



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:31 AM UTC

PDB ID : 3F8S / pdb_00003f8s
Title : Crystal structure of dipeptidyl peptidase IV in complex with inhibitor
Authors : Ammirati, M.J.; Liu, S.; Piotrowski, D.W.
Deposited on : 2008-11-13
Resolution : 2.43 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

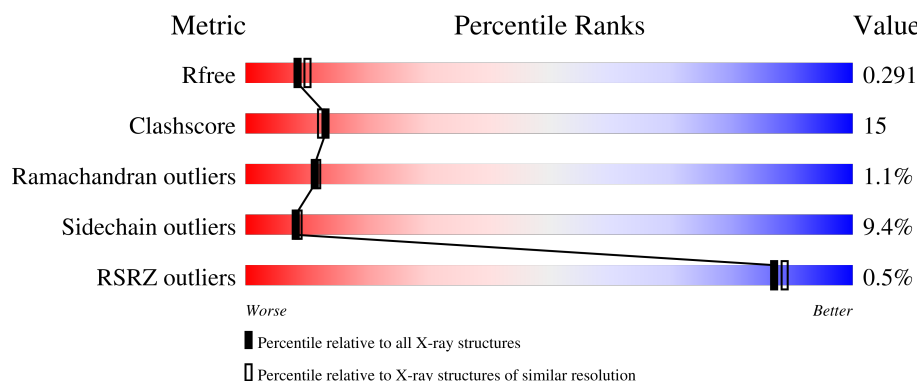
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

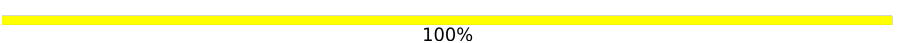
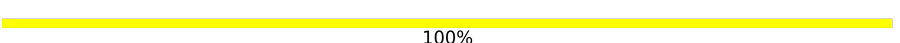
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	748	 66% 27% 5% •
1	B	748	 65% 27% 5% •
2	C	2	 100%
2	D	2	 100%
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%

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
3	NAG	B	799	X	-	-	-
4	PF2	B	900	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12132 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	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

There are 24 discrepancies between the modelled and reference sequences:

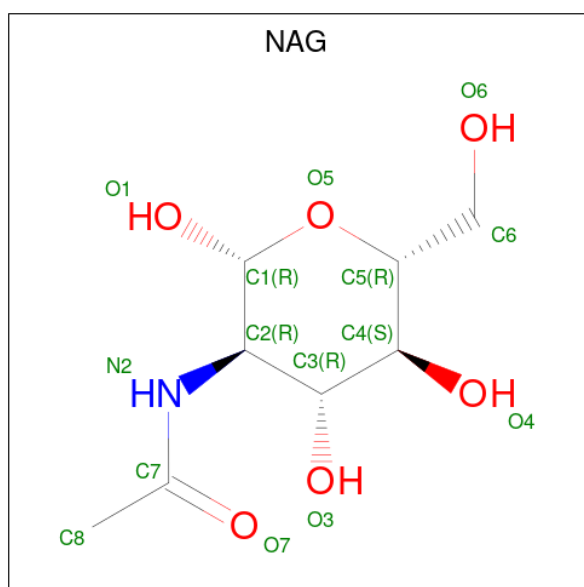
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	expression tag	UNP P27487
A	768	VAL	-	expression tag	UNP P27487
A	769	PRO	-	expression tag	UNP P27487
A	770	ARG	-	expression tag	UNP P27487
A	771	GLY	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	HIS	-	expression tag	UNP P27487
A	775	HIS	-	expression tag	UNP P27487
A	776	HIS	-	expression tag	UNP P27487
A	777	HIS	-	expression tag	UNP P27487
A	778	HIS	-	expression tag	UNP P27487
B	767	LEU	-	expression tag	UNP P27487
B	768	VAL	-	expression tag	UNP P27487
B	769	PRO	-	expression tag	UNP P27487
B	770	ARG	-	expression tag	UNP P27487
B	771	GLY	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	HIS	-	expression tag	UNP P27487
B	775	HIS	-	expression tag	UNP P27487
B	776	HIS	-	expression tag	UNP P27487
B	777	HIS	-	expression tag	UNP P27487
B	778	HIS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called 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	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

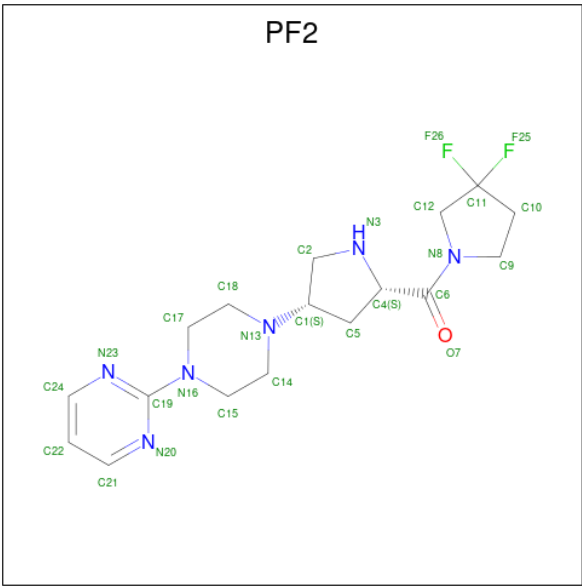
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	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 2-(4-{(3S,5S)-5-[(3,3-difluoropyrrolidin-1-yl)carbonyl]pyrrolidin-3-yl}piperazin

-1-yl)pyrimidine (CCD ID: PF2) (formula: C₁₇H₂₄F₂N₆O).

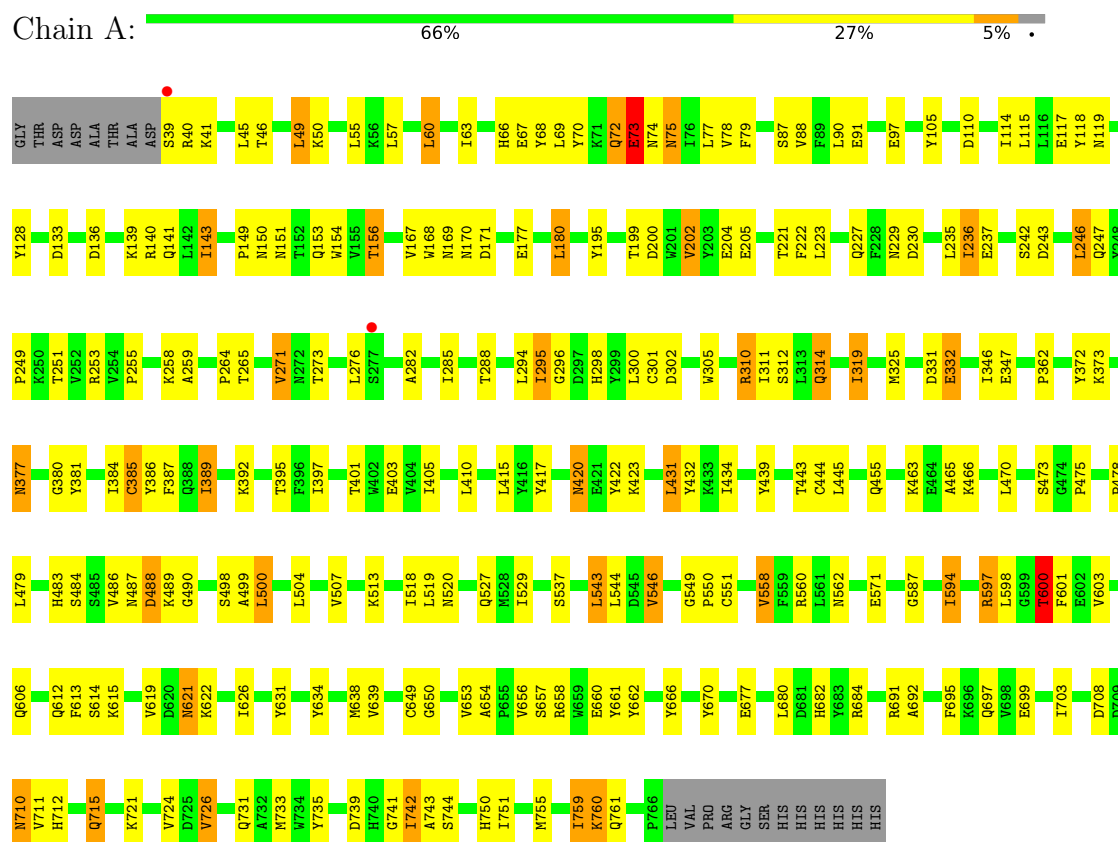


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	17	2	6	1		
4	B	1	Total	C	F	N	O	0	0
			26	17	2	6	1		

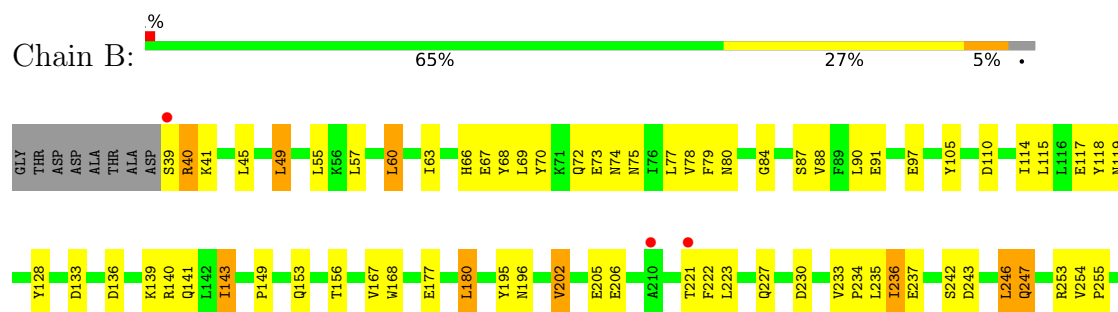
3 Residue-property plots

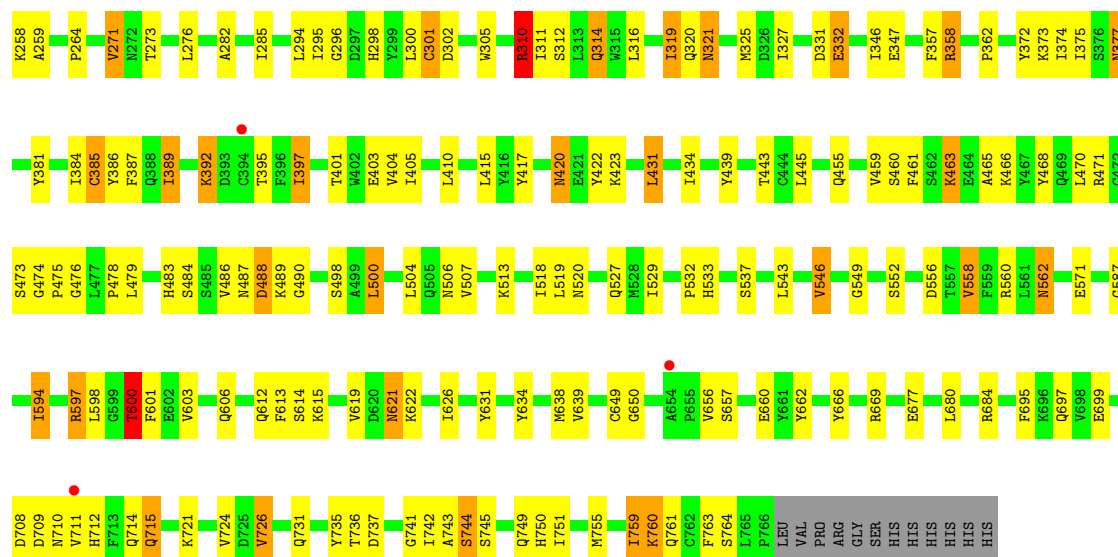
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Dipeptidyl peptidase 4





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.43Å 67.14Å 421.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.43 50.00 – 2.43	Depositor EDS
% Data completeness (in resolution range)	47.8 (50.00-2.43) 47.8 (50.00-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.243 , 0.295 0.249 , 0.291	Depositor DCC
R_{free} test set	1685 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	1.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12132	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, PF2

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	0.68	0/6135	0.92	6/8344 (0.1%)
1	B	0.72	0/6135	0.96	11/8344 (0.1%)
All	All	0.70	0/12270	0.94	17/16688 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ARG	NE-CZ-NH1	-11.39	110.11	121.50
1	B	310	ARG	NE-CZ-NH2	10.09	128.28	119.20
1	B	310	ARG	CD-NE-CZ	9.21	137.29	124.40
1	A	310	ARG	NE-CZ-NH2	-9.17	110.95	119.20
1	B	389	ILE	N-CA-C	8.98	119.78	110.62
1	A	310	ARG	CD-NE-CZ	8.54	136.36	124.40
1	A	389	ILE	N-CA-C	7.24	118.00	110.62
1	A	310	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	B	744	SER	N-CA-C	-6.37	101.97	110.24
1	B	202	VAL	CB-CA-C	-5.64	104.52	112.14
1	B	254	VAL	N-CA-C	5.58	114.09	107.73
1	B	254	VAL	CB-CA-C	-5.57	104.44	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	GLN	N-CA-C	5.56	117.02	111.07
1	A	562	ASN	N-CA-C	5.34	115.18	108.45
1	A	202	VAL	CB-CA-C	-5.29	104.93	112.22
1	B	397	ILE	CB-CA-C	-5.18	105.30	112.24
1	B	463	LYS	N-CA-C	-5.11	103.59	110.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	ARG	Sidechain
1	B	310	ARG	Sidechain

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	5963	0	5682	168	0
1	B	5963	0	5682	184	1
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	14	0	13	0	0
3	B	28	0	26	10	0
4	A	26	0	24	4	0
4	B	26	0	24	12	0
All	All	12132	0	11551	353	1

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 15.

All (353) 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:321:ASN:OD1	3:B:800:NAG:C1	2.04	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:CG	3:B:800:NAG:C1	2.33	1.01
3:B:799:NAG:H83	3:B:799:NAG:H3	1.41	1.01
1:A:470:LEU:HD12	1:A:483:HIS:HE1	1.30	0.96
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.04	0.93
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.02	0.93
1:B:470:LEU:HD12	1:B:483:HIS:HE1	1.33	0.92
1:A:558:VAL:HG12	1:A:560:ARG:NH1	1.83	0.91
1:B:321:ASN:ND2	3:B:800:NAG:C1	2.33	0.91
1:A:253:ARG:HH12	1:B:253:ARG:HH12	0.96	0.90
1:B:558:VAL:HG12	1:B:560:ARG:NH1	1.86	0.90
1:B:662:TYR:CE2	4:B:900:PF2:H9	2.08	0.89
1:B:39:SER:O	1:B:40:ARG:HD3	1.71	0.89
1:A:253:ARG:NH1	1:B:253:ARG:HH12	1.73	0.87
1:A:39:SER:O	1:A:40:ARG:HD3	1.76	0.86
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.58	0.85
1:A:445:LEU:HD22	1:A:488:ASP:OD2	1.77	0.85
1:A:312:SER:OG	1:A:325:MET:HE2	1.79	0.83
1:B:39:SER:C	1:B:40:ARG:HD3	2.05	0.81
1:B:312:SER:OG	1:B:325:MET:HE2	1.81	0.80
1:B:136:ASP:O	1:B:139:LYS:O	1.99	0.80
1:A:347:GLU:OE2	1:A:373:LYS:NZ	2.14	0.79
1:A:253:ARG:HH12	1:B:253:ARG:NH1	1.80	0.78
1:A:39:SER:C	1:A:40:ARG:HD3	2.08	0.78
1:A:558:VAL:CG1	1:A:560:ARG:CZ	2.61	0.77
1:B:372:TYR:CE2	1:B:397:ILE:HD11	2.21	0.76
3:B:799:NAG:O4	3:B:799:NAG:O6	1.90	0.76
1:A:397:ILE:CG2	1:A:434:ILE:HG21	2.17	0.75
1:B:487:ASN:O	1:B:489:LYS:N	2.20	0.74
1:B:397:ILE:CG2	1:B:434:ILE:HG21	2.17	0.74
1:A:558:VAL:HG11	1:A:560:ARG:CZ	2.18	0.74
1:B:558:VAL:CG1	1:B:560:ARG:CZ	2.65	0.74
1:A:558:VAL:CG1	1:A:560:ARG:NH1	2.51	0.73
1:B:662:TYR:HE2	4:B:900:PF2:H9	1.52	0.73
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.72	0.73
1:A:372:TYR:CE2	1:A:397:ILE:HD11	2.23	0.72
1:A:597:ARG:HD3	1:A:600:THR:HG21	1.70	0.72
1:B:487:ASN:O	1:B:488:ASP:C	2.32	0.72
1:B:321:ASN:HD21	3:B:800:NAG:C1	2.00	0.72
1:B:445:LEU:HD22	1:B:488:ASP:OD2	1.90	0.71
1:A:136:ASP:O	1:A:139:LYS:O	2.07	0.71
1:B:39:SER:O	1:B:40:ARG:CD	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:SER:H	1:B:715:GLN:NE2	1.89	0.70
1:A:312:SER:HG	1:A:325:MET:HE2	1.55	0.70
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.27	0.70
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.57	0.70
1:B:666:TYR:CE1	4:B:900:PF2:H10	2.27	0.69
1:A:558:VAL:HG11	1:A:560:ARG:NH2	2.07	0.69
1:B:558:VAL:CG1	1:B:560:ARG:NH1	2.54	0.69
1:B:597:ARG:HD3	1:B:600:THR:HG21	1.75	0.69
1:B:518:ILE:O	1:B:519:LEU:HD23	1.93	0.69
1:B:666:TYR:CZ	4:B:900:PF2:C10	2.77	0.68
4:A:900:PF2:H9A	4:A:900:PF2:H5	1.74	0.68
1:A:518:ILE:O	1:A:519:LEU:HD23	1.95	0.67
1:B:558:VAL:HG11	1:B:560:ARG:CZ	2.23	0.67
1:A:657:SER:H	1:A:715:GLN:NE2	1.92	0.67
1:A:118:TYR:O	1:A:119:ASN:HB2	1.93	0.67
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.24	0.66
3:B:799:NAG:H3	3:B:799:NAG:C8	2.19	0.66
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.61	0.66
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.31	0.66
1:B:117:GLU:OE1	1:B:128:TYR:CE1	2.48	0.65
1:A:39:SER:O	1:A:40:ARG:CD	2.44	0.65
1:B:236:ILE:HG13	1:B:712:HIS:CE1	2.31	0.65
1:A:249:PRO:HD3	1:B:714:GLN:NE2	2.12	0.64
1:B:117:GLU:OE1	1:B:128:TYR:HE1	1.79	0.64
1:B:558:VAL:HG11	1:B:560:ARG:NH2	2.13	0.64
1:A:139:LYS:O	1:A:141:GLN:N	2.30	0.64
1:A:39:SER:O	1:A:40:ARG:HB2	1.98	0.64
1:A:401:THR:O	1:A:401:THR:HG22	1.97	0.64
1:A:397:ILE:HG21	1:A:434:ILE:HG21	1.80	0.64
1:A:680:LEU:HD11	1:A:684:ARG:NE	2.13	0.63
1:B:562:ASN:N	1:B:562:ASN:HD22	1.95	0.63
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.80	0.63
1:B:347:GLU:OE2	1:B:373:LYS:NZ	2.32	0.63
1:A:487:ASN:O	1:A:489:LYS:N	2.32	0.63
4:A:900:PF2:H9A	4:A:900:PF2:C5	2.28	0.62
1:B:321:ASN:OD1	3:B:800:NAG:N2	2.32	0.62
1:B:377:ASN:HD21	1:B:381:TYR:H	1.48	0.62
1:B:666:TYR:CZ	4:B:900:PF2:H10	2.35	0.62
1:B:666:TYR:CE2	4:B:900:PF2:H9A	2.34	0.62
1:B:403:GLU:OE2	1:B:587:GLY:HA2	1.99	0.62
1:A:710:ASN:HD22	1:A:710:ASN:C	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.81	0.61
1:A:377:ASN:C	1:A:377:ASN:HD22	2.08	0.61
1:B:403:GLU:H	1:B:420:ASN:HD21	1.48	0.61
1:B:310:ARG:HD3	1:B:327:ILE:HG23	1.81	0.61
1:A:487:ASN:O	1:A:488:ASP:C	2.42	0.61
1:A:372:TYR:HE2	1:A:397:ILE:HD11	1.65	0.60
1:B:546:VAL:HG23	1:B:606:GLN:OE1	2.01	0.60
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.83	0.60
1:A:621:ASN:C	1:A:621:ASN:HD22	2.09	0.60
4:B:900:PF2:H9A	4:B:900:PF2:C5	2.32	0.60
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.83	0.59
1:A:417:TYR:HE1	1:A:434:ILE:HG13	1.67	0.59
1:B:372:TYR:HE2	1:B:397:ILE:HD11	1.63	0.59
1:B:39:SER:O	1:B:40:ARG:HB2	2.03	0.59
1:B:431:LEU:HD13	1:B:445:LEU:HD12	1.84	0.59
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.85	0.59
1:B:483:HIS:HD2	1:B:490:GLY:HA2	1.67	0.58
1:B:473:SER:HB2	1:B:558:VAL:HG23	1.84	0.58
1:B:626:ILE:O	1:B:650:GLY:HA2	2.04	0.58
1:A:649:CYS:HB3	1:A:699:GLU:HB2	1.86	0.58
1:B:417:TYR:HE1	1:B:434:ILE:HG13	1.69	0.58
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.04	0.58
1:B:397:ILE:HG21	1:B:434:ILE:HG21	1.84	0.58
1:B:296:GLY:O	1:B:298:HIS:HD2	1.87	0.57
1:B:312:SER:HG	1:B:325:MET:HE2	1.66	0.57
1:B:357:PHE:O	1:B:358:ARG:HB3	2.04	0.57
1:B:680:LEU:HD11	1:B:684:ARG:NE	2.19	0.57
1:B:206:GLU:OE2	4:B:900:PF2:N3	2.38	0.57
1:B:735:TYR:OH	1:B:750:HIS:CD2	2.50	0.57
1:B:242:SER:OG	1:B:243:ASP:N	2.38	0.56
1:B:377:ASN:ND2	1:B:381:TYR:H	2.03	0.56
4:B:900:PF2:H9A	4:B:900:PF2:H5	1.88	0.56
1:A:463:LYS:C	1:A:465:ALA:H	2.13	0.56
1:B:55:LEU:HD22	1:B:478:PRO:HG2	1.87	0.56
1:A:68:TYR:CD1	1:A:68:TYR:C	2.84	0.56
1:B:139:LYS:O	1:B:141:GLN:N	2.34	0.56
1:A:236:ILE:HG13	1:A:712:HIS:CE1	2.41	0.56
1:B:463:LYS:C	1:B:465:ALA:H	2.13	0.56
1:A:621:ASN:HD22	1:A:622:LYS:N	2.04	0.56
1:B:562:ASN:HD22	1:B:562:ASN:H	1.53	0.55
1:A:403:GLU:OE2	1:A:587:GLY:HA2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ILE:HG23	1:A:598:LEU:HD23	1.88	0.55
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.36	0.55
1:A:73:GLU:O	1:A:74:ASN:HB2	2.07	0.55
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.89	0.55
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.89	0.55
1:A:237:GLU:OE2	1:A:253:ARG:HD3	2.07	0.54
1:B:285:ILE:HD12	1:B:285:ILE:N	2.22	0.54
1:B:401:THR:HG22	1:B:401:THR:O	2.07	0.54
1:A:296:GLY:O	1:A:298:HIS:HD2	1.91	0.54
1:A:445:LEU:CD2	1:A:488:ASP:OD2	2.53	0.54
1:A:68:TYR:CD1	1:A:68:TYR:O	2.61	0.54
1:A:319:ILE:HD12	1:A:319:ILE:H	1.71	0.54
1:B:666:TYR:CD2	4:B:900:PF2:H9A	2.43	0.54
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.89	0.54
1:B:621:ASN:C	1:B:621:ASN:HD22	2.15	0.54
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.89	0.54
1:A:39:SER:O	1:A:40:ARG:CB	2.54	0.54
1:A:117:GLU:OE1	1:A:128:TYR:CE1	2.61	0.54
1:A:69:LEU:HD23	1:A:78:VAL:HG22	1.90	0.53
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.90	0.53
1:B:319:ILE:HD12	1:B:319:ILE:H	1.74	0.53
1:A:384:ILE:CG2	1:A:397:ILE:HD12	2.39	0.53
1:A:710:ASN:C	1:A:710:ASN:ND2	2.65	0.53
1:B:662:TYR:OH	4:B:900:PF2:C6	2.57	0.53
1:A:69:LEU:CD2	1:A:78:VAL:HG22	2.39	0.53
1:A:626:ILE:O	1:A:650:GLY:HA2	2.08	0.53
1:B:594:ILE:HG23	1:B:594:ILE:O	2.09	0.52
1:B:743:ALA:O	1:B:744:SER:C	2.52	0.52
1:A:242:SER:OG	1:A:243:ASP:N	2.40	0.52
1:A:403:GLU:H	1:A:420:ASN:HD21	1.58	0.52
1:B:483:HIS:CD2	1:B:490:GLY:HA2	2.45	0.52
1:A:432:TYR:CE2	1:A:444:CYS:SG	3.02	0.52
1:B:66:HIS:ND1	1:B:67:GLU:HG3	2.25	0.52
1:A:626:ILE:O	1:A:650:GLY:CA	2.58	0.52
1:A:695:PHE:C	1:A:697:GLN:H	2.18	0.52
1:B:39:SER:O	1:B:40:ARG:CB	2.57	0.51
1:A:473:SER:HB2	1:A:558:VAL:HG23	1.92	0.51
1:B:634:TYR:O	1:B:638:MET:HG2	2.10	0.51
1:B:301:CYS:SG	1:B:316:LEU:HB2	2.51	0.51
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.93	0.51
1:B:60:LEU:C	1:B:60:LEU:CD2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:O	1:B:143:ILE:CG1	2.60	0.50
1:B:195:TYR:O	1:B:227:GLN:HA	2.11	0.50
1:B:221:THR:O	1:B:273:THR:OG1	2.26	0.50
1:A:150:ASN:O	1:A:151:ASN:HB2	2.11	0.50
1:A:247:GLN:HG2	1:B:258:LYS:HD2	1.94	0.50
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.12	0.50
1:A:253:ARG:NH1	1:B:253:ARG:NH1	2.51	0.50
1:A:377:ASN:HD21	1:A:381:TYR:H	1.58	0.50
1:B:513:LYS:O	1:B:527:GLN:HA	2.12	0.50
1:B:397:ILE:HG22	1:B:434:ILE:HG21	1.92	0.50
1:A:285:ILE:N	1:A:285:ILE:HD12	2.26	0.50
1:B:597:ARG:O	1:B:600:THR:OG1	2.15	0.50
1:B:626:ILE:O	1:B:650:GLY:CA	2.60	0.50
1:B:594:ILE:HG23	1:B:598:LEU:HD23	1.94	0.50
1:A:258:LYS:HD2	1:B:247:GLN:HG2	1.94	0.49
1:B:656:VAL:HG13	1:B:715:GLN:HE22	1.77	0.49
1:A:597:ARG:O	1:A:600:THR:OG1	2.23	0.49
1:A:410:LEU:HD12	1:A:415:LEU:HD12	1.95	0.49
1:A:377:ASN:ND2	1:A:381:TYR:H	2.09	0.49
1:A:543:LEU:HD22	1:A:544:LEU:N	2.28	0.49
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.47	0.49
1:A:735:TYR:OH	1:A:750:HIS:CD2	2.61	0.49
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.95	0.49
1:B:666:TYR:CE2	4:B:900:PF2:H5	2.47	0.49
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.94	0.49
1:B:205:GLU:OE1	1:B:205:GLU:HA	2.12	0.49
1:A:612:GLN:HA	1:A:615:LYS:HE2	1.95	0.49
1:A:55:LEU:HD22	1:A:478:PRO:HG2	1.93	0.49
1:A:751:ILE:O	1:A:755:MET:HG3	2.13	0.49
1:B:118:TYR:O	1:B:119:ASN:HB2	2.12	0.49
1:A:499:ALA:O	1:A:500:LEU:C	2.57	0.48
1:B:484:SER:O	1:B:488:ASP:HA	2.12	0.48
1:B:612:GLN:HA	1:B:615:LYS:HE2	1.95	0.48
1:A:154:TRP:NE1	1:A:156:THR:HG22	2.29	0.48
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.43	0.48
1:B:235:LEU:HD23	1:B:255:PRO:HA	1.95	0.48
1:B:763:PHE:O	1:B:764:SER:HB2	2.13	0.48
1:A:484:SER:O	1:A:488:ASP:HA	2.13	0.48
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.14	0.48
1:A:60:LEU:HB2	1:A:68:TYR:CD1	2.49	0.47
1:B:613:PHE:O	1:B:619:VAL:HG21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:O	1:A:75:ASN:C	2.57	0.47
1:A:149:PRO:HB2	1:A:168:TRP:CD1	2.48	0.47
1:A:546:VAL:HG23	1:A:606:GLN:OE1	2.15	0.47
1:B:397:ILE:HG23	1:B:439:TYR:CD1	2.49	0.47
1:A:384:ILE:HG21	1:A:397:ILE:HD12	1.97	0.47
1:A:422:TYR:CE2	1:A:423:LYS:HD2	2.50	0.47
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.96	0.47
1:A:386:TYR:N	1:A:395:THR:O	2.46	0.47
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.14	0.47
1:B:741:GLY:O	1:B:742:ILE:C	2.58	0.47
1:A:251:THR:HG21	1:A:253:ARG:NH1	2.30	0.47
1:A:695:PHE:C	1:A:697:GLN:N	2.73	0.47
3:B:799:NAG:H83	3:B:799:NAG:C3	2.29	0.47
1:A:550:PRO:O	1:A:551:CYS:CB	2.64	0.46
1:B:60:LEU:HB2	1:B:68:TYR:CD1	2.50	0.46
1:A:167:VAL:HA	1:A:171:ASP:O	2.16	0.46
1:A:372:TYR:CE1	1:A:410:LEU:HD11	2.51	0.46
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.97	0.46
1:A:703:ILE:HA	1:A:733:MET:O	2.15	0.46
1:B:377:ASN:C	1:B:377:ASN:HD22	2.23	0.46
1:A:662:TYR:HE1	1:A:710:ASN:ND2	2.14	0.46
1:A:483:HIS:CD2	1:A:490:GLY:HA2	2.51	0.46
1:B:422:TYR:CE2	1:B:423:LYS:HD2	2.51	0.46
1:A:66:HIS:ND1	1:A:67:GLU:HG3	2.30	0.46
1:A:594:ILE:HG23	1:A:594:ILE:O	2.16	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.51	0.46
1:A:377:ASN:C	1:A:377:ASN:ND2	2.71	0.46
1:A:571:GLU:CD	1:A:760:LYS:HD3	2.40	0.46
1:B:556:ASP:C	1:B:556:ASP:OD1	2.58	0.46
1:A:658:ARG:HB3	1:A:661:TYR:CD2	2.51	0.45
1:A:45:LEU:HG	1:A:49:LEU:HD22	1.97	0.45
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.50	0.45
1:A:199:THR:OG1	1:A:204:GLU:HB2	2.17	0.45
1:B:68:TYR:CD1	1:B:68:TYR:C	2.95	0.45
1:B:751:ILE:O	1:B:755:MET:HG3	2.17	0.45
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.46	0.45
1:A:325:MET:CE	1:A:362:PRO:HG3	2.47	0.45
1:B:331:ASP:O	1:B:332:GLU:C	2.59	0.45
1:A:741:GLY:O	1:A:742:ILE:C	2.59	0.45
1:B:600:THR:HB	1:B:601:PHE:H	1.51	0.45
1:A:549:GLY:HA2	1:A:631:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ALA:O	1:A:744:SER:C	2.56	0.45
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.99	0.45
1:A:55:LEU:HD23	1:A:500:LEU:HD12	1.99	0.44
1:B:657:SER:H	1:B:715:GLN:HE21	1.62	0.44
1:A:544:LEU:HD21	1:A:606:GLN:OE1	2.17	0.44
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.53	0.44
1:A:513:LYS:O	1:A:527:GLN:HA	2.17	0.44
1:B:325:MET:CE	1:B:362:PRO:HG3	2.47	0.44
1:B:759:ILE:HG22	1:B:760:LYS:N	2.32	0.44
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.99	0.44
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.99	0.44
1:A:153:GLN:OE1	1:A:167:VAL:HG12	2.17	0.43
1:B:73:GLU:O	1:B:74:ASN:HB2	2.17	0.43
1:B:372:TYR:CE1	1:B:410:LEU:HD11	2.53	0.43
1:B:562:ASN:N	1:B:562:ASN:ND2	2.65	0.43
1:B:621:ASN:HD22	1:B:622:LYS:N	2.16	0.43
1:A:603:VAL:HG13	1:A:639:VAL:HG23	2.00	0.43
1:A:656:VAL:HG13	1:A:715:GLN:HE22	1.83	0.43
1:B:276:LEU:CD2	1:B:282:ALA:HB2	2.48	0.43
1:A:331:ASP:O	1:A:332:GLU:C	2.61	0.43
1:A:653:VAL:O	1:A:654:ALA:C	2.62	0.43
1:B:55:LEU:HD23	1:B:500:LEU:HD12	2.00	0.43
1:B:90:LEU:HD23	1:B:91:GLU:N	2.34	0.43
1:B:695:PHE:C	1:B:697:GLN:H	2.25	0.43
1:B:384:ILE:CG2	1:B:397:ILE:HD12	2.48	0.43
1:A:558:VAL:HG12	1:A:560:ARG:HH12	1.71	0.43
1:B:445:LEU:CD2	1:B:488:ASP:OD2	2.63	0.43
1:A:143:ILE:O	1:A:143:ILE:CG1	2.66	0.43
1:A:634:TYR:O	1:A:638:MET:HG2	2.19	0.43
1:B:372:TYR:CD2	1:B:397:ILE:HD11	2.53	0.43
1:B:410:LEU:HD12	1:B:415:LEU:HD12	1.99	0.43
1:B:745:SER:O	1:B:749:GLN:HG3	2.19	0.43
1:B:759:ILE:CG2	1:B:760:LYS:N	2.81	0.43
1:A:74:ASN:O	1:A:75:ASN:O	2.36	0.43
1:A:222:PHE:HA	1:A:271:VAL:O	2.19	0.43
1:B:471:ARG:O	1:B:471:ARG:HG3	2.19	0.43
1:A:72:GLN:O	1:A:73:GLU:HB2	2.17	0.42
1:A:276:LEU:CD2	1:A:282:ALA:HB2	2.48	0.42
1:B:386:TYR:N	1:B:395:THR:O	2.49	0.42
1:B:708:ASP:CG	1:B:711:VAL:O	2.63	0.42
1:A:200:ASP:OD1	1:A:200:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:O	1:A:273:THR:OG1	2.26	0.42
1:A:691:ARG:O	1:A:692:ALA:C	2.62	0.42
1:A:739:ASP:OD1	1:A:739:ASP:C	2.61	0.42
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.53	0.42
1:B:474:GLY:HA2	1:B:476:GLY:N	2.34	0.42
1:A:258:LYS:O	1:A:259:ALA:C	2.62	0.42
1:A:666:TYR:O	1:A:670:TYR:CD2	2.73	0.42
1:A:708:ASP:CG	1:A:711:VAL:O	2.62	0.42
1:B:77:LEU:HD23	1:B:88:VAL:HA	2.01	0.42
1:B:743:ALA:C	1:B:744:SER:O	2.61	0.42
1:A:600:THR:HB	1:A:601:PHE:H	1.59	0.42
1:B:60:LEU:C	1:B:60:LEU:HD23	2.44	0.42
1:B:153:GLN:OE1	1:B:167:VAL:HG12	2.19	0.42
1:A:658:ARG:HD2	1:A:661:TYR:CZ	2.55	0.42
1:B:222:PHE:HA	1:B:271:VAL:O	2.20	0.42
1:A:662:TYR:CE1	1:A:710:ASN:ND2	2.88	0.42
1:B:347:GLU:OE1	1:B:375:ILE:HD13	2.19	0.42
1:B:532:PRO:O	1:B:533:HIS:C	2.61	0.42
1:A:295:ILE:O	1:A:295:ILE:HG12	2.19	0.42
1:B:695:PHE:C	1:B:697:GLN:N	2.77	0.42
1:B:321:ASN:OD1	3:B:800:NAG:C2	2.65	0.41
1:B:374:ILE:HD11	1:B:404:VAL:HG12	2.01	0.41
1:A:483:HIS:HD2	1:A:490:GLY:HA2	1.86	0.41
1:A:662:TYR:OH	4:A:900:PF2:C6	2.68	0.41
1:B:558:VAL:HG12	1:B:560:ARG:HH12	1.75	0.41
1:B:571:GLU:CD	1:B:760:LYS:HD3	2.45	0.41
1:B:709:ASP:O	1:B:712:HIS:NE2	2.53	0.41
1:A:90:LEU:HD23	1:A:91:GLU:N	2.35	0.41
1:A:169:ASN:O	1:A:170:ASN:HB2	2.21	0.41
1:B:233:VAL:HA	1:B:234:PRO:HD3	1.94	0.41
1:B:377:ASN:ND2	1:B:377:ASN:C	2.78	0.41
1:A:377:ASN:HD22	1:A:380:GLY:H	1.68	0.41
1:A:613:PHE:O	1:A:619:VAL:HG21	2.19	0.41
1:A:759:ILE:HG22	1:A:760:LYS:N	2.35	0.41
1:A:372:TYR:CD2	1:A:397:ILE:HD11	2.56	0.41
1:A:397:ILE:HG23	1:A:439:TYR:CD1	2.55	0.41
1:B:372:TYR:CD1	1:B:410:LEU:HD11	2.55	0.41
1:A:455:GLN:HB2	1:A:475:PRO:HD3	2.02	0.41
1:B:724:VAL:C	1:B:726:VAL:H	2.29	0.41
1:A:195:TYR:O	1:A:227:GLN:HA	2.21	0.41
1:A:305:TRP:CZ3	1:A:311:ILE:CG1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLU:OE2	1:B:587:GLY:CA	2.66	0.41
1:A:46:THR:O	1:A:50:LYS:HB2	2.20	0.41
1:B:549:GLY:HA2	1:B:631:TYR:CE1	2.55	0.41
1:A:205:GLU:OE2	4:A:900:PF2:N3	2.52	0.41
1:A:235:LEU:HD23	1:A:255:PRO:HA	2.01	0.41
1:B:258:LYS:O	1:B:259:ALA:C	2.63	0.41
1:A:377:ASN:ND2	1:A:380:GLY:N	2.68	0.40
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.21	0.40
1:A:420:ASN:C	1:A:420:ASN:HD22	2.29	0.40
1:A:543:LEU:CD2	1:A:544:LEU:N	2.84	0.40
1:B:420:ASN:C	1:B:420:ASN:HD22	2.29	0.40
1:B:459:VAL:HG22	1:B:460:SER:N	2.36	0.40
1:B:621:ASN:C	1:B:621:ASN:ND2	2.80	0.40
1:A:724:VAL:C	1:A:726:VAL:H	2.30	0.40
1:B:90:LEU:HD23	1:B:91:GLU:O	2.21	0.40
1:B:710:ASN:ND2	1:B:710:ASN:C	2.80	0.40
1:B:80:ASN:O	1:B:84:GLY:N	2.54	0.40
1:B:149:PRO:HB2	1:B:168:TRP:CD1	2.55	0.40
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.22	0.40
1:B:549:GLY:O	1:B:552:SER:OG	2.37	0.40
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.56	0.40
1:B:463:LYS:C	1:B:465:ALA:N	2.77	0.40
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.87	0.40
1:B:736:THR:O	1:B:737:ASP:HB2	2.21	0.40

All (1) 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)
1:B:392:LYS:CE	1:B:506:ASN:OD1[1_545]	2.08	0.12

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	726/748 (97%)	667 (92%)	51 (7%)	8 (1%)	11	12
1	B	726/748 (97%)	669 (92%)	49 (7%)	8 (1%)	11	12
All	All	1452/1496 (97%)	1336 (92%)	100 (7%)	16 (1%)	11	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	140	ARG
1	A	488	ASP
1	B	140	ARG
1	B	488	ASP
1	A	332	GLU
1	B	75	ASN
1	B	332	GLU
1	A	486	VAL
1	B	486	VAL
1	B	600	THR
1	A	73	GLU
1	A	600	THR
1	B	40	ARG
1	B	358	ARG
1	A	742	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	653/669 (98%)	591 (90%)	62 (10%)	8	8
1	B	653/669 (98%)	592 (91%)	61 (9%)	8	9
All	All	1306/1338 (98%)	1183 (91%)	123 (9%)	8	9

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	49	LEU
1	A	57	LEU
1	A	60	LEU
1	A	63	ILE
1	A	72	GLN
1	A	73	GLU
1	A	87	SER
1	A	97	GLU
1	A	110	ASP
1	A	115	LEU
1	A	133	ASP
1	A	143	ILE
1	A	156	THR
1	A	180	LEU
1	A	202	VAL
1	A	223	LEU
1	A	236	ILE
1	A	246	LEU
1	A	271	VAL
1	A	288	THR
1	A	294	LEU
1	A	295	ILE
1	A	300	LEU
1	A	301	CYS
1	A	314	GLN
1	A	319	ILE
1	A	346	ILE
1	A	377	ASN
1	A	385	CYS
1	A	389	ILE
1	A	392	LYS
1	A	405	ILE
1	A	420	ASN
1	A	431	LEU
1	A	443	THR
1	A	466	LYS
1	A	479	LEU
1	A	498	SER
1	A	500	LEU
1	A	507	VAL
1	A	520	ASN
1	A	529	ILE

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Mol	Chain	Res	Type
1	A	537	SER
1	A	543	LEU
1	A	546	VAL
1	A	558	VAL
1	A	594	ILE
1	A	597	ARG
1	A	600	THR
1	A	614	SER
1	A	621	ASN
1	A	660	GLU
1	A	677	GLU
1	A	710	ASN
1	A	715	GLN
1	A	721	LYS
1	A	726	VAL
1	A	731	GLN
1	A	759	ILE
1	A	760	LYS
1	A	761	GLN
1	B	41	LYS
1	B	49	LEU
1	B	57	LEU
1	B	60	LEU
1	B	63	ILE
1	B	72	GLN
1	B	87	SER
1	B	97	GLU
1	B	110	ASP
1	B	115	LEU
1	B	133	ASP
1	B	143	ILE
1	B	156	THR
1	B	180	LEU
1	B	202	VAL
1	B	223	LEU
1	B	236	ILE
1	B	246	LEU
1	B	271	VAL
1	B	294	LEU
1	B	295	ILE
1	B	300	LEU
1	B	301	CYS

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Mol	Chain	Res	Type
1	B	314	GLN
1	B	319	ILE
1	B	321	ASN
1	B	346	ILE
1	B	377	ASN
1	B	385	CYS
1	B	389	ILE
1	B	392	LYS
1	B	405	ILE
1	B	420	ASN
1	B	431	LEU
1	B	443	THR
1	B	466	LYS
1	B	479	LEU
1	B	498	SER
1	B	500	LEU
1	B	507	VAL
1	B	520	ASN
1	B	529	ILE
1	B	537	SER
1	B	543	LEU
1	B	546	VAL
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	597	ARG
1	B	600	THR
1	B	614	SER
1	B	621	ASN
1	B	660	GLU
1	B	677	GLU
1	B	715	GLN
1	B	721	LYS
1	B	726	VAL
1	B	731	GLN
1	B	759	ILE
1	B	760	LYS
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	100	HIS
1	A	103	ASN
1	A	123	GLN
1	A	169	ASN
1	A	227	GLN
1	A	263	ASN
1	A	272	ASN
1	A	298	HIS
1	A	363	HIS
1	A	377	ASN
1	A	383	HIS
1	A	420	ASN
1	A	435	GLN
1	A	450	ASN
1	A	483	HIS
1	A	487	ASN
1	A	586	GLN
1	A	595	ASN
1	A	621	ASN
1	A	679	ASN
1	A	710	ASN
1	A	715	GLN
1	A	750	HIS
1	B	72	GLN
1	B	100	HIS
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	363	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	450	ASN
1	B	483	HIS
1	B	487	ASN
1	B	562	ASN
1	B	586	GLN
1	B	592	HIS
1	B	621	ASN
1	B	679	ASN
1	B	694	ASN

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Mol	Chain	Res	Type
1	B	710	ASN
1	B	715	GLN
1	B	750	HIS

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 ⓘ

8 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	1,2	14,14,15	0.58	0	17,19,21	1.18	3 (17%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.98	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.86	1 (7%)	17,19,21	2.46	6 (35%)
2	NAG	D	2	2	14,14,15	0.49	0	17,19,21	1.37	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	1.49	2 (11%)
2	NAG	E	2	2	14,14,15	0.64	0	17,19,21	1.17	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.63	0	17,19,21	1.53	4 (23%)
2	NAG	F	2	2	14,14,15	0.51	0	17,19,21	1.03	1 (5%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C1-C2	2.82	1.56	1.52
2	E	1	NAG	O5-C1	-2.45	1.39	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	7.32	122.00	112.19
2	C	2	NAG	C1-O5-C5	5.83	120.00	112.19
2	E	1	NAG	O5-C1-C2	-4.80	103.86	111.29
2	D	1	NAG	C4-C3-C2	3.90	116.73	111.02
2	D	2	NAG	C1-O5-C5	3.73	117.19	112.19
2	C	2	NAG	O5-C5-C4	3.33	118.93	110.83
2	F	1	NAG	O5-C5-C6	3.07	113.64	107.66
2	F	1	NAG	O5-C1-C2	-2.84	106.89	111.29
2	C	2	NAG	C3-C4-C5	2.82	115.34	110.23
2	D	1	NAG	O7-C7-N2	2.60	126.57	121.98
2	F	2	NAG	C2-N2-C7	-2.54	119.50	122.90
2	D	1	NAG	C1-C2-N2	2.53	114.42	110.43
2	E	2	NAG	C2-N2-C7	-2.52	119.52	122.90
2	E	2	NAG	C1-O5-C5	2.48	115.51	112.19
2	D	1	NAG	C2-N2-C7	2.42	126.14	122.90
2	C	1	NAG	C6-C5-C4	-2.41	107.11	113.02
2	C	1	NAG	C2-N2-C7	-2.38	119.71	122.90
2	F	1	NAG	C6-C5-C4	-2.35	107.25	113.02
2	F	1	NAG	C2-N2-C7	-2.29	119.83	122.90
2	D	2	NAG	O5-C1-C2	-2.27	107.79	111.29
2	E	1	NAG	C1-O5-C5	2.23	115.17	112.19
2	D	1	NAG	C6-C5-C4	-2.19	107.64	113.02
2	C	1	NAG	C3-C4-C5	2.03	113.91	110.23

There are no chirality outliers.

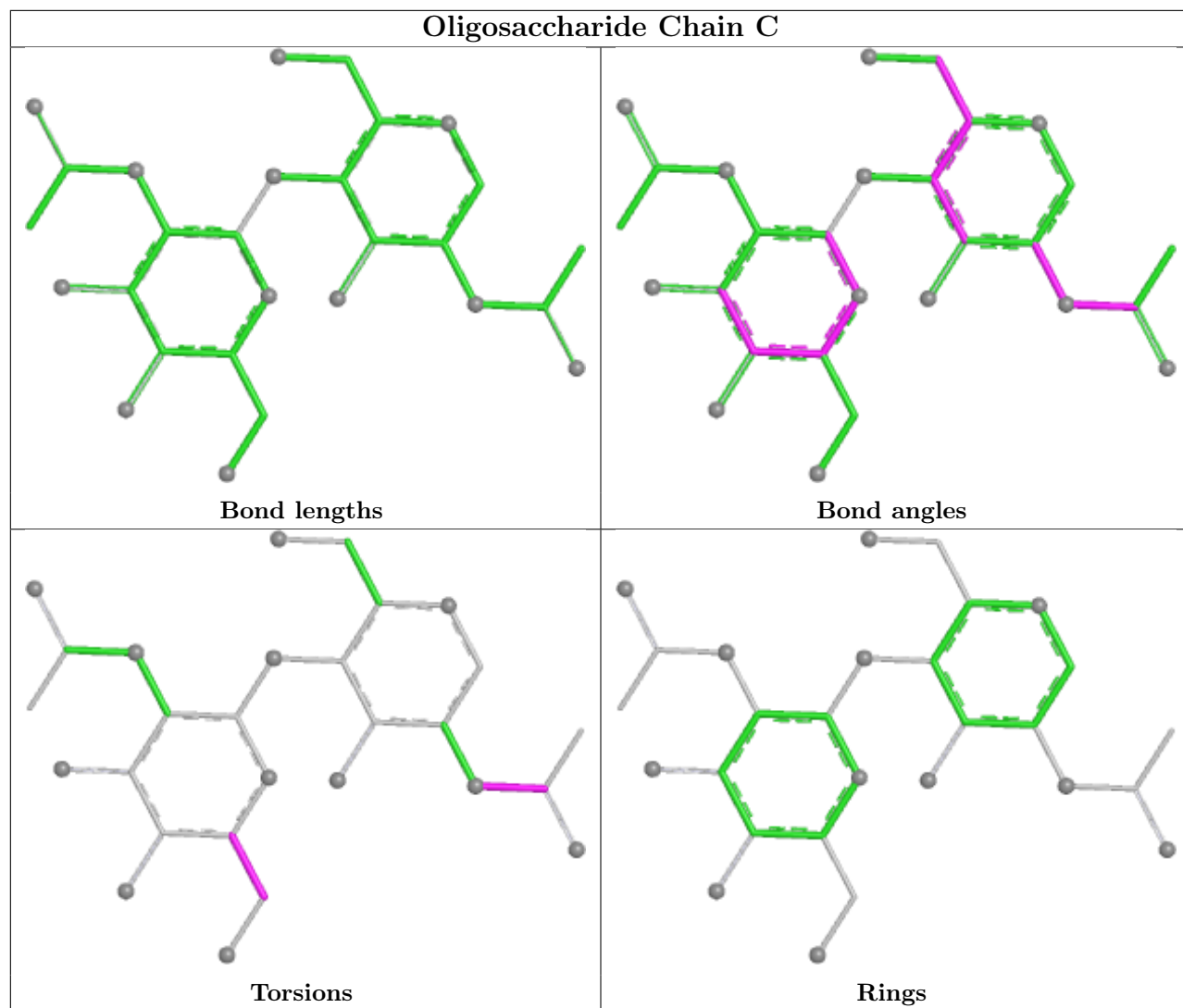
All (13) torsion outliers are listed below:

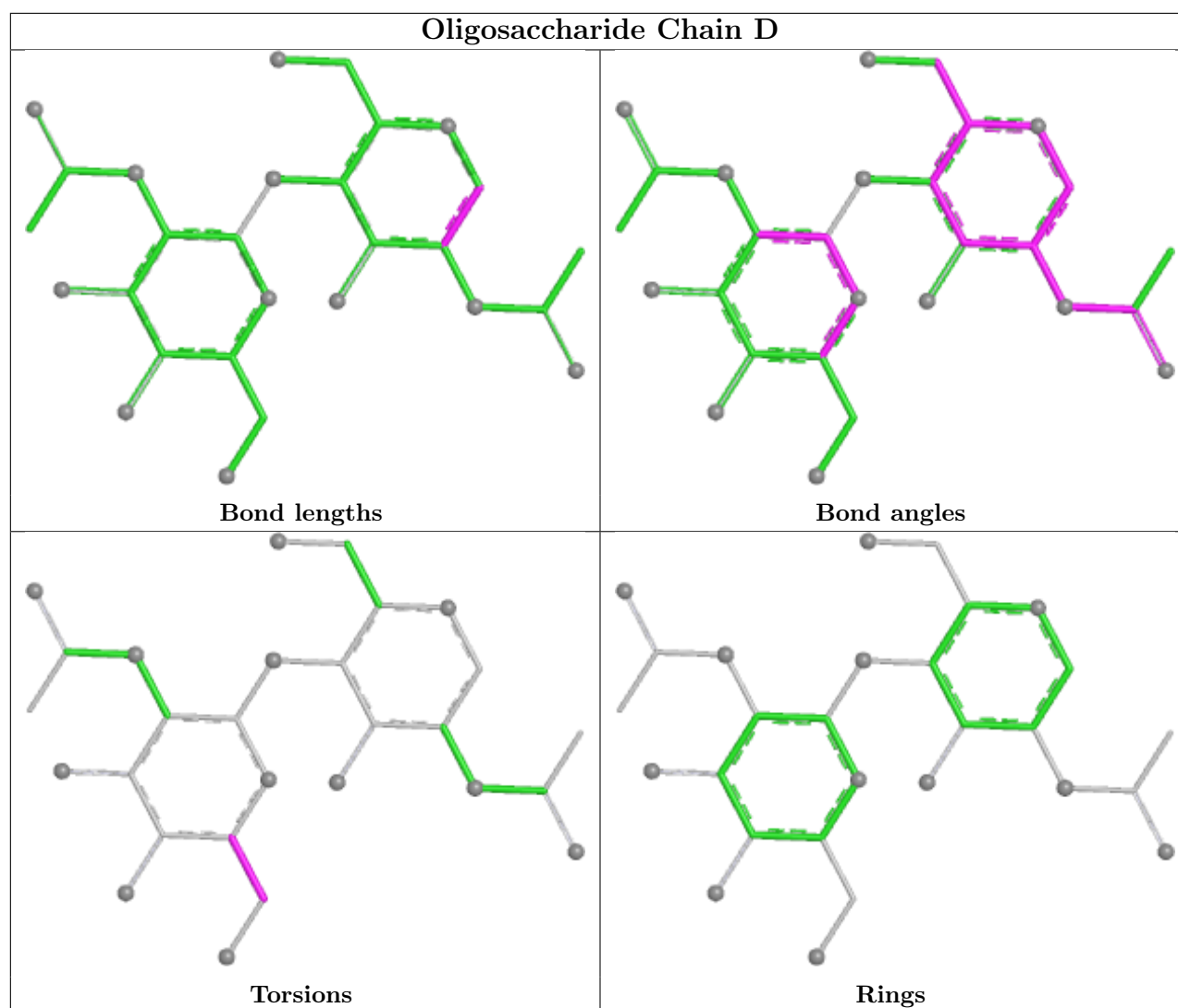
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	F	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6

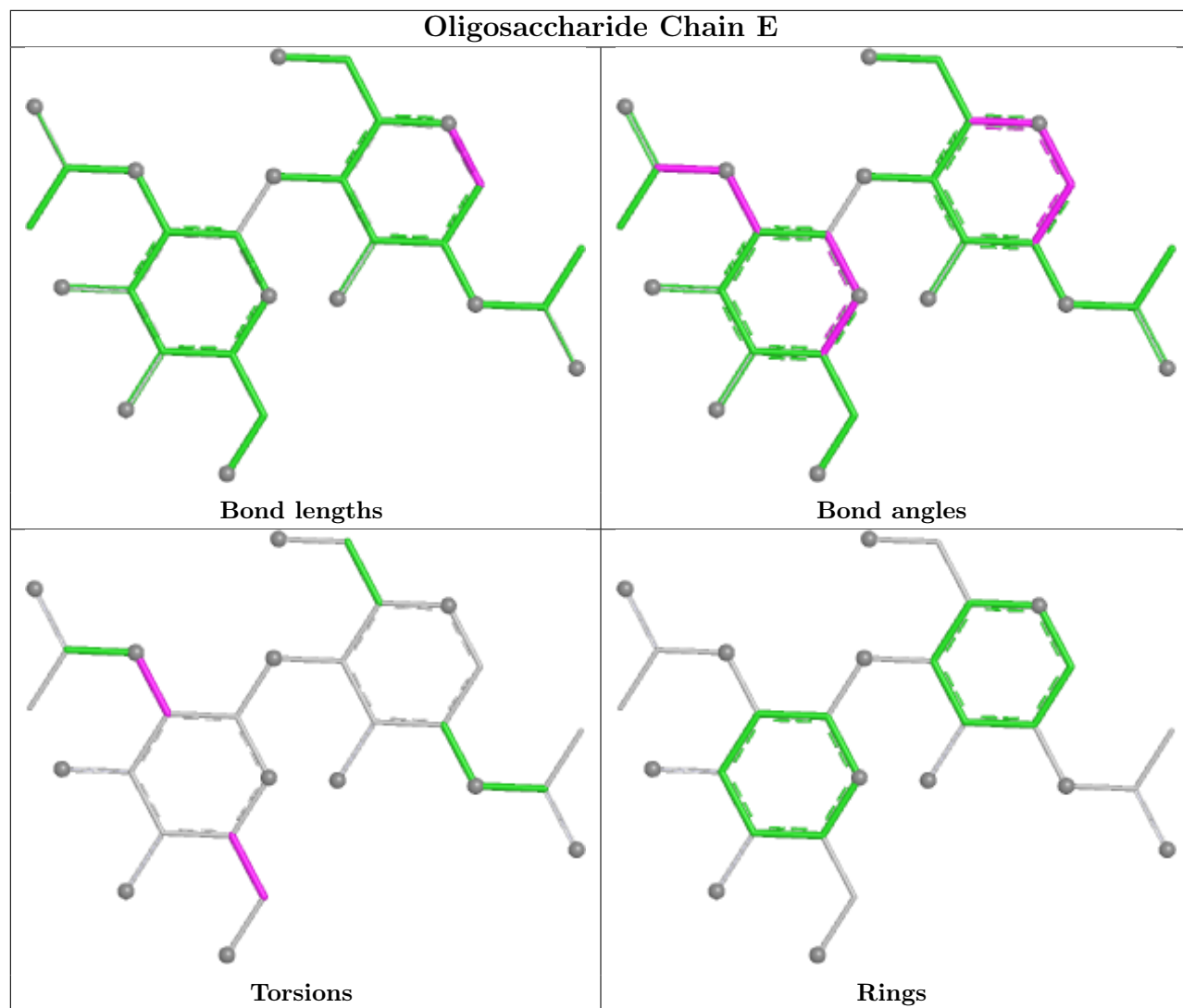
There are no ring outliers.

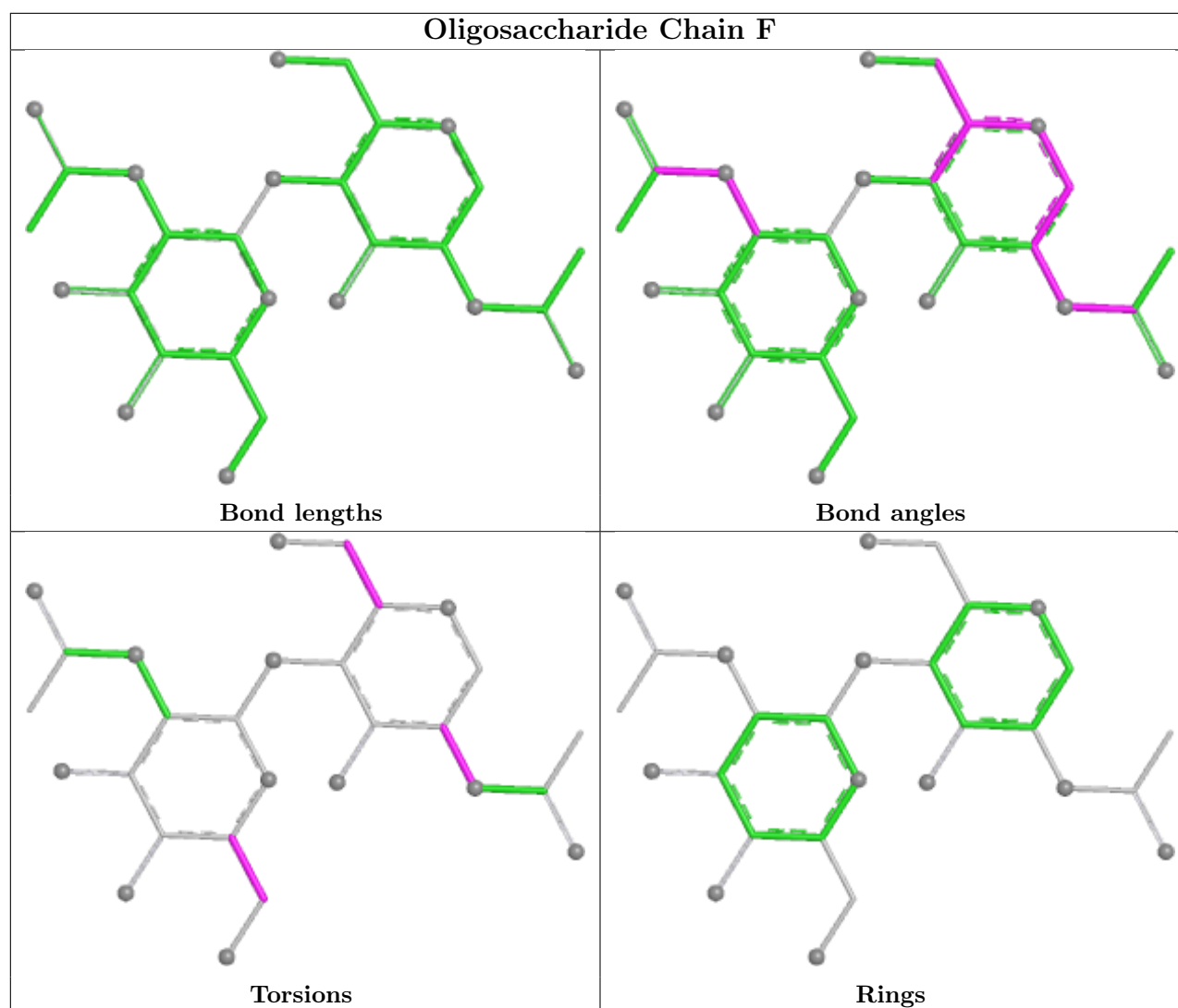
No monomer is involved in short contacts.

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](#)

5 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	B	799	1	14,14,15	0.71	0	17,19,21	1.78	3 (17%)
4	PF2	B	900	-	27,29,29	0.81	0	35,42,42	2.24	13 (37%)
3	NAG	A	796	1	14,14,15	0.62	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PF2	A	900	-	27,29,29	0.98	1 (3%)	35,42,42	2.43	12 (34%)
3	NAG	B	800	-	14,14,15	0.60	0	17,19,21	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	799	1	1/1/5/7	4/6/23/26	0/1/1/1
4	PF2	B	900	-	-	0/16/46/46	0/4/4/4
3	NAG	A	796	1	-	4/6/23/26	0/1/1/1
4	PF2	A	900	-	-	0/16/46/46	0/4/4/4
3	NAG	B	800	-	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	PF2	C19-N23	2.06	1.37	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	PF2	C24-N23-C19	6.86	121.85	115.13
4	A	900	PF2	C15-N16-C17	5.21	123.28	111.57
4	B	900	PF2	O7-C6-N8	4.92	127.48	121.61
4	B	900	PF2	C15-N16-C17	4.85	122.47	111.57
4	A	900	PF2	N20-C19-N23	-4.36	120.29	127.06
4	B	900	PF2	C4-C6-N8	-4.35	112.29	118.85
3	B	799	NAG	C6-C5-C4	-4.22	102.66	113.02
4	B	900	PF2	C24-N23-C19	4.10	119.15	115.13
4	A	900	PF2	C21-N20-C19	4.01	119.06	115.13
4	A	900	PF2	C10-C9-N8	-3.89	100.05	103.53
4	B	900	PF2	C21-N20-C19	3.50	118.56	115.13
4	A	900	PF2	N20-C19-N16	3.48	120.51	116.90
3	B	799	NAG	O5-C5-C6	3.36	114.19	107.66
4	A	900	PF2	C4-C6-N8	-3.33	113.83	118.85
4	A	900	PF2	C22-C24-N23	-2.96	118.74	123.42
4	B	900	PF2	C21-C22-C24	2.84	120.33	116.63
4	A	900	PF2	C17-N16-C19	-2.71	116.30	121.67
4	B	900	PF2	C22-C24-N23	-2.66	119.21	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	PF2	C14-C15-N16	-2.53	105.45	110.78
4	B	900	PF2	C22-C21-N20	-2.49	119.47	123.42
4	B	900	PF2	C14-N13-C1	-2.48	106.47	112.79
4	B	900	PF2	C18-C17-N16	-2.48	105.56	110.78
4	B	900	PF2	N20-C19-N23	-2.44	123.27	127.06
3	B	799	NAG	C2-N2-C7	2.27	125.94	122.90
3	A	796	NAG	C2-N2-C7	-2.24	119.89	122.90
4	A	900	PF2	O7-C6-N8	2.24	124.29	121.61
4	A	900	PF2	N23-C19-N16	2.21	119.20	116.90
4	A	900	PF2	C12-N8-C6	2.19	131.52	124.01
4	B	900	PF2	C5-C1-N13	-2.12	108.70	113.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	799	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	799	NAG	C3-C2-N2-C7
3	B	799	NAG	C8-C7-N2-C2
3	B	799	NAG	O7-C7-N2-C2
3	A	796	NAG	O5-C5-C6-O6
3	A	796	NAG	C4-C5-C6-O6
3	B	799	NAG	O5-C5-C6-O6
3	A	796	NAG	C8-C7-N2-C2
3	A	796	NAG	O7-C7-N2-C2
3	B	800	NAG	C8-C7-N2-C2
3	B	800	NAG	O7-C7-N2-C2

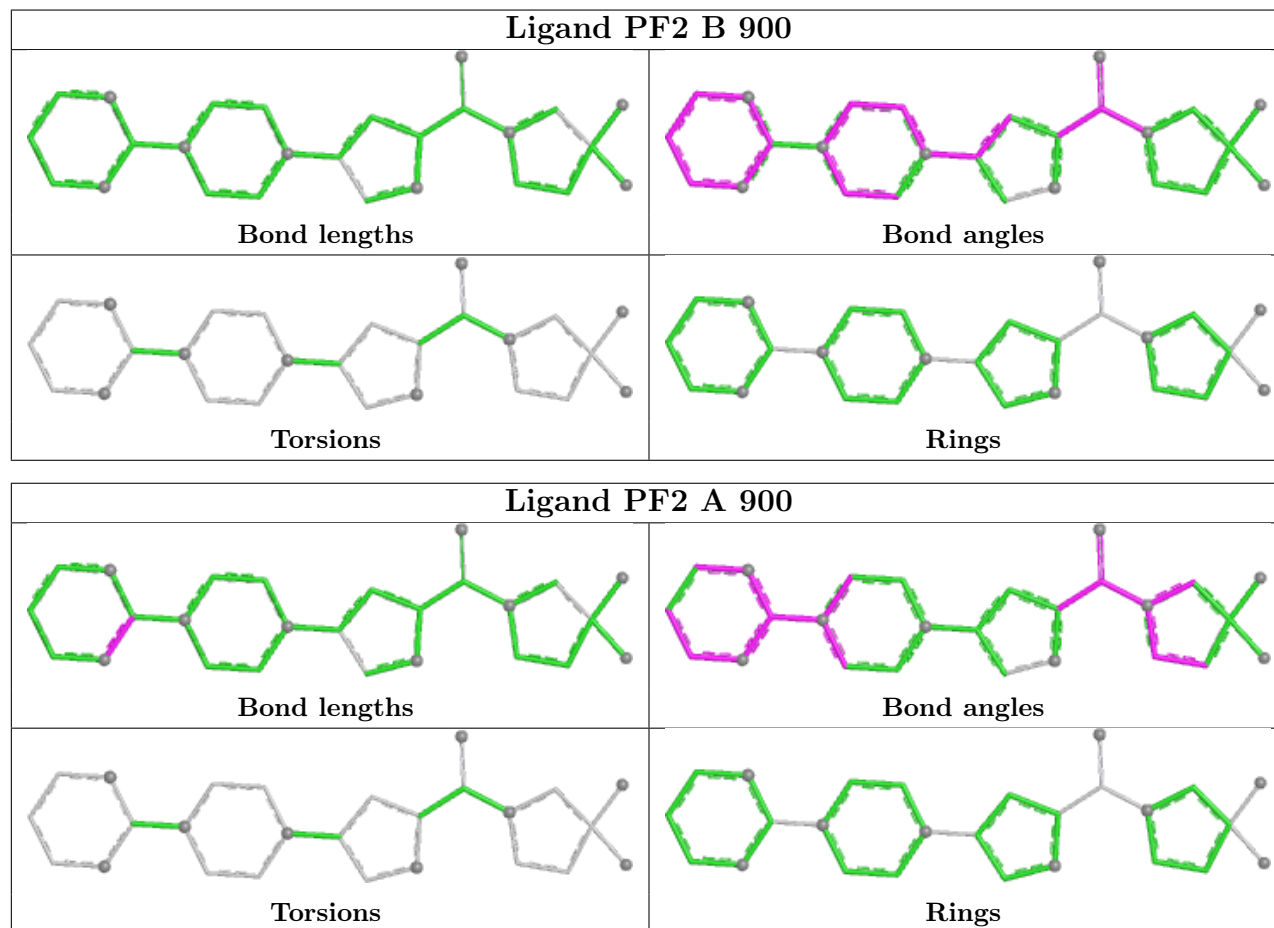
There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	799	NAG	4	0
4	B	900	PF2	12	0
4	A	900	PF2	4	0
3	B	800	NAG	6	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 [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	728/748 (97%)	0.06	2 (0%) 90 91	72, 84, 97, 104	0
1	B	728/748 (97%)	0.15	6 (0%) 82 83	72, 84, 97, 104	0
All	All	1456/1496 (97%)	0.10	8 (0%) 87 89	72, 84, 97, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	4.1
1	B	39	SER	3.0
1	B	654	ALA	2.5
1	B	221	THR	2.2
1	B	711	VAL	2.2
1	A	277	SER	2.1
1	B	394	CYS	2.1
1	B	210	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](#)

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.

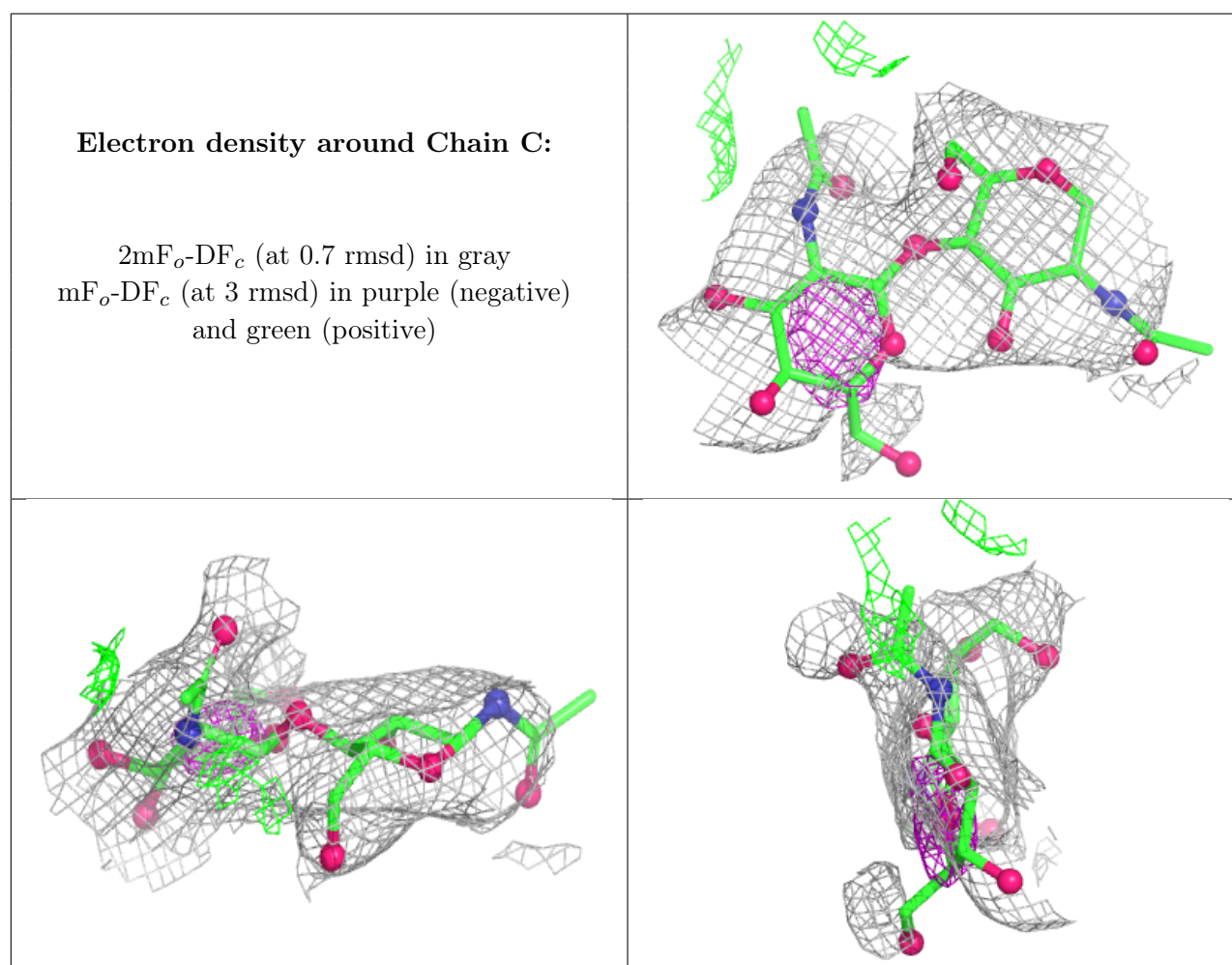
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.55	0.12	114,117,119,119	0

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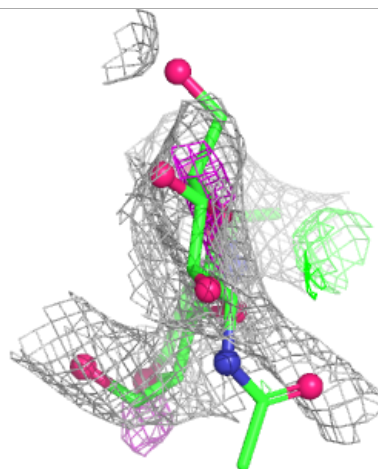
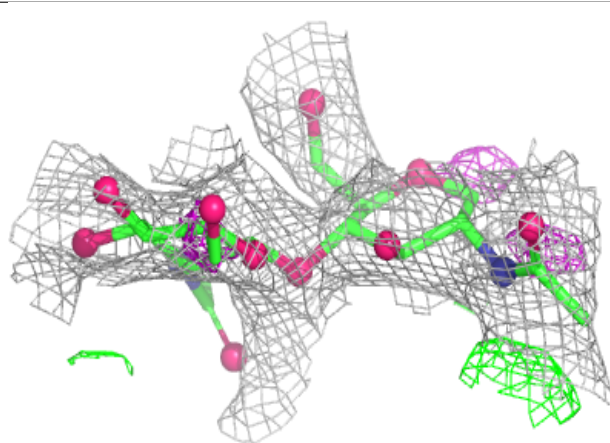
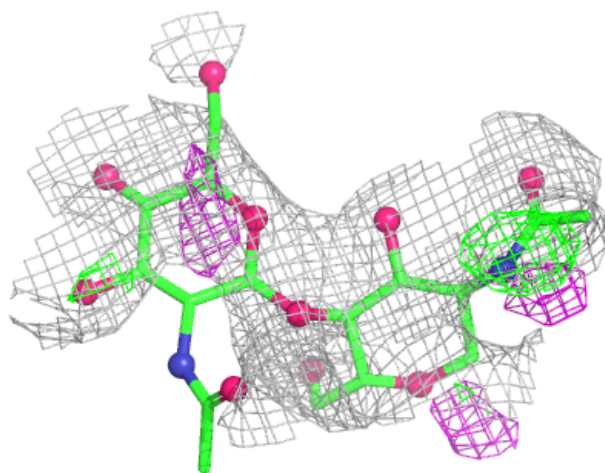
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	1	14/15	0.61	0.13	103,106,110,113	0
2	NAG	D	2	14/15	0.64	0.11	117,120,121,122	0
2	NAG	C	2	14/15	0.71	0.12	113,115,116,116	0
2	NAG	E	2	14/15	0.80	0.13	91,93,96,96	0
2	NAG	F	1	14/15	0.88	0.09	89,93,100,108	0
2	NAG	C	1	14/15	0.88	0.09	97,101,104,109	0
2	NAG	E	1	14/15	0.91	0.08	78,83,89,89	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.



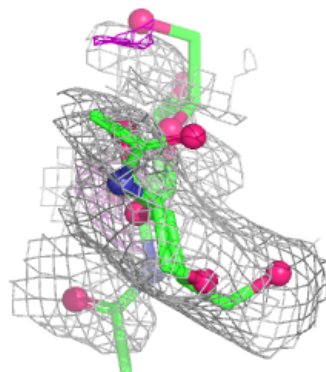
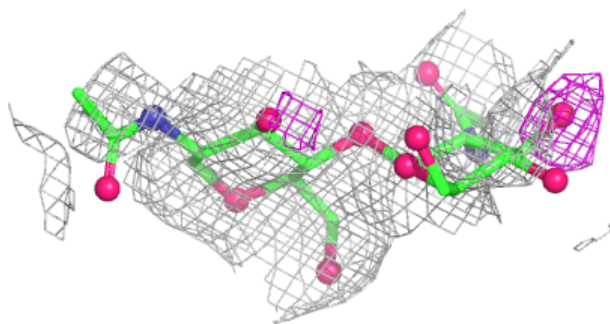
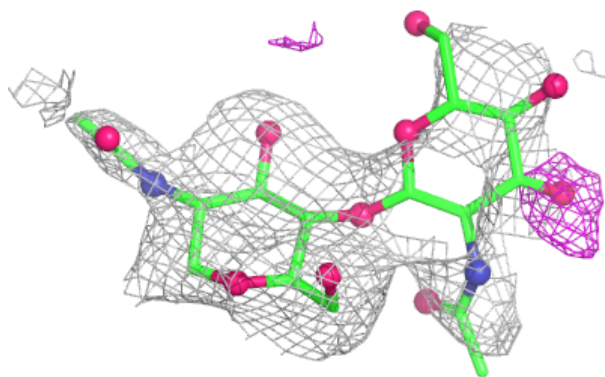
Electron density around Chain D:

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

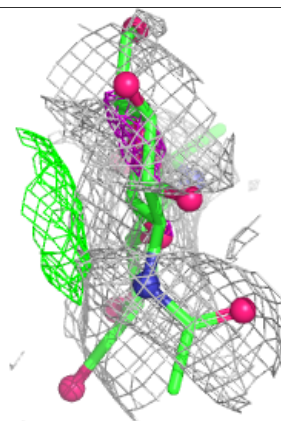
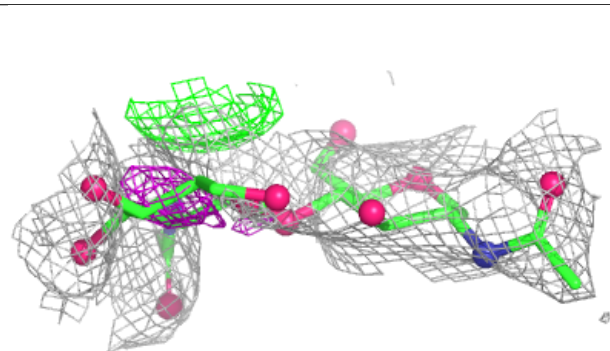
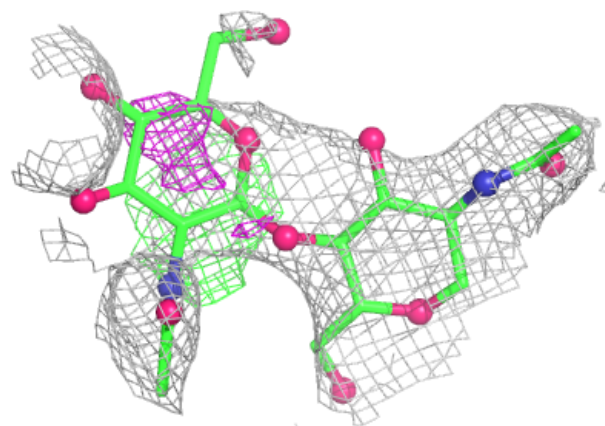


Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands ⓘ

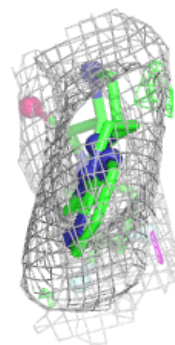
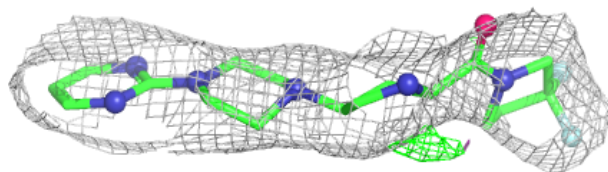
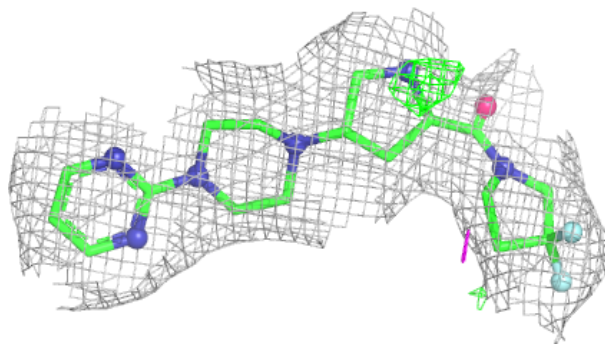
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	799	14/15	0.76	0.10	100,104,105,106	0
3	NAG	A	796	14/15	0.80	0.11	85,89,92,92	0
3	NAG	B	800	14/15	0.81	0.10	108,109,110,111	0
4	PF2	A	900	26/26	0.91	0.09	73,77,79,81	0
4	PF2	B	900	26/26	0.91	0.10	71,73,78,78	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.

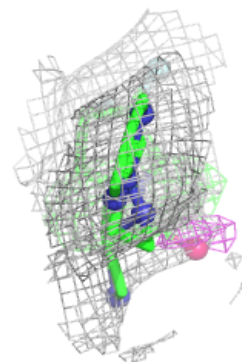
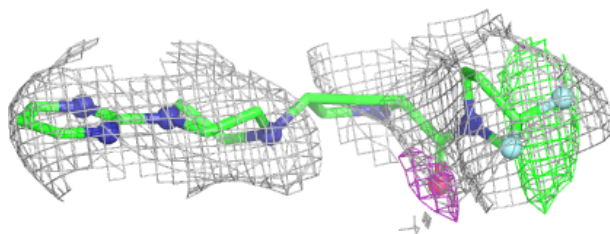
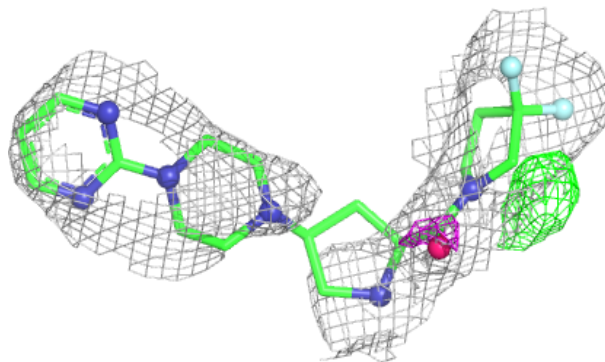
Electron density around PF2 A 900:

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 PF2 B 900:

$2mF_o - DF_c$ (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.