continued from previous page...

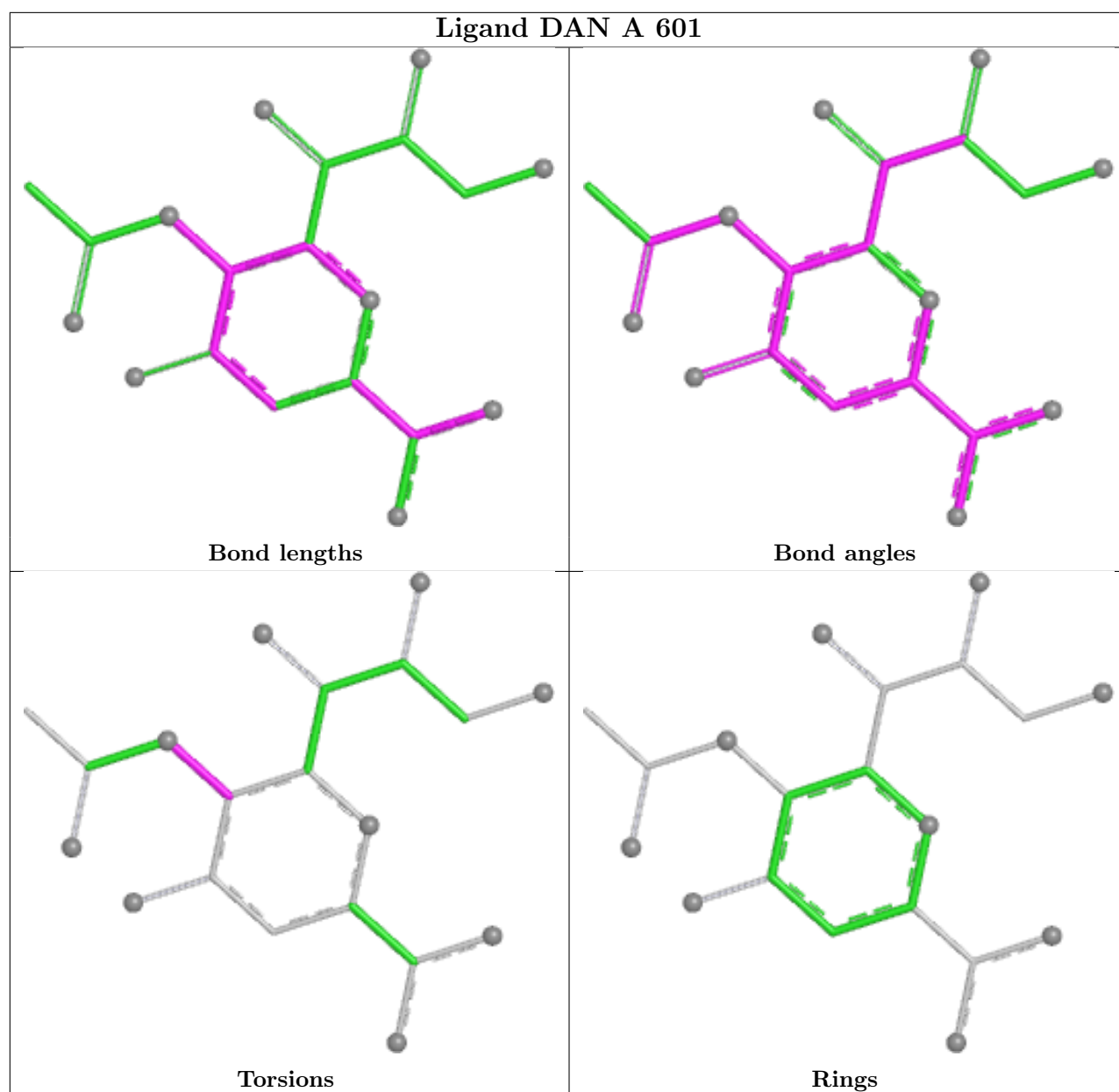
Mol	Chain	Res	Type	Atoms
2	A	601	DAN	C4-C5-N5-C10
2	D	601	DAN	C6-C5-N5-C10
2	C	601	DAN	C4-C5-N5-C10
2	B	601	DAN	C7-C8-C9-O9
2	D	601	DAN	C4-C5-N5-C10
2	B	601	DAN	O8-C8-C9-O9
2	C	601	DAN	C6-C5-N5-C10

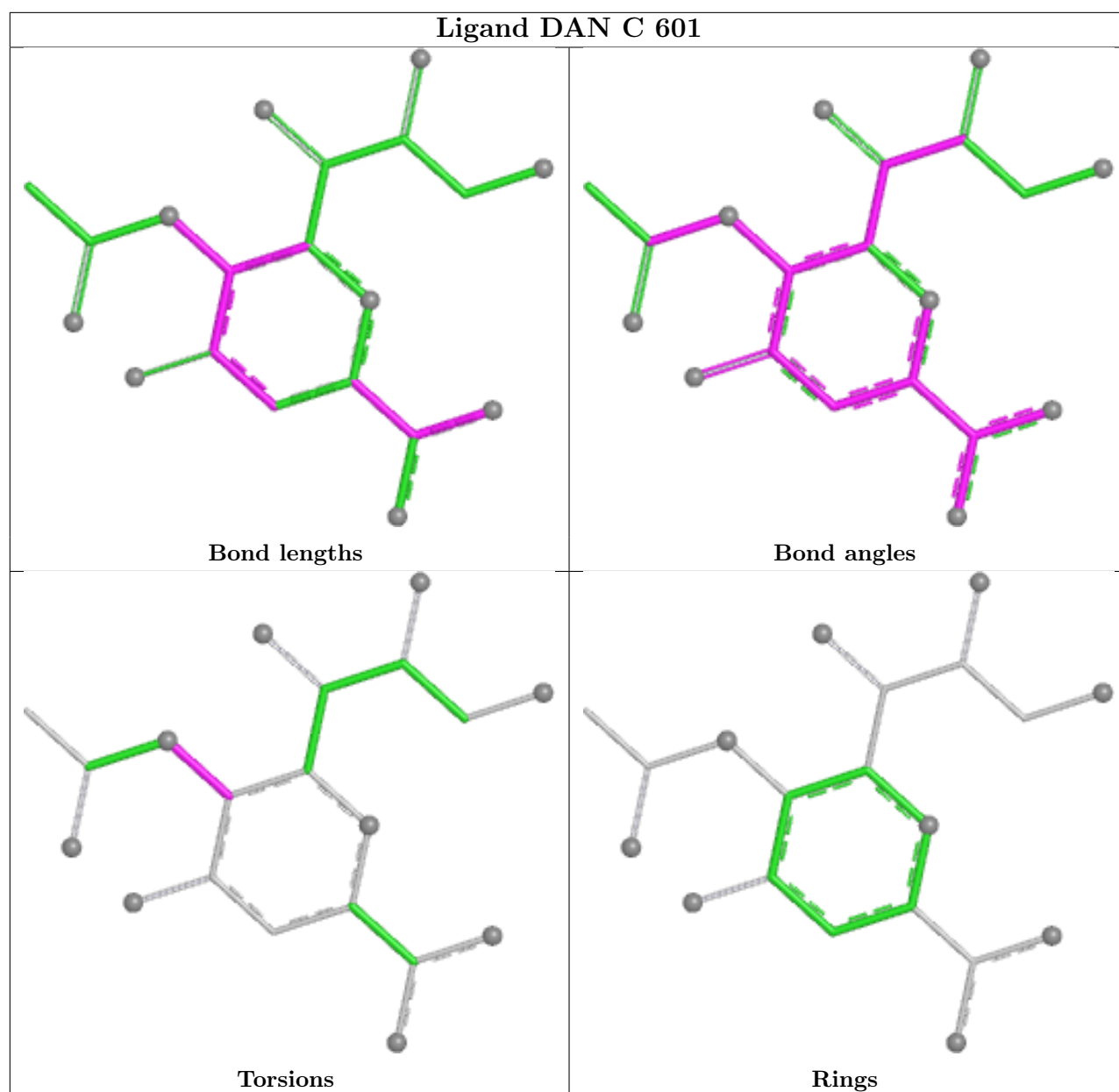
There are no ring outliers.

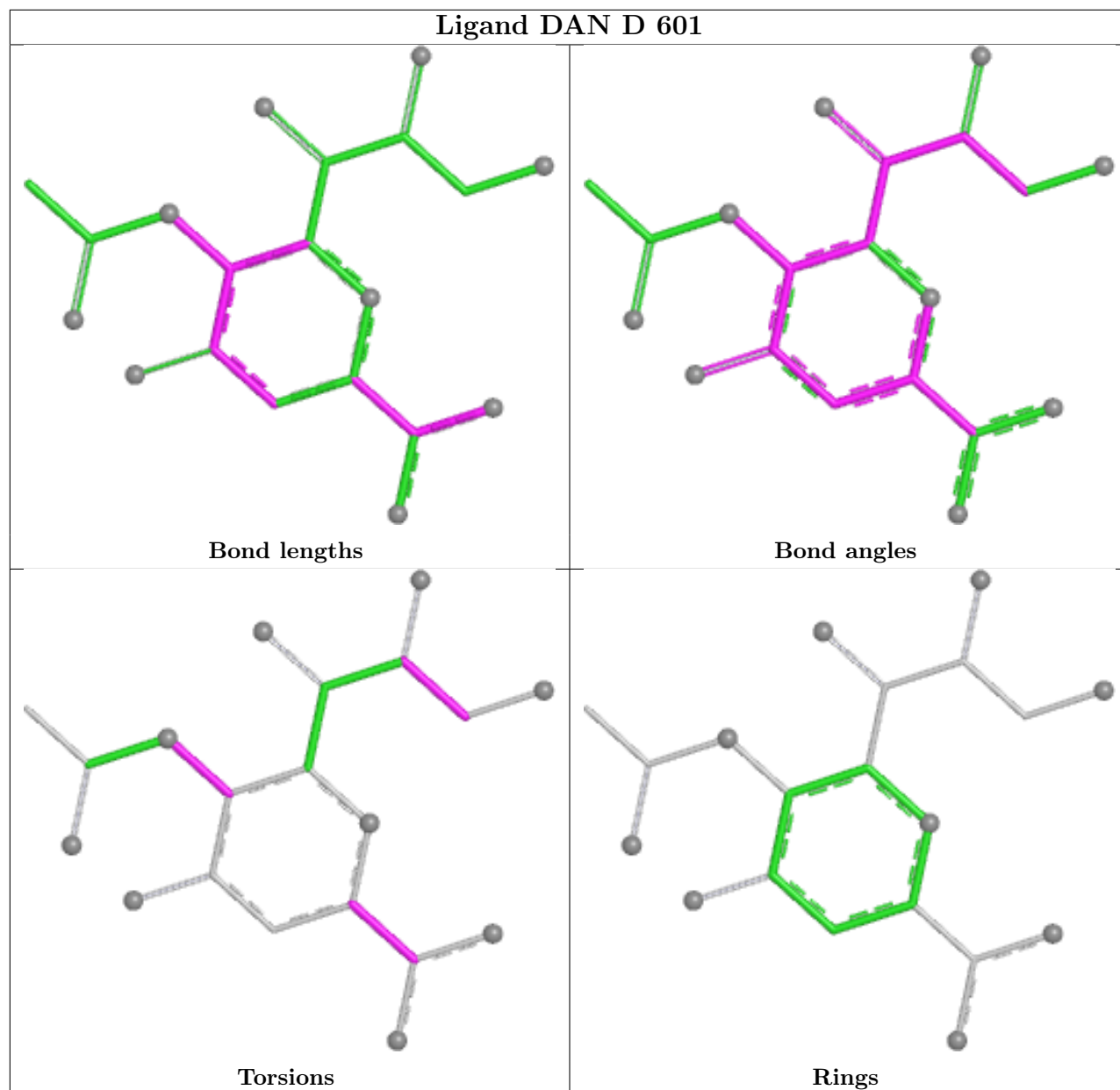
3 monomers are involved in 6 short contacts:

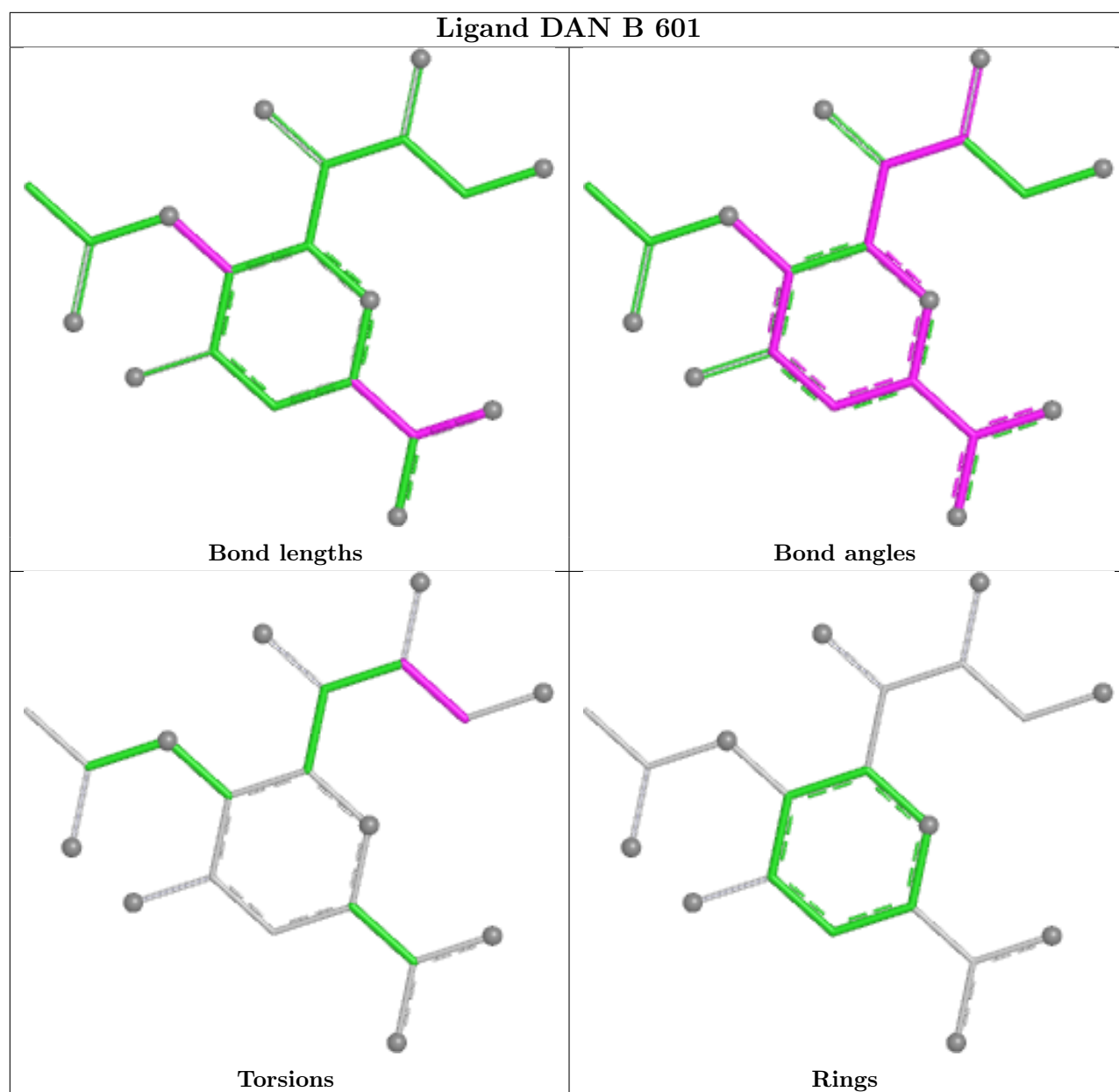
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	DAN	2	0
2	C	601	DAN	1	0
2	B	601	DAN	3	0

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	521/540 (96%)	0.25	26 (4%) 34 36	27, 40, 65, 89	0
1	B	521/540 (96%)	0.14	18 (3%) 47 49	27, 39, 58, 79	0
1	C	521/540 (96%)	0.33	21 (4%) 42 44	30, 41, 72, 88	0
1	D	521/540 (96%)	0.66	27 (5%) 33 35	33, 48, 67, 91	0
All	All	2084/2160 (96%)	0.35	92 (4%) 39 41	27, 42, 67, 91	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	ALA	5.3
1	B	430	ASN	4.5
1	A	11	VAL	4.3
1	D	54	PRO	4.2
1	A	10	THR	3.9
1	D	9	ASP	3.8
1	D	52	SER	3.7
1	A	73	HIS	3.6
1	A	75	ASP	3.5
1	D	374	MET	3.5
1	D	50	SER	3.5
1	D	53	THR	3.4
1	C	9	ASP	3.2
1	D	11	VAL	3.1
1	B	52	SER	3.1
1	A	9	ASP	3.1
1	C	75	ASP	3.1
1	B	428	ALA	3.0
1	D	286	TRP	3.0
1	B	53	THR	3.0
1	D	372	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	52	SER	2.9
1	D	114	VAL	2.9
1	C	10	THR	2.9
1	A	54	PRO	2.9
1	C	457	ASN	2.9
1	D	117	LYS	2.8
1	C	375	HIS	2.8
1	D	56	HIS	2.8
1	C	47	LEU	2.7
1	A	47	LEU	2.7
1	A	74	ARG	2.7
1	A	71	LEU	2.7
1	D	245	TYR	2.6
1	A	427	LYS	2.6
1	D	370	LYS	2.6
1	A	49	PHE	2.6
1	B	50	SER	2.6
1	A	56	HIS	2.6
1	B	54	PRO	2.6
1	C	78	ARG	2.6
1	D	375	HIS	2.5
1	C	71	LEU	2.5
1	C	39	SER	2.5
1	C	428	ALA	2.5
1	C	54	PRO	2.5
1	A	374	MET	2.5
1	A	12	PHE	2.5
1	C	51	LYS	2.5
1	A	76	LYS	2.4
1	A	235	LYS	2.4
1	A	157	LYS	2.4
1	D	417	LYS	2.4
1	C	56	HIS	2.4
1	B	149	LEU	2.4
1	B	429	LEU	2.4
1	B	138	GLY	2.3
1	B	374	MET	2.3
1	A	375	HIS	2.3
1	A	53	THR	2.3
1	D	47	LEU	2.3
1	D	49	PHE	2.3
1	A	52	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	104	CYS	2.3
1	B	47	LEU	2.3
1	D	312	TRP	2.3
1	A	121	LYS	2.3
1	D	109	ARG	2.3
1	B	75	ASP	2.3
1	B	55	LEU	2.3
1	A	162	LYS	2.2
1	D	51	LYS	2.2
1	B	36	ALA	2.2
1	D	253	ASN	2.2
1	A	302	MET	2.2
1	C	302	MET	2.2
1	C	374	MET	2.2
1	C	73	HIS	2.2
1	D	58	ILE	2.2
1	D	55	LEU	2.1
1	B	286	TRP	2.1
1	B	375	HIS	2.1
1	C	76	LYS	2.1
1	C	11	VAL	2.1
1	A	161	CYS	2.1
1	A	163	TYR	2.1
1	D	156	GLY	2.1
1	D	167	LYS	2.1
1	B	10	THR	2.0
1	C	169	ILE	2.0
1	B	38	ASP	2.0
1	D	161	CYS	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

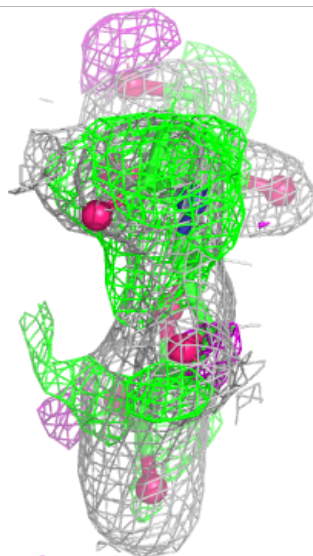
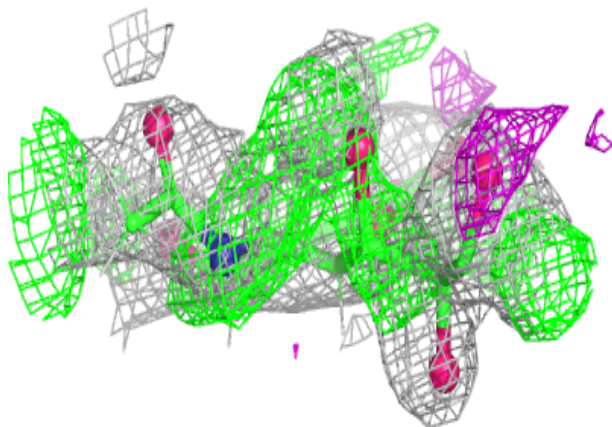
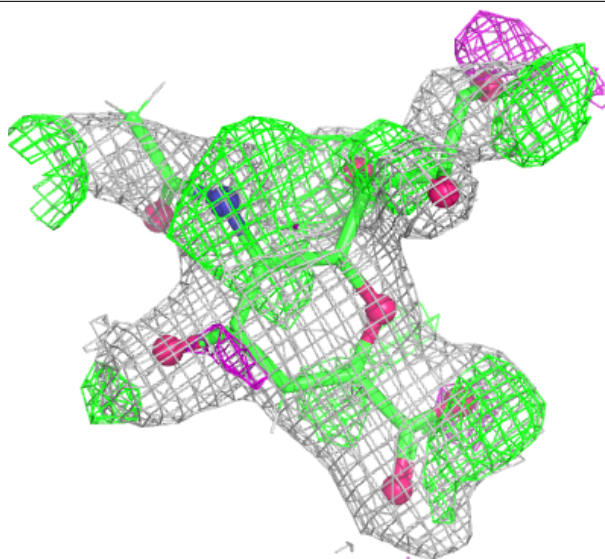
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DAN	B	601	20/20	0.66	0.23	33,49,61,63	10
2	DAN	C	601	20/20	0.67	0.21	33,47,59,62	10
2	DAN	D	601	20/20	0.67	0.25	37,51,62,64	10
2	DAN	A	601	20/20	0.71	0.22	33,52,63,73	10

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.

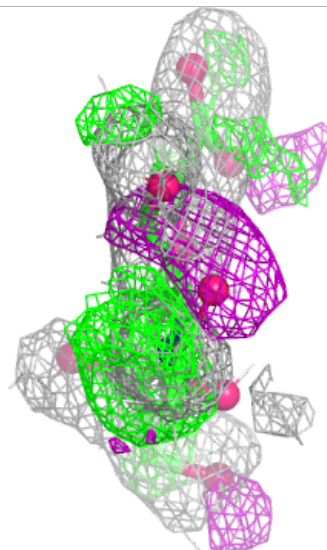
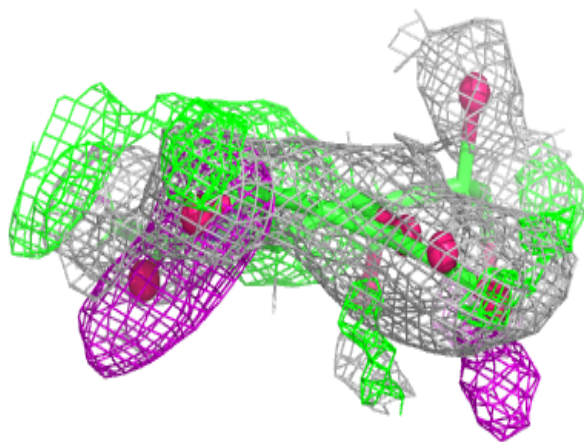
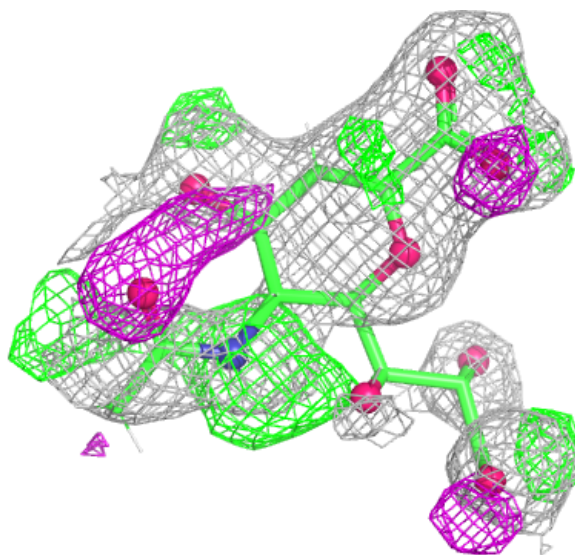
Electron density around DAN B 601:

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



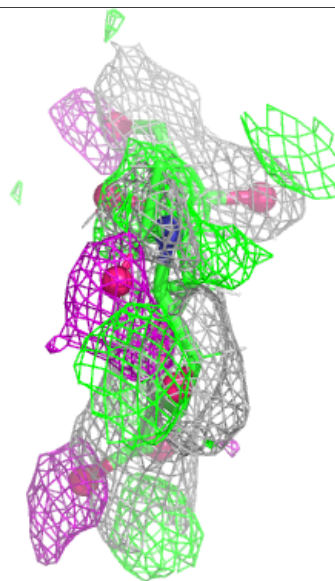
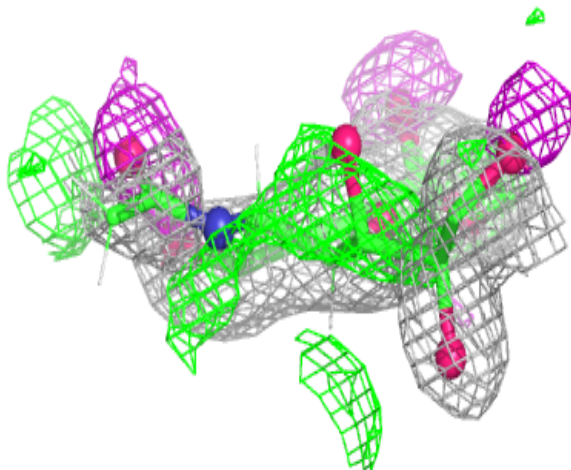
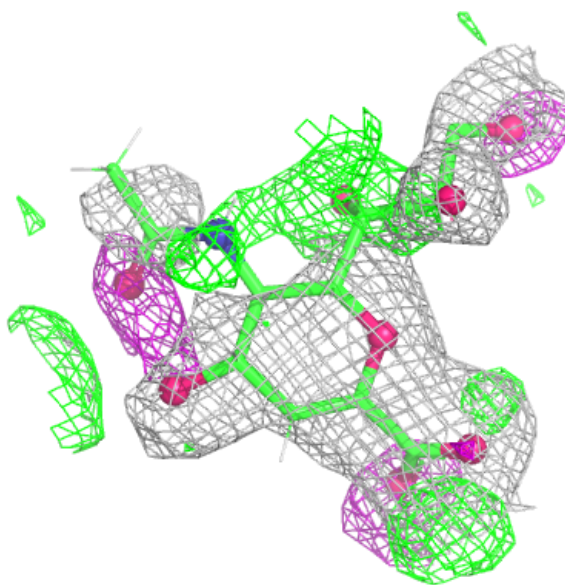
Electron density around DAN C 601:

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



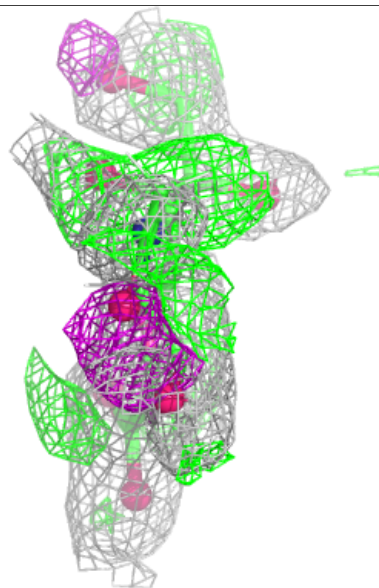
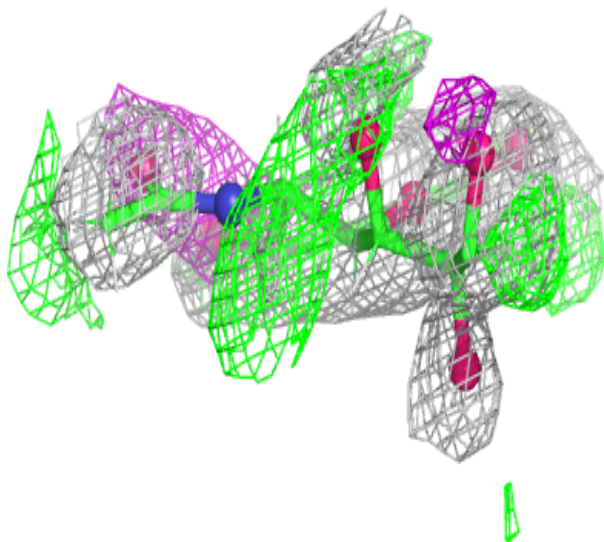
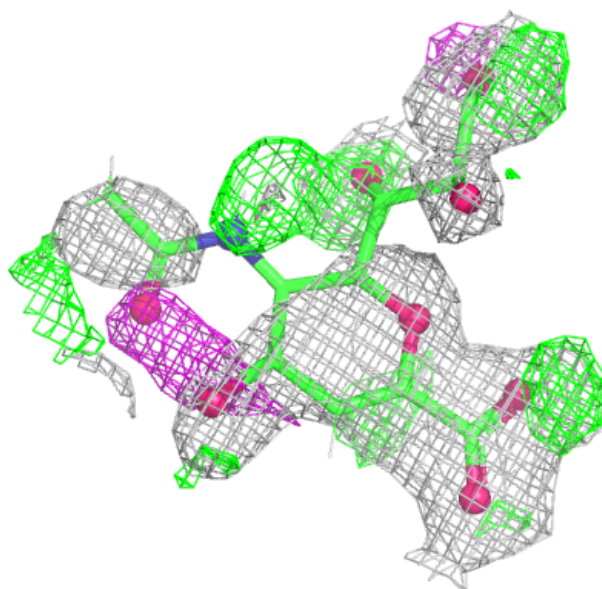
Electron density around DAN D 601:

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



Electron density around DAN A 601:

$2mF_o-DF_c$ (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.