



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:26 AM UTC

PDB ID : 4N8E / pdb_00004n8e
Title : DPP4 complexed with compound 12a
Authors : Ostermann, N.; Zink, F.; Kroemer, M.
Deposited on : 2013-10-17
Resolution : 2.30 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

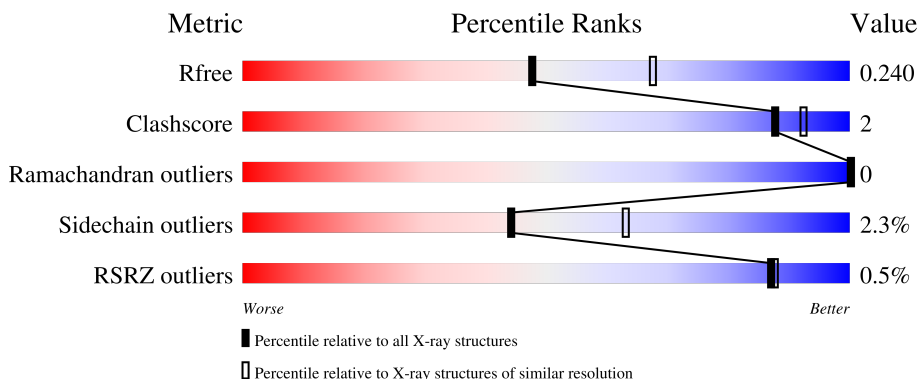
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

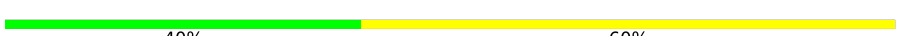
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	740	 90% 8% ..
1	B	740	 % 90% 9% .
2	C	5	 40% 60%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13353 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5959	3827	981	1125	26			
1	B	734	Total	C	N	O	S	0	0	0
			6006	3856	989	1135	26			

There are 26 discrepancies between the modelled and reference sequences:

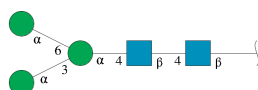
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	ILE	SER	conflict	UNP P27487
A	767	ALA	-	expression tag	UNP P27487
A	768	ALA	-	expression tag	UNP P27487
A	769	ALA	-	expression tag	UNP P27487
A	770	SER	-	expression tag	UNP P27487
A	771	TRP	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	PRO	-	expression tag	UNP P27487
A	775	GLN	-	expression tag	UNP P27487
A	776	PHE	-	expression tag	UNP P27487
A	777	GLU	-	expression tag	UNP P27487
A	778	LYS	-	expression tag	UNP P27487
B	437	ILE	SER	conflict	UNP P27487
B	767	ALA	-	expression tag	UNP P27487
B	768	ALA	-	expression tag	UNP P27487
B	769	ALA	-	expression tag	UNP P27487
B	770	SER	-	expression tag	UNP P27487
B	771	TRP	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	PRO	-	expression tag	UNP P27487
B	775	GLN	-	expression tag	UNP P27487
B	776	PHE	-	expression tag	UNP P27487
B	777	GLU	-	expression tag	UNP P27487

Continued on next page...

Continued from previous page...

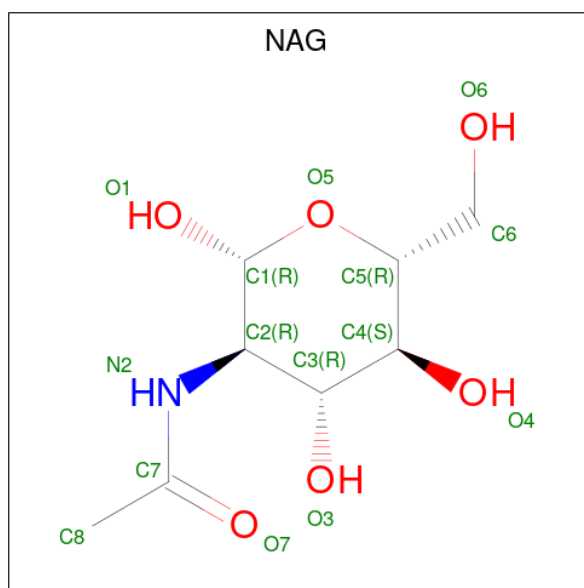
Chain	Residue	Modelled	Actual	Comment	Reference
B	778	LYS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



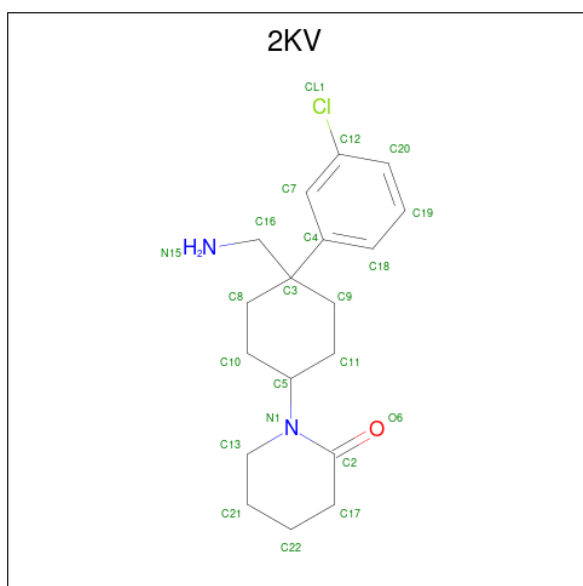
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1-[cis-4-(aminomethyl)-4-(3-chlorophenyl)cyclohexyl]piperidin-2-one (CCD ID: 2KV) (formula: C₁₈H₂₅ClN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			22	18	1	2	1		
5	B	1	Total	C	Cl	N	O	0	0
			22	18	1	2	1		

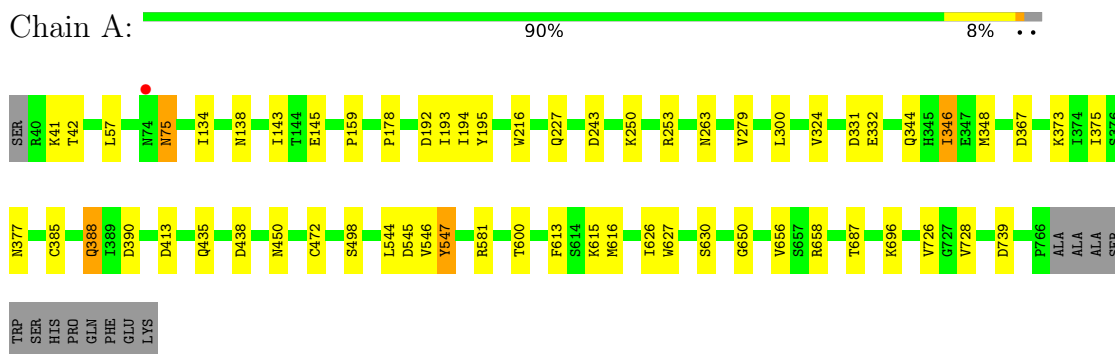
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	583	Total	O	0	0
			583	583		
6	B	502	Total	O	0	0
			502	502		

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: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.09Å 122.05Å 191.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.30 49.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.88-2.30) 98.3 (49.88-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.172 , 0.218 0.191 , 0.240	Depositor DCC
R_{free} test set	4589 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13353	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: NAG, 2KV, SO4, MAN

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	0.88	2/6131 (0.0%)	1.21	20/8339 (0.2%)
1	B	0.86	0/6180	1.21	21/8407 (0.2%)
All	All	0.87	2/12311 (0.0%)	1.21	41/16746 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	600	THR	CA-C	7.14	1.55	1.52
1	A	348	MET	SD-CE	-5.13	1.66	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ASP	CA-CB-CG	7.61	120.21	112.60
1	B	92	ASN	CA-CB-CG	7.46	120.06	112.60
1	B	739	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	615	LYS	CA-C-N	6.51	133.23	121.89
1	A	615	LYS	C-N-CA	6.51	133.23	121.89
1	A	739	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	450	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	367	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	367	ASP	CA-CB-CG	6.38	118.97	112.60
1	A	390	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	656	VAL	N-CA-C	-6.13	100.88	109.21
1	B	136	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	656	VAL	N-CA-C	-6.04	101.00	109.21
1	B	104	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	243	ASP	CA-C-N	5.80	128.84	120.38
1	A	243	ASP	C-N-CA	5.80	128.84	120.38
1	A	300	LEU	N-CA-C	-5.71	99.89	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	545	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	192	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	340	LEU	CA-C-N	5.55	128.35	120.53
1	B	340	LEU	C-N-CA	5.55	128.35	120.53
1	B	243	ASP	CA-C-N	5.40	128.27	120.38
1	B	243	ASP	C-N-CA	5.40	128.27	120.38
1	B	148	ILE	N-CA-C	-5.37	103.69	108.95
1	A	75	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	146	GLU	CA-C-N	5.29	128.59	120.82
1	B	146	GLU	C-N-CA	5.29	128.59	120.82
1	B	546	VAL	N-CA-C	5.23	116.11	108.53
1	A	377	ASN	CA-C-N	5.22	127.80	120.28
1	A	377	ASN	C-N-CA	5.22	127.80	120.28
1	A	388	GLN	N-CA-C	-5.20	100.77	109.24
1	B	421	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	113	PHE	N-CA-C	5.09	116.73	109.14
1	B	300	LEU	N-CA-C	-5.09	100.87	108.96
1	A	546	VAL	N-CA-C	5.08	115.89	108.53
1	A	331	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	545	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	713	PHE	CA-C-N	5.04	128.39	120.82
1	B	713	PHE	C-N-CA	5.04	128.39	120.82
1	A	377	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

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	5959	0	5679	24	0
1	B	6006	0	5720	25	0
2	C	61	0	52	0	0
3	A	84	0	78	2	0
3	B	84	0	78	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	22	0	25	0	0
5	B	22	0	25	1	0
6	A	583	0	0	3	0
6	B	502	0	0	2	0
All	All	13353	0	11657	48	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 2.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.63	0.81
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.63	0.79
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.29	0.77
1:B:434:ILE:HG22	1:B:442:VAL:HG22	1.69	0.73
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.71	0.72
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.86	0.58
1:A:435:GLN:HE21	1:A:438:ASP:HB3	1.69	0.57
1:B:434:ILE:CG2	1:B:442:VAL:HG22	2.35	0.56
1:A:658:ARG:HG3	1:A:687:THR:HG22	1.89	0.55
1:B:658:ARG:HG3	1:B:687:THR:HG22	1.91	0.53
1:A:613:PHE:O	1:A:616:MET:HB2	2.10	0.52
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.92	0.51
1:B:630:SER:HB3	5:B:810:2KV:C19	2.42	0.50
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.92	0.50
1:A:250:LYS:HD2	6:A:1383:HOH:O	2.12	0.49
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.95	0.49
1:A:544:LEU:HD23	1:A:626:ILE:HD12	1.94	0.47
1:B:626:ILE:O	1:B:650:GLY:HA2	2.14	0.47
1:A:435:GLN:NE2	1:A:438:ASP:HB3	2.29	0.47
1:B:324:VAL:HG22	1:B:346:ILE:HG13	1.95	0.47
1:A:581:ARG:NE	3:A:811:NAG:H82	2.30	0.47
1:B:378:GLU:CD	1:B:378:GLU:H	2.23	0.46
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.98	0.46
1:A:324:VAL:CG1	1:A:344:GLN:HG2	2.46	0.45
1:A:195:TYR:O	1:A:227:GLN:HA	2.17	0.45
1:A:324:VAL:HG22	1:A:346:ILE:HG13	1.99	0.45
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LYS:HD2	6:B:1125:HOH:O	2.17	0.44
1:A:41:LYS:HE3	1:A:42:THR:O	2.18	0.44
1:A:626:ILE:O	1:A:650:GLY:HA2	2.18	0.44
1:B:112:GLN:HG2	1:B:138:ASN:HD21	1.83	0.44
1:B:127:SER:HB3	1:B:211:TYR:CG	2.54	0.43
1:A:373:LYS:HD3	1:A:375:ILE:HD11	2.00	0.43
1:B:373:LYS:HD3	1:B:375:ILE:HD11	2.01	0.43
1:B:41:LYS:HE3	1:B:42:THR:O	2.19	0.43
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.01	0.42
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.01	0.42
1:B:739:ASP:HB2	6:B:940:HOH:O	2.19	0.42
1:B:345:HIS:HE1	1:B:389:ILE:O	2.03	0.42
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.51	0.41
1:B:352:GLY:HA2	1:B:595:ASN:ND2	2.36	0.41
1:B:614:SER:HB3	1:B:624:ILE:HD11	2.03	0.41
1:B:195:TYR:O	1:B:227:GLN:HA	2.22	0.41
1:A:581:ARG:NH1	3:A:811:NAG:HN2	2.19	0.40
1:A:279:VAL:HA	6:A:1283:HOH:O	2.20	0.40
1:A:547:TYR:C	1:A:547:TYR:CD1	2.99	0.40
1:A:630:SER:HB2	6:A:1156:HOH:O	2.21	0.40
1:B:414:TYR:CE1	1:B:435:GLN:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/740 (98%)	693 (96%)	32 (4%)	0	100	100
1	B	732/740 (99%)	695 (95%)	37 (5%)	0	100	100
All	All	1457/1480 (98%)	1388 (95%)	69 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	652/662 (98%)	638 (98%)	14 (2%)	47	66
1	B	656/662 (99%)	640 (98%)	16 (2%)	43	62
All	All	1308/1324 (99%)	1278 (98%)	30 (2%)	44	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	75	ASN
1	A	138	ASN
1	A	143	ILE
1	A	145	GLU
1	A	263	ASN
1	A	332	GLU
1	A	346	ILE
1	A	385	CYS
1	A	388	GLN
1	A	472	CYS
1	A	498	SER
1	A	547	TYR
1	A	627	TRP
1	B	39	SER
1	B	57	LEU
1	B	97	GLU
1	B	101	SER
1	B	114	ILE
1	B	145	GLU
1	B	263	ASN
1	B	332	GLU
1	B	341	VAL
1	B	385	CYS
1	B	434	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	448	GLU
1	B	472	CYS
1	B	484	SER
1	B	547	TYR
1	B	627	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	123	GLN
1	A	196	ASN
1	A	227	GLN
1	A	263	ASN
1	A	314	GLN
1	A	363	HIS
1	A	430	ASN
1	A	435	GLN
1	A	455	GLN
1	A	506	ASN
1	A	553	GLN
1	A	606	GLN
1	B	51	ASN
1	B	72	GLN
1	B	227	GLN
1	B	263	ASN
1	B	314	GLN
1	B	338	ASN
1	B	344	GLN
1	B	345	HIS
1	B	363	HIS
1	B	430	ASN
1	B	435	GLN
1	B	450	ASN
1	B	506	ASN
1	B	595	ASN
1	B	606	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 ⓘ

5 monosaccharides 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	NAG	C	1	2,1	14,14,15	0.38	0	17,19,21	0.65	0
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.40	4 (23%)
2	MAN	C	3	2	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
2	MAN	C	4	2	11,11,12	0.44	0	15,15,17	0.63	0
2	MAN	C	5	2	11,11,12	0.42	0	15,15,17	0.97	1 (6%)

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	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	1/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C1-C2	-2.73	107.07	111.29
2	C	5	MAN	C1-O5-C5	2.61	115.69	112.19
2	C	2	NAG	O3-C3-C2	-2.59	104.02	109.40
2	C	3	MAN	C1-O5-C5	2.46	115.49	112.19
2	C	2	NAG	O4-C4-C5	-2.23	103.82	109.32
2	C	2	NAG	C1-C2-N2	2.21	113.91	110.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

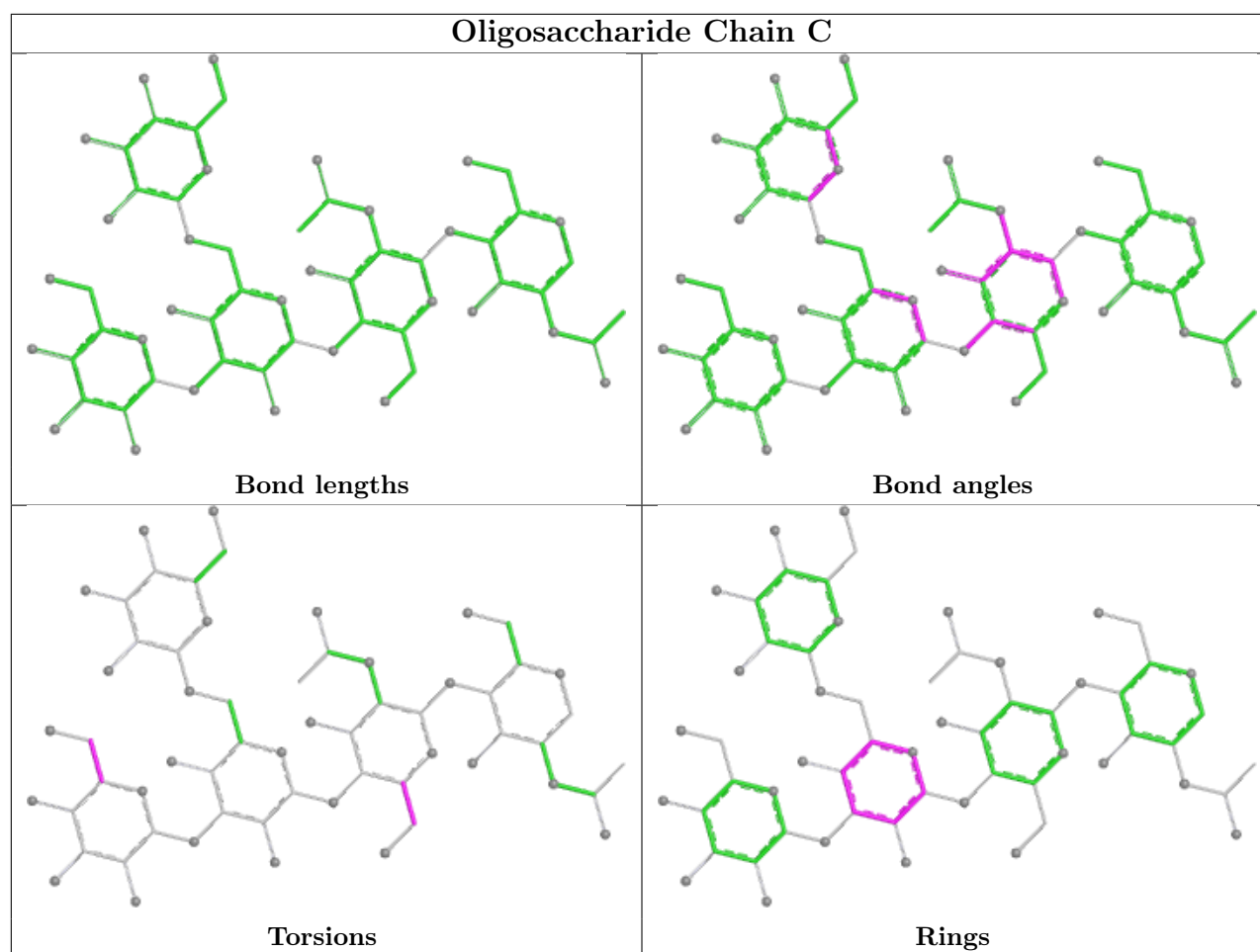
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
3	NAG	A	809	1	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
3	NAG	B	805	1	14,14,15	0.36	0	17,19,21	0.86	1 (5%)
3	NAG	A	807	1	14,14,15	0.31	0	17,19,21	0.44	0
4	SO4	B	808	-	4,4,4	0.28	0	6,6,6	0.25	0
3	NAG	B	804	1	14,14,15	0.29	0	17,19,21	1.12	3 (17%)
3	NAG	A	808	1	14,14,15	0.34	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	809	-	4,4,4	0.26	0	6,6,6	0.15	0
4	SO4	A	813	-	4,4,4	0.24	0	6,6,6	0.20	0
4	SO4	B	807	-	4,4,4	0.38	0	6,6,6	0.19	0
3	NAG	A	806	1	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	NAG	A	810	1	14,14,15	0.25	0	17,19,21	1.04	1 (5%)
4	SO4	A	812	-	4,4,4	0.25	0	6,6,6	0.18	0
3	NAG	B	803	1	14,14,15	0.34	0	17,19,21	0.37	0
3	NAG	B	801	1	14,14,15	0.46	0	17,19,21	1.12	1 (5%)
5	2KV	A	815	-	23,24,24	1.42	3 (13%)	30,34,34	1.90	9 (30%)
4	SO4	A	814	-	4,4,4	0.26	0	6,6,6	0.09	0
5	2KV	B	810	-	23,24,24	1.16	1 (4%)	30,34,34	1.93	9 (30%)
3	NAG	B	802	1	14,14,15	0.35	0	17,19,21	0.62	1 (5%)
3	NAG	B	806	1	14,14,15	0.36	0	17,19,21	1.36	3 (17%)
3	NAG	A	811	1	14,14,15	0.34	0	17,19,21	1.34	3 (17%)

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	NAG	A	808	1	-	0/6/23/26	0/1/1/1
3	NAG	A	809	1	-	0/6/23/26	0/1/1/1
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
3	NAG	B	806	1	-	0/6/23/26	0/1/1/1
3	NAG	B	805	1	-	1/6/23/26	0/1/1/1
3	NAG	A	807	1	-	0/6/23/26	0/1/1/1
3	NAG	A	811	1	-	3/6/23/26	0/1/1/1
3	NAG	A	810	1	-	0/6/23/26	0/1/1/1
5	2KV	A	815	-	-	0/13/36/36	0/3/3/3
5	2KV	B	810	-	-	1/13/36/36	0/3/3/3
3	NAG	B	803	1	-	1/6/23/26	0/1/1/1
3	NAG	B	804	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	815	2KV	C11-C5	2.32	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	815	2KV	C10-C5	2.28	1.58	1.52
5	A	815	2KV	C3-C4	2.20	1.57	1.53
5	B	810	2KV	C10-C5	2.09	1.57	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	810	2KV	C12-C7-C4	4.52	123.13	119.48
5	A	815	2KV	C21-C13-N1	4.24	117.21	110.65
3	A	811	NAG	C1-C2-N2	3.94	116.64	110.43
3	B	801	NAG	C1-O5-C5	3.75	117.21	112.19
5	A	815	2KV	C12-C7-C4	3.66	122.44	119.48
3	A	810	NAG	O5-C1-C2	-3.45	105.95	111.29
5	A	815	2KV	O6-C2-C17	-3.32	113.93	121.35
5	A	815	2KV	C9-C11-C5	3.24	115.48	110.99
5	B	810	2KV	O6-C2-C17	-3.22	114.17	121.35
5	B	810	2KV	C17-C2-N1	3.20	122.93	118.42
3	B	806	NAG	O5-C1-C2	3.18	116.20	111.29
5	B	810	2KV	C10-C5-C11	3.10	118.18	111.17
5	B	810	2KV	C21-C13-N1	3.07	115.40	110.65
5	A	815	2KV	C17-C2-N1	3.01	122.66	118.42
3	B	806	NAG	C1-C2-N2	-2.97	105.75	110.43
3	A	806	NAG	C1-O5-C5	2.86	116.01	112.19
3	B	804	NAG	O5-C1-C2	-2.83	106.91	111.29
3	B	806	NAG	C1-O5-C5	2.82	115.97	112.19
5	B	810	2KV	C9-C11-C5	2.76	114.82	110.99
5	A	815	2KV	C10-C5-N1	2.73	115.63	111.83
3	B	805	NAG	C1-C2-N2	-2.57	106.38	110.43
5	B	810	2KV	C8-C3-C16	2.52	114.51	109.39
3	B	804	NAG	C1-O5-C5	2.48	115.51	112.19
3	A	811	NAG	C2-N2-C7	2.42	126.15	122.90
5	A	815	2KV	C10-C5-C11	2.32	116.41	111.17
3	A	811	NAG	O5-C1-C2	-2.24	107.83	111.29
5	A	815	2KV	C20-C12-CL1	2.22	122.63	119.36
3	B	804	NAG	C1-C2-N2	2.20	113.90	110.43
5	A	815	2KV	C7-C12-CL1	-2.20	116.41	119.17
3	A	809	NAG	C1-O5-C5	2.17	115.09	112.19
5	B	810	2KV	C11-C9-C3	2.17	116.94	113.39
5	B	810	2KV	C20-C12-CL1	2.12	122.49	119.36
3	B	802	NAG	C1-O5-C5	2.03	114.90	112.19
3	A	808	NAG	O5-C1-C2	-2.02	108.16	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	811	NAG	C1-C2-N2-C7
3	A	811	NAG	C8-C7-N2-C2
5	B	810	2KV	N15-C16-C3-C9
3	B	803	NAG	C1-C2-N2-C7
3	A	811	NAG	O7-C7-N2-C2
3	B	805	NAG	C4-C5-C6-O6

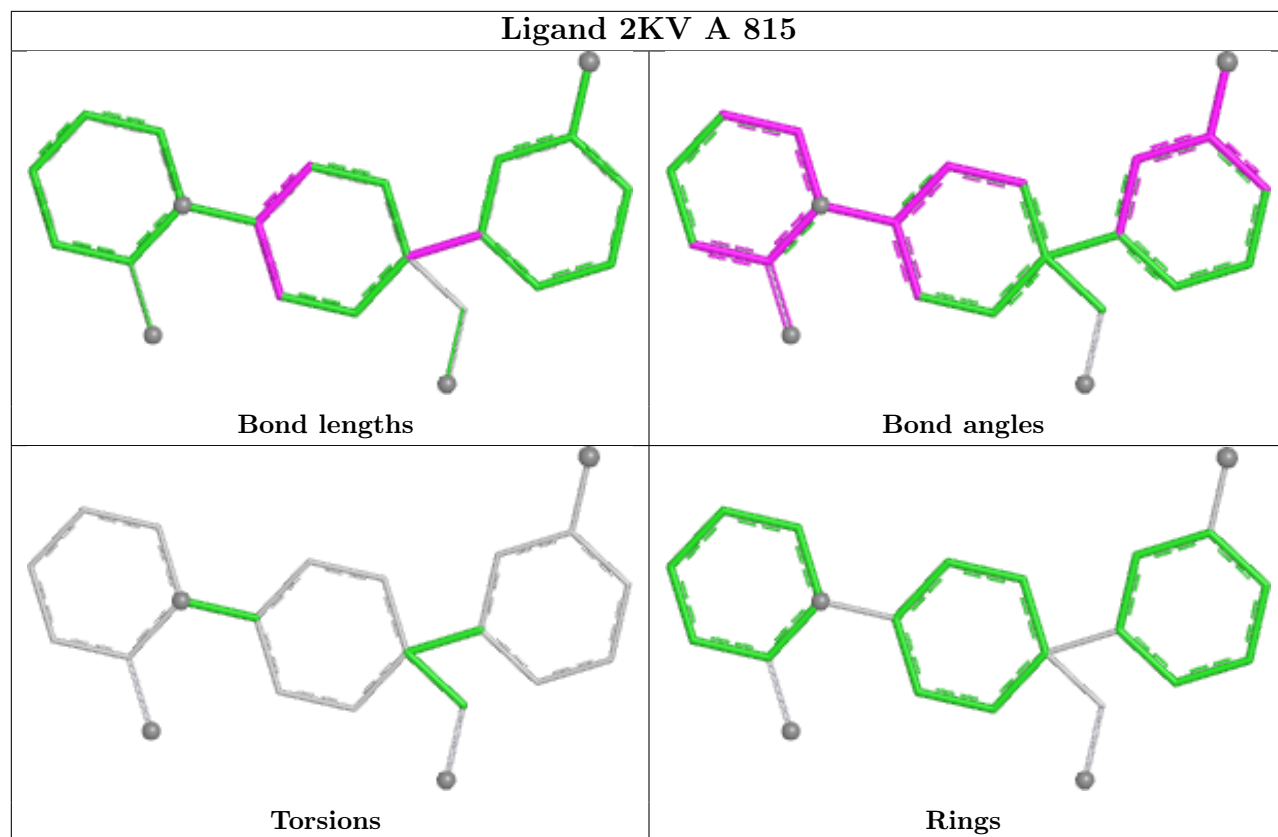
There are no ring outliers.

2 monomers are involved in 3 short contacts:

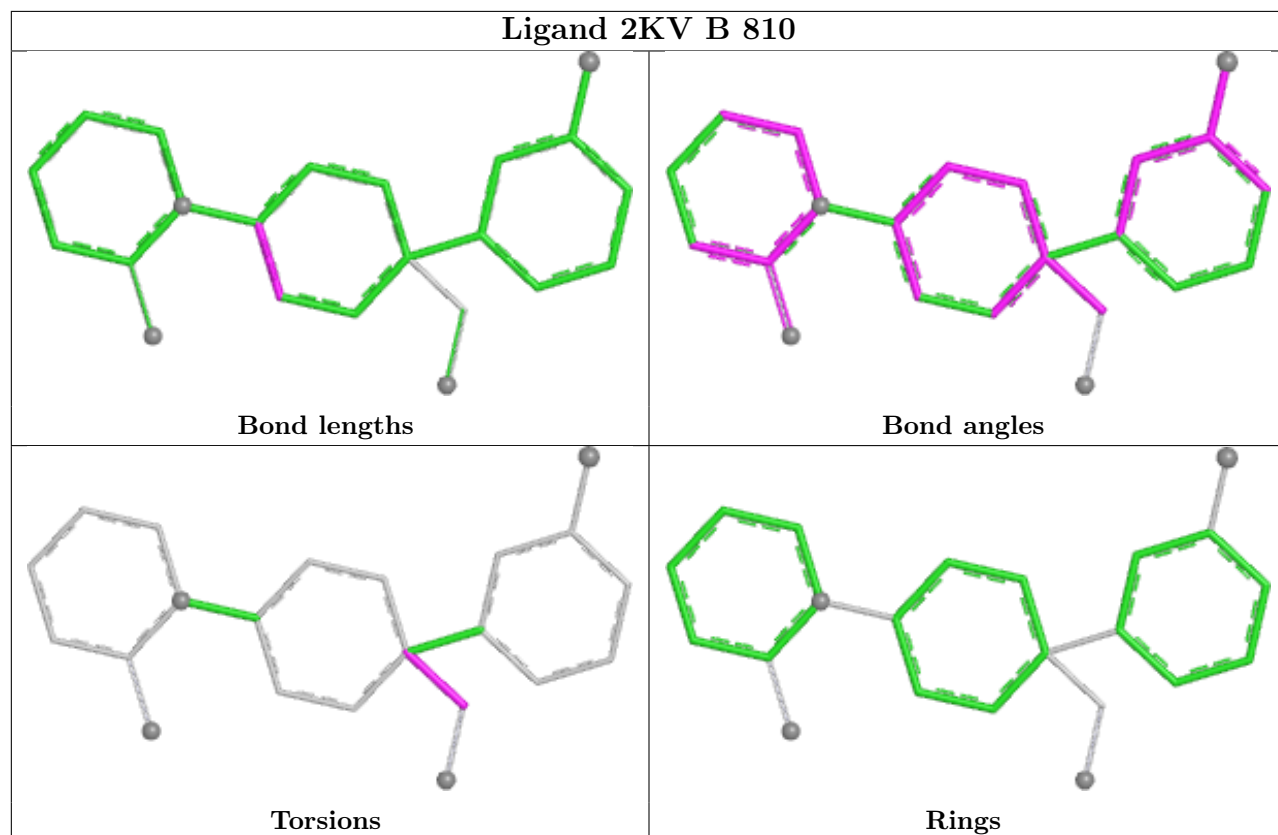
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	810	2KV	1	0
3	A	811	NAG	2	0

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.

Ligand 2KV A 815



Ligand 2KV B 810



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	727/740 (98%)	-0.51	1 (0%) 92 91	8, 20, 43, 73	0
1	B	734/740 (99%)	-0.36	7 (0%) 79 80	10, 24, 50, 78	0
All	All	1461/1480 (98%)	-0.43	8 (0%) 87 87	8, 22, 47, 78	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	GLY	3.1
1	B	98	PHE	3.0
1	B	772	SER	2.8
1	B	466	LYS	2.4
1	A	74	ASN	2.1
1	B	519	LEU	2.1
1	B	97	GLU	2.1
1	B	95	PHE	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](#)

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.

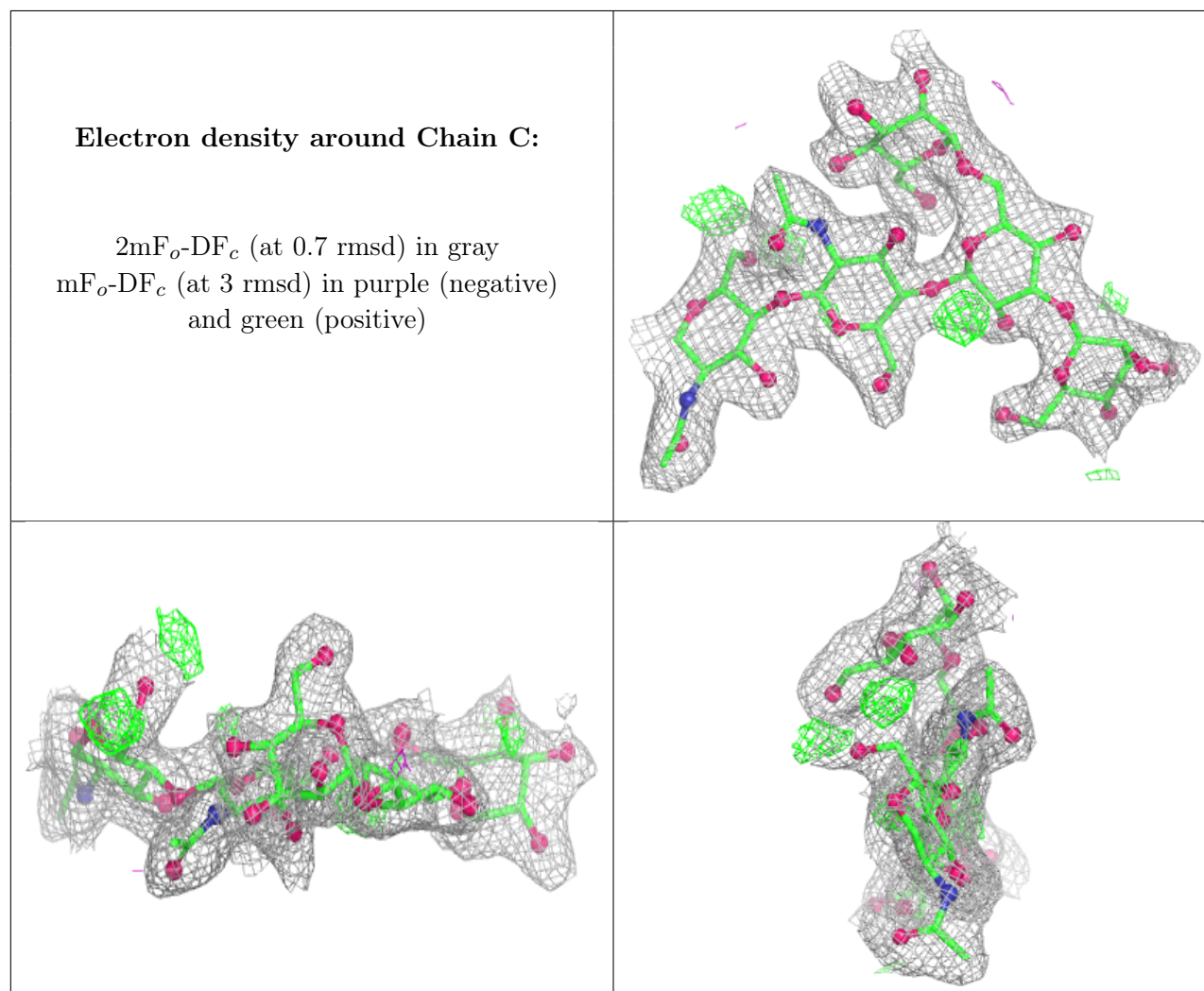
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	4	11/12	0.85	0.12	53,55,59,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.89	0.10	36,41,46,48	0
2	MAN	C	3	11/12	0.90	0.09	37,41,43,49	0
2	NAG	C	1	14/15	0.92	0.09	14,30,42,47	0
2	MAN	C	5	11/12	0.93	0.08	25,37,39,40	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

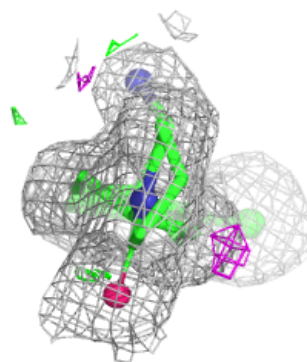
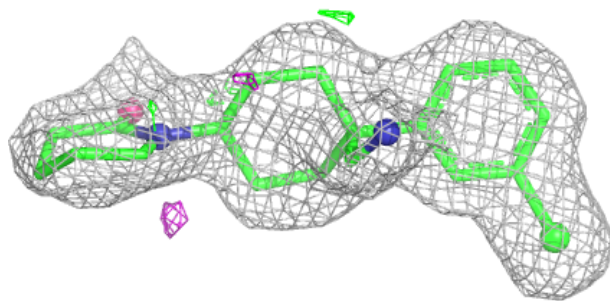
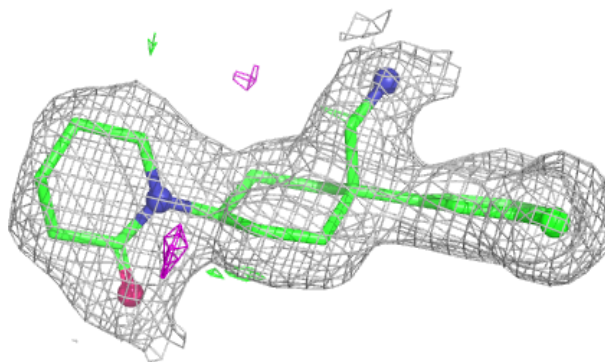
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	814	5/5	0.68	0.20	135,135,135,136	0
3	NAG	B	802	14/15	0.77	0.15	55,64,68,70	0
4	SO4	B	809	5/5	0.77	0.19	110,111,112,113	0
3	NAG	A	807	14/15	0.81	0.14	47,55,61,64	0
3	NAG	B	801	14/15	0.83	0.14	54,62,64,65	0
3	NAG	A	806	14/15	0.83	0.12	41,44,55,57	0
4	SO4	B	808	5/5	0.84	0.14	96,96,97,98	0
4	SO4	B	807	5/5	0.84	0.12	81,82,82,84	0
3	NAG	B	803	14/15	0.85	0.14	47,58,63,64	0
3	NAG	B	805	14/15	0.88	0.10	43,49,51,51	0
3	NAG	B	806	14/15	0.88	0.11	33,40,46,47	0
3	NAG	A	808	14/15	0.90	0.09	30,34,37,39	0
4	SO4	A	812	5/5	0.90	0.14	83,84,84,87	0
3	NAG	A	811	14/15	0.91	0.10	34,40,48,53	0
3	NAG	A	809	14/15	0.92	0.09	31,42,46,47	0
3	NAG	A	810	14/15	0.93	0.08	33,37,42,43	0
3	NAG	B	804	14/15	0.94	0.07	24,29,32,33	0
4	SO4	A	813	5/5	0.95	0.15	49,54,57,58	0
5	2KV	A	815	22/22	0.97	0.06	5,16,22,24	0
5	2KV	B	810	22/22	0.97	0.06	9,17,20,22	0

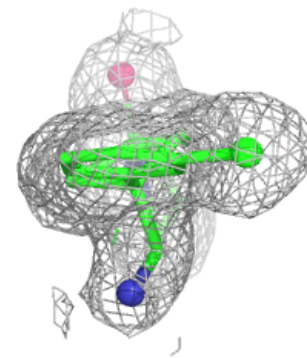
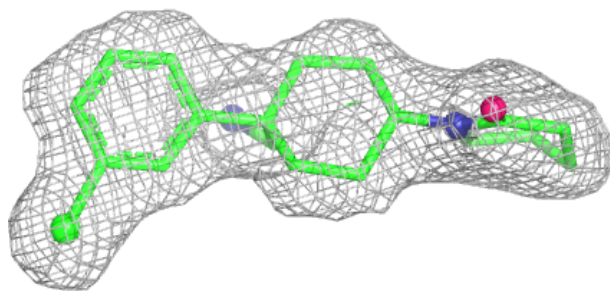
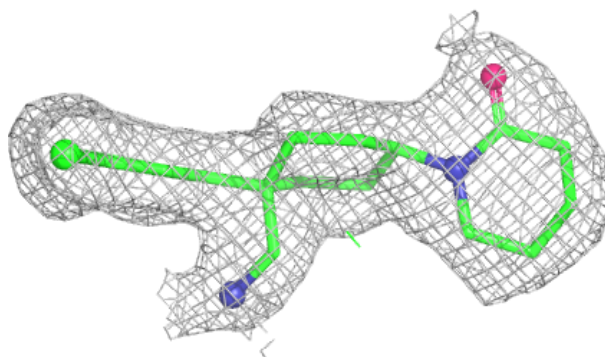
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2KV A 815:

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

**Electron density around 2KV B 810:**

$2mF_o-DF_c$ (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.