Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:39 pm GMT

PDB ID	:	4BTY
Title	:	Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors
Authors	:	Bligt-Linden, E.; Pihlavisto, M.; Szatmari, I.; Otwinowski, Z.; Smith, D.J.; Lazar, L.; Fulop, F.; Salminen, T.A.
Deposited on	:	2013-06-19
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

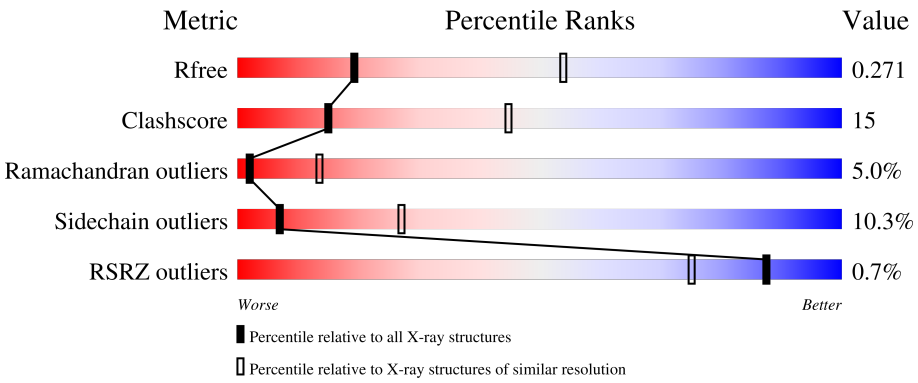
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	737	62% 28% 6% •
1	B	737	% 61% 29% 5% • •
2	C	2	50% 50%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
3	D	5	60% 40%

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
2	NAG	E	2	X	-	-	-
3	NAG	D	1	X	-	-	-
3	BMA	D	3	-	-	X	-
3	MAN	D	4	X	-	-	-
3	MAN	D	5	X	-	X	-
6	NAG	A	1768	X	-	-	-
6	NAG	A	1769	-	-	-	X
6	NAG	A	1770	-	-	-	X
6	NAG	B	1773	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11484 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.

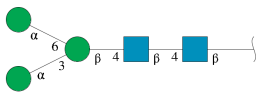
- Molecule 1 is a protein called MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	711	5604	3595	968	1021	20	0	0	0
1	B	707	5567	3574	957	1016	20	0	0	0

- 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-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
			Total	C	N	O			
3	D	5	61	34	2	25	0	0	0

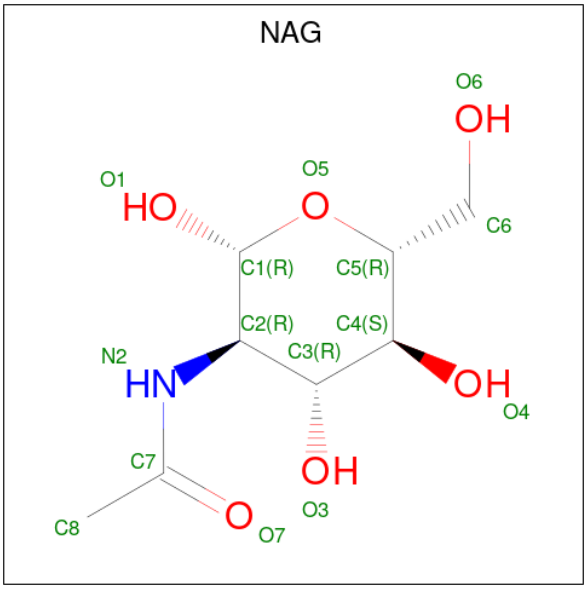
- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0
4	B	1	Total Cu 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	2	Total Ca 2 2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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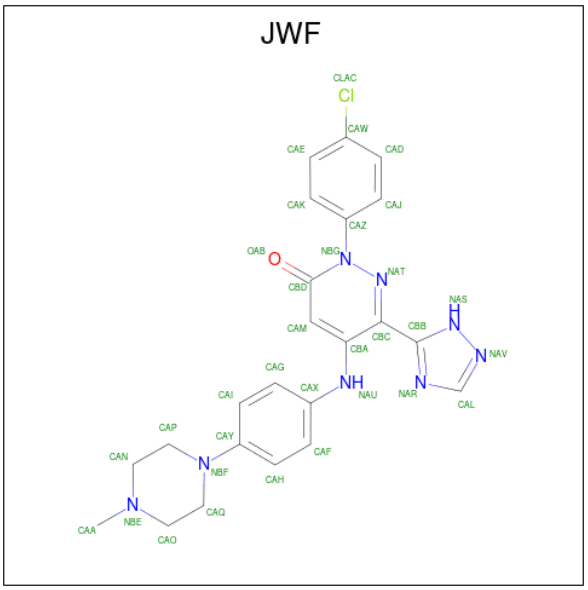
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0

- Molecule 7 is 5-[4-(4-methylpiperazin-1-yl)phenylamino]-2-(4-chlorophenyl)-6-(1H-1,2,4-triazol-5-yl)-3(2H)-pyridazinone (three-letter code: JWF) (formula: $C_{23}H_{23}ClN_8O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
7	A	1	33	23	1	8	1	0	0
			Total	C	Cl	N	O		
7	B	1	33	23	1	8	1	0	0

- Molecule 8 is water.

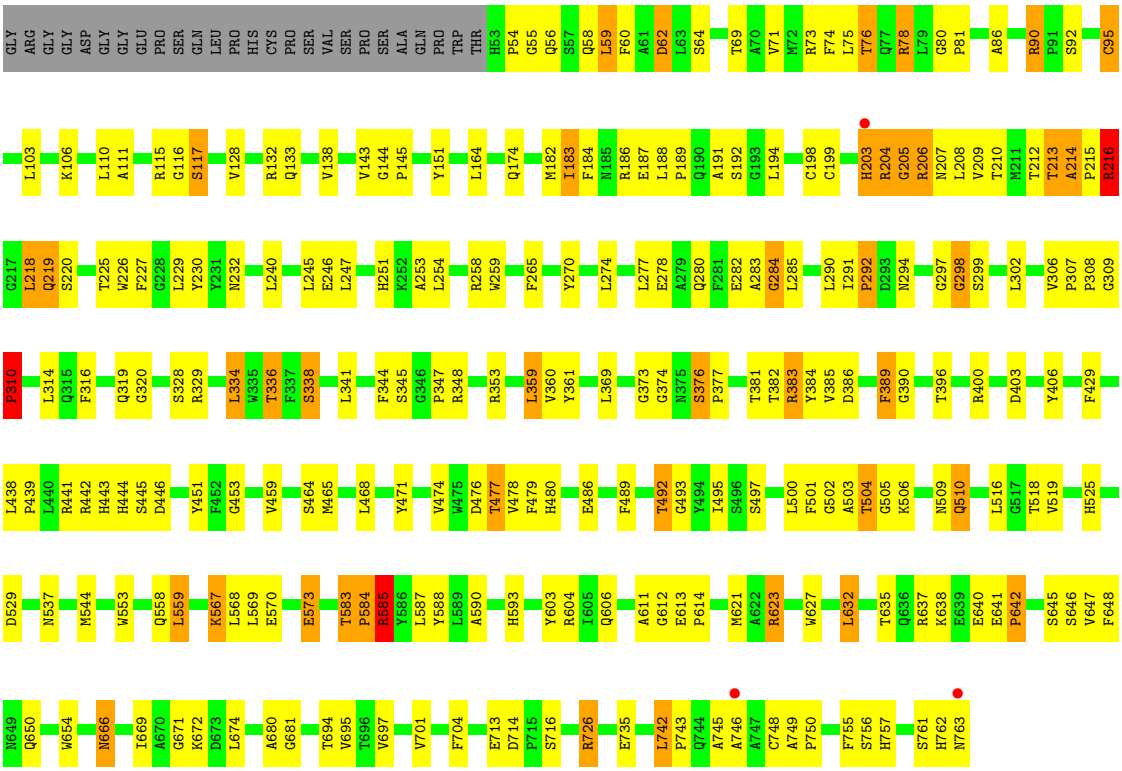
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	26	26	26	0	0
			Total	O		
8	B	14	14	14	0	0

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.

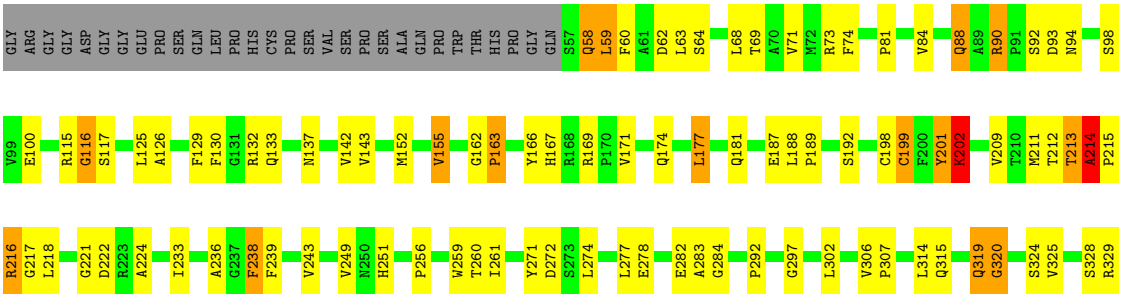
• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

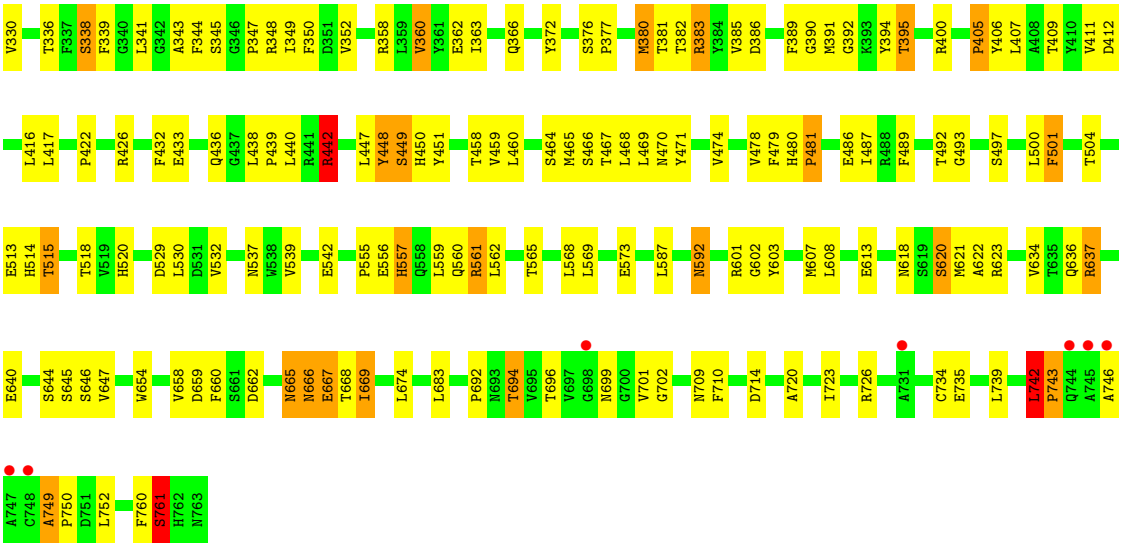
Chain A: 62% 28% 6% •



• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

Chain B: % 61% 29% 5% • •





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

Chain C: 50% 50%

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

Chain E: 100%

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 60% 40%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	226.74Å 226.74Å 218.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.20 – 3.10 49.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	76.2 (49.20-3.10) 76.2 (49.15-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.246 0.217 , 0.271	Depositor DCC
R_{free} test set	2314 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	88.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN, JWF, TPQ, CA, CU

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	0.67	1/5769 (0.0%)	0.89	5/7867 (0.1%)
1	B	0.66	1/5730 (0.0%)	0.88	1/7815 (0.0%)
All	All	0.66	2/11499 (0.0%)	0.88	6/15682 (0.0%)

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	2
1	B	0	7
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	ASN	CG-ND2	6.88	1.50	1.32
1	B	592	ASN	CG-ND2	5.50	1.46	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	585	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	A	529	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	529	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	258	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	585	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	216	ARG	N-CA-C	-5.19	96.99	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	PRO	Peptide
1	A	438	LEU	Peptide
1	B	162	GLY	Peptide
1	B	202	LYS	Peptide
1	B	213	THR	Peptide
1	B	214	ALA	Peptide
1	B	480	HIS	Peptide
1	B	742	LEU	Peptide
1	B	761	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5604	0	5335	169	0
1	B	5567	0	5299	182	0
2	C	28	0	25	1	0
2	E	28	0	25	1	0
3	D	61	0	52	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	56	0	52	1	0
6	B	28	0	26	4	0
7	A	33	0	23	5	0
7	B	33	0	23	3	0
8	A	26	0	0	2	0
8	B	14	0	0	4	0
All	All	11484	0	10860	337	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 15.

All (337) 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:592:ASN:ND2	6:B:1772:NAG:C1	1.90	1.35
1:B:592:ASN:ND2	6:B:1772:NAG:O5	1.62	1.32
3:D:3:BMA:O4	3:D:5:MAN:H2	1.33	1.25
3:D:3:BMA:C4	3:D:5:MAN:H2	1.79	1.13
1:B:592:ASN:HD22	6:B:1772:NAG:C1	1.59	1.00
1:B:58:GLN:HE21	1:B:58:GLN:HA	1.26	0.99
1:B:592:ASN:HD21	6:B:1772:NAG:C1	1.70	0.96
3:D:3:BMA:C4	3:D:5:MAN:C2	2.48	0.92
1:B:492:THR:HG23	1:B:694:THR:O	1.71	0.90
1:B:749:ALA:HB1	1:B:750:PRO:CD	2.02	0.88
1:A:205:GLY:O	1:A:207:ASN:N	2.10	0.85
1:B:376:SER:O	1:B:380:MET:HG2	1.79	0.82
1:B:749:ALA:HB1	1:B:750:PRO:HD2	1.60	0.82
1:A:389:PHE:CE2	7:A:2000:JWF:HAE	2.20	0.77
1:A:204:ARG:HD3	1:A:206:ARG:N	2.00	0.76
1:B:407:LEU:HD21	1:B:752:LEU:HD22	1.69	0.74
1:B:64:SER:O	1:B:68:LEU:HG	1.89	0.72
1:A:374:GLY:O	1:B:561:ARG:NH2	2.23	0.72
1:A:495:ILE:HD12	1:A:495:ILE:N	2.05	0.72
1:B:556:GLU:HB2	1:B:557:HIS:HB2	1.72	0.71
3:D:3:BMA:H4	3:D:5:MAN:O2	1.90	0.71
3:D:3:BMA:H4	3:D:5:MAN:C2	2.19	0.71
1:B:115:ARG:O	1:B:117:SER:N	2.23	0.71
3:D:3:BMA:O4	3:D:5:MAN:C2	2.28	0.70
1:B:163:PRO:HB3	3:D:1:NAG:H82	1.74	0.70
1:A:265:PHE:HD2	1:A:270:TYR:CE1	2.12	0.68
1:B:400:ARG:NH1	1:B:406:TYR:O	2.26	0.67
1:A:214:ALA:HB2	1:A:382:THR:HG23	1.77	0.66
1:B:319:GLN:O	1:B:320:GLY:O	2.11	0.66
1:A:749:ALA:H	1:B:749:ALA:HB2	1.60	0.66
1:A:58:GLN:O	1:A:60:PHE:N	2.23	0.66
1:A:519:VAL:HG13	1:B:562:LEU:HD23	1.76	0.66
1:B:58:GLN:HA	1:B:58:GLN:NE2	1.98	0.66
1:A:251:HIS:HA	1:A:259:TRP:CD1	2.31	0.66
1:A:204:ARG:HD3	1:A:206:ARG:H	1.60	0.65
1:A:504:THR:OG1	1:A:505:GLY:N	2.30	0.65
1:A:640:GLU:OE1	1:A:640:GLU:N	2.26	0.65
1:B:360:VAL:HG13	1:B:530:LEU:HD23	1.77	0.65
1:A:441:ARG:HA	1:B:492:THR:HG21	1.79	0.65
1:A:214:ALA:CB	1:A:215:PRO:CD	2.76	0.64
1:B:71:VAL:HG13	1:B:143:VAL:HG11	1.80	0.64
1:A:573:GLU:OE2	1:A:666:ASN:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ARG:HG3	1:B:561:ARG:HH11	1.62	0.63
1:B:381:THR:HG21	8:B:2003:HOH:O	1.97	0.63
1:B:256:PRO:HA	1:B:259:TRP:CE2	2.34	0.63
1:A:695:VAL:HG13	1:B:440:LEU:HG	1.81	0.62
1:B:665:ASN:O	1:B:667:GLU:N	2.32	0.62
1:A:115:ARG:O	1:A:117:SER:N	2.32	0.62
1:A:214:ALA:CB	1:A:215:PRO:HD2	2.30	0.62
1:B:637:ARG:HG2	1:B:637:ARG:HH11	1.63	0.62
1:A:214:ALA:HB1	1:A:215:PRO:CD	2.30	0.61
1:B:59:LEU:H	1:B:59:LEU:HD12	1.65	0.61
1:B:381:THR:CG2	8:B:2003:HOH:O	2.47	0.61
1:A:377:PRO:O	1:A:381:THR:HG22	2.00	0.61
1:B:556:GLU:N	1:B:557:HIS:HB2	2.15	0.61
1:B:343:ALA:HA	1:B:392:GLY:HA3	1.83	0.61
1:A:680:ALA:HB1	1:A:701:VAL:HG13	1.82	0.60
1:B:63:LEU:HB2	1:B:68:LEU:HD21	1.83	0.60
1:B:447:LEU:O	1:B:449:SER:N	2.34	0.60
1:A:588:TYR:HB3	1:A:604:ARG:HA	1.83	0.59
1:B:501:PHE:O	1:B:501:PHE:CD2	2.55	0.59
1:A:585:ARG:HH11	1:A:585:ARG:HG2	1.67	0.59
3:D:3:BMA:C5	3:D:5:MAN:C2	2.80	0.59
1:A:373:GLY:HA3	1:B:562:LEU:HB3	1.85	0.59
1:A:477:THR:HG22	1:A:479:PHE:CE1	2.38	0.58
1:B:212:THR:HG22	1:B:213:THR:N	2.17	0.58
1:B:58:GLN:HE21	1:B:58:GLN:CA	2.08	0.57
1:B:129:PHE:CZ	1:B:169:ARG:HB2	2.39	0.57
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.86	0.57
1:A:762:HIS:CE1	7:A:2000:JWF:HAA1	2.40	0.57
3:D:3:BMA:C5	3:D:5:MAN:H2	2.35	0.57
1:A:735:GLU:CD	1:A:735:GLU:H	2.09	0.57
1:B:556:GLU:CB	1:B:557:HIS:HB2	2.35	0.57
1:A:585:ARG:HH11	1:A:585:ARG:CG	2.19	0.56
1:A:74:PHE:O	1:A:78:ARG:NH1	2.38	0.56
1:B:352:VAL:HB	1:B:360:VAL:HG23	1.87	0.56
1:B:251:HIS:HA	1:B:259:TRP:CD1	2.41	0.56
1:B:749:ALA:CB	1:B:750:PRO:CD	2.81	0.56
1:B:696:THR:O	1:B:699:ASN:HB2	2.06	0.56
1:B:212:THR:CG2	1:B:216:ARG:NH2	2.68	0.56
1:A:306:VAL:HG23	1:A:307:PRO:HD2	1.86	0.55
1:B:214:ALA:HB2	1:B:382:THR:HA	1.89	0.55
1:B:201:TYR:O	1:B:202:LYS:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:CG1	1:B:448:TYR:CE2	2.90	0.55
1:B:669:ILE:HG22	1:B:674:LEU:HD22	1.88	0.55
1:A:389:PHE:CD2	7:A:2000:JWF:HAE	2.41	0.54
1:B:352:VAL:HB	1:B:360:VAL:CG2	2.37	0.54
1:A:492:THR:OG1	1:A:493:GLY:N	2.34	0.54
1:B:556:GLU:CA	1:B:557:HIS:HB2	2.38	0.54
1:A:58:GLN:C	1:A:59:LEU:HD23	2.28	0.54
1:B:63:LEU:CB	1:B:68:LEU:HD21	2.38	0.54
1:B:487:ILE:O	1:B:702:GLY:HA3	2.07	0.54
2:E:1:NAG:O6	2:E:2:NAG:C1	2.56	0.54
1:A:640:GLU:C	1:A:642:PRO:HD3	2.28	0.54
1:B:385:VAL:HG12	1:B:385:VAL:O	2.07	0.53
1:B:386:ASP:HB3	1:B:468:LEU:CD1	2.38	0.53
1:A:78:ARG:HH11	1:A:78:ARG:HB2	1.73	0.53
1:A:569:LEU:HD12	1:A:569:LEU:N	2.23	0.53
1:A:369:LEU:HD12	1:A:384:TYR:O	2.09	0.53
1:A:132:ARG:HB2	1:A:132:ARG:CZ	2.39	0.53
1:A:213:THR:HG22	1:A:225:THR:HG23	1.90	0.53
1:B:451:TYR:HA	1:B:726:ARG:HA	1.90	0.53
1:B:587:LEU:C	1:B:587:LEU:HD23	2.29	0.53
1:A:245:LEU:HD12	1:A:265:PHE:O	2.09	0.53
1:A:191:ALA:HA	1:A:278:GLU:CG	2.39	0.52
1:B:214:ALA:HB1	1:B:215:PRO:CD	2.39	0.52
1:B:636:GLN:NE2	1:B:668:THR:O	2.42	0.52
1:A:183:ILE:HG22	1:A:184:PHE:N	2.25	0.52
1:B:637:ARG:HH11	1:B:637:ARG:CG	2.20	0.52
1:B:735:GLU:OE1	1:B:735:GLU:N	2.42	0.52
1:A:623:ARG:CZ	1:A:623:ARG:HA	2.39	0.52
1:B:58:GLN:OE1	1:B:329:ARG:NH1	2.43	0.52
1:B:349:ILE:HD11	1:B:363:ILE:HB	1.91	0.52
1:A:314:LEU:HD12	8:A:2009:HOH:O	2.10	0.52
1:B:459:VAL:HG11	1:B:478:VAL:CG1	2.40	0.52
1:B:314:LEU:HD12	1:B:315:GLN:N	2.25	0.52
1:B:660:PHE:O	1:B:662:ASP:N	2.43	0.52
1:B:167:HIS:CE1	1:B:221:GLY:HA2	2.45	0.52
1:A:133:GLN:OE1	2:C:1:NAG:O6	2.28	0.51
1:A:214:ALA:HB3	1:A:215:PRO:HD2	1.92	0.51
1:A:632:LEU:HD23	1:A:632:LEU:C	2.30	0.51
1:A:62:ASP:OD1	1:A:348:ARG:NH2	2.42	0.51
1:B:142:VAL:HG23	1:B:155:VAL:CG2	2.40	0.51
1:B:623:ARG:HD3	1:B:659:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:ALA:N	1:B:749:ALA:HB2	2.26	0.51
1:A:309:GLY:O	1:A:310:PRO:O	2.28	0.51
1:B:187:GLU:HB3	1:B:274:LEU:CD1	2.40	0.51
1:A:400:ARG:NH1	1:A:406:TYR:O	2.42	0.51
1:B:239:PHE:CD1	1:B:470:ASN:HB3	2.46	0.51
1:B:478:VAL:HB	1:B:486:GLU:HB3	1.91	0.51
1:B:640:GLU:OE1	1:B:640:GLU:N	2.41	0.51
1:B:602:GLY:O	1:B:710:PHE:HB2	2.10	0.51
1:A:306:VAL:CG2	1:A:307:PRO:HD2	2.41	0.51
1:A:309:GLY:H	1:B:720:ALA:HB1	1.76	0.51
1:A:465:MET:HG2	1:A:474:VAL:HG22	1.93	0.50
1:B:601:ARG:HA	1:B:709:ASN:O	2.11	0.50
1:B:742:LEU:O	1:B:743:PRO:C	2.50	0.50
1:A:218:LEU:O	1:A:219:GLN:CB	2.59	0.50
1:A:214:ALA:HB3	1:A:382:THR:HA	1.93	0.50
1:A:544:MET:HE2	1:B:683:LEU:HD13	1.94	0.50
1:B:94:ASN:HA	1:B:129:PHE:O	2.11	0.50
1:B:497:SER:HB2	1:B:515:THR:HG22	1.94	0.50
1:A:669:ILE:O	1:A:674:LEU:HD11	2.13	0.49
1:A:75:LEU:O	1:A:76:THR:C	2.50	0.49
1:A:204:ARG:NE	1:A:206:ARG:HB3	2.28	0.49
1:A:382:THR:C	1:A:383:ARG:HD3	2.33	0.49
1:A:396:THR:OG1	1:B:442:ARG:NH2	2.44	0.49
1:A:78:ARG:NH1	1:A:78:ARG:HB2	2.27	0.49
1:A:583:THR:HG23	1:A:583:THR:O	2.12	0.49
1:B:556:GLU:N	1:B:557:HIS:CB	2.76	0.49
1:A:403:ASP:OD2	1:B:442:ARG:NH1	2.44	0.48
1:B:58:GLN:HG2	1:B:329:ARG:HD3	1.95	0.48
1:B:360:VAL:CG1	1:B:530:LEU:HD23	2.42	0.48
1:A:213:THR:HB	1:A:226:TRP:O	2.11	0.48
1:A:218:LEU:HD12	1:B:557:HIS:ND1	2.28	0.48
1:A:328:SER:O	1:A:338:SER:HA	2.13	0.48
1:A:334:LEU:HD12	1:A:334:LEU:N	2.28	0.48
1:A:671:GLY:C	1:A:672:LYS:HD2	2.34	0.48
1:B:224:ALA:HA	1:B:249:VAL:O	2.13	0.48
1:A:95:CYS:O	1:A:128:VAL:HA	2.13	0.48
1:B:328:SER:O	1:B:338:SER:HA	2.13	0.48
1:A:187:GLU:HB3	1:A:274:LEU:HD12	1.96	0.48
1:A:443:HIS:HB2	1:B:493:GLY:HA2	1.95	0.48
1:B:171:VAL:HG23	1:B:216:ARG:NH1	2.29	0.48
1:B:214:ALA:CB	1:B:382:THR:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:ILE:HG22	1:B:674:LEU:CD2	2.43	0.48
1:A:86:ALA:HA	1:A:95:CYS:SG	2.54	0.47
1:A:106:LYS:HG3	1:A:361:TYR:CZ	2.49	0.47
1:B:565:THR:HG22	1:B:565:THR:O	2.15	0.47
1:A:218:LEU:O	1:A:219:GLN:HB2	2.13	0.47
1:A:385:VAL:HG12	1:A:385:VAL:O	2.14	0.47
1:A:537:ASN:HA	1:A:590:ALA:O	2.14	0.47
1:A:453:GLY:HA3	1:B:302:LEU:HD13	1.96	0.47
1:A:480:HIS:NE2	1:A:486:GLU:OE1	2.48	0.47
1:B:62:ASP:OD1	1:B:348:ARG:NH2	2.46	0.47
1:B:344:PHE:HA	1:B:390:GLY:HA2	1.97	0.47
1:B:59:LEU:CD1	1:B:60:PHE:CD2	2.97	0.47
1:A:383:ARG:N	1:A:383:ARG:CD	2.78	0.47
1:B:59:LEU:HD11	1:B:60:PHE:CE2	2.50	0.47
1:B:212:THR:HG23	1:B:216:ARG:HH21	1.80	0.47
1:B:256:PRO:HA	1:B:259:TRP:CD2	2.50	0.47
1:A:106:LYS:HB2	1:A:637:ARG:NH2	2.30	0.47
1:A:726:ARG:HB2	1:A:726:ARG:CZ	2.45	0.47
1:A:745:ALA:O	1:A:746:ALA:HB3	2.15	0.46
1:B:90:ARG:N	1:B:90:ARG:HD2	2.29	0.46
1:B:433:GLU:HA	1:B:459:VAL:O	2.15	0.46
1:A:611:ALA:HA	1:A:681:GLY:O	2.15	0.46
1:B:395:THR:HA	1:B:466:SER:HA	1.97	0.46
1:B:520:HIS:CE1	8:B:2006:HOH:O	2.68	0.46
1:A:194:LEU:HD12	1:A:277:LEU:HG	1.98	0.46
1:A:525:HIS:HB2	1:A:627:TRP:CE3	2.50	0.46
1:A:381:THR:HG23	8:A:2006:HOH:O	2.14	0.46
1:A:495:ILE:N	1:A:495:ILE:CD1	2.73	0.46
1:A:341:LEU:HB2	1:A:429:PHE:HZ	1.81	0.46
1:B:238:PHE:CD1	1:B:238:PHE:C	2.89	0.46
1:B:556:GLU:H	1:B:557:HIS:CB	2.28	0.46
1:A:214:ALA:HB1	1:A:215:PRO:HD2	1.95	0.46
1:B:243:VAL:O	1:B:243:VAL:CG1	2.64	0.46
1:B:233:ILE:HG21	1:B:236:ALA:HB3	1.97	0.46
1:B:447:LEU:HG	1:B:448:TYR:CD2	2.51	0.46
1:A:138:VAL:HB	1:A:164:LEU:HB2	1.98	0.45
1:A:641:GLU:N	1:A:642:PRO:HD3	2.29	0.45
1:B:130:PHE:HB2	1:B:137:ASN:O	2.16	0.45
1:B:465:MET:HG2	1:B:474:VAL:HG22	1.98	0.45
1:A:389:PHE:CD2	7:A:2000:JWF:CAE	3.00	0.45
1:A:90:ARG:HA	1:A:90:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MET:HA	1:A:186:ARG:HD3	1.98	0.45
1:B:438:LEU:HD23	1:B:439:PRO:HD2	1.98	0.45
1:B:500:LEU:O	1:B:501:PHE:HB3	2.16	0.45
1:A:444:HIS:O	1:B:467:THR:HG21	2.17	0.45
1:B:116:GLY:O	1:B:117:SER:C	2.55	0.45
1:B:646:SER:HB3	1:B:658:VAL:HG23	1.99	0.45
1:A:492:THR:HB	1:A:694:THR:O	2.16	0.44
1:A:478:VAL:HB	1:A:486:GLU:HB3	1.98	0.44
1:A:567:LYS:HE2	1:A:568:LEU:N	2.33	0.44
1:A:583:THR:HA	1:A:584:PRO:HD2	1.54	0.44
1:A:588:TYR:HB2	1:A:603:TYR:O	2.18	0.44
1:B:59:LEU:CD1	1:B:60:PHE:CE2	3.00	0.44
1:B:142:VAL:O	1:B:152:MET:HA	2.17	0.44
1:A:204:ARG:CD	1:A:205:GLY:H	2.31	0.44
1:A:297:GLY:O	1:A:298:GLY:C	2.56	0.44
1:B:561:ARG:HH11	1:B:561:ARG:CG	2.31	0.44
1:A:294:ASN:OD1	6:A:1768:NAG:H61	2.17	0.44
1:B:306:VAL:HG13	1:B:307:PRO:HD2	1.99	0.44
1:A:389:PHE:HE1	1:A:650:GLN:HE21	1.64	0.44
1:B:187:GLU:HB3	1:B:274:LEU:HD11	1.99	0.44
1:B:532:VAL:HB	1:B:537:ASN:OD1	2.16	0.44
1:A:442:ARG:CD	1:B:465:MET:SD	3.07	0.43
1:A:500:LEU:HD21	1:A:510:GLN:HG3	1.99	0.43
1:B:350:PHE:CE1	1:B:362:GLU:HG3	2.53	0.43
1:B:513:GLU:O	1:B:514:HIS:HB2	2.17	0.43
1:B:349:ILE:HD12	1:B:349:ILE:O	2.19	0.43
1:A:92:SER:O	1:A:132:ARG:N	2.51	0.43
1:A:198:CYS:SG	1:A:199:CYS:N	2.91	0.43
1:A:567:LYS:HE2	1:A:568:LEU:H	1.83	0.43
1:B:372:TYR:CD2	1:B:520:HIS:HB3	2.53	0.43
1:B:416:LEU:O	1:B:417:LEU:HD23	2.19	0.43
1:A:501:PHE:O	1:A:503:ALA:N	2.51	0.43
1:A:646:SER:O	1:A:648:PHE:N	2.50	0.43
1:A:714:ASP:OD2	1:A:716:SER:OG	2.36	0.43
1:B:88:GLN:HA	1:B:174:GLN:HB2	2.00	0.43
1:A:632:LEU:HD23	1:A:632:LEU:O	2.19	0.43
1:B:212:THR:CG2	1:B:216:ARG:HH21	2.31	0.43
1:B:492:THR:HG22	1:B:493:GLY:N	2.33	0.43
1:B:542:GLU:HA	1:B:565:THR:O	2.17	0.43
1:A:106:LYS:HG3	1:A:361:TYR:CE1	2.54	0.43
1:A:209:VAL:HG11	1:B:448:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:CD2	1:A:750:PRO:HD3	2.54	0.43
1:A:671:GLY:O	1:A:672:LYS:HD2	2.19	0.43
1:A:755:PHE:CE2	1:A:757:HIS:HB2	2.54	0.43
1:B:416:LEU:HD23	1:B:416:LEU:C	2.39	0.43
1:B:487:ILE:N	1:B:487:ILE:HD12	2.34	0.43
1:A:336:THR:HG23	1:A:353:ARG:HB2	2.01	0.43
1:A:445:SER:HB3	1:A:451:TYR:CE2	2.54	0.43
1:B:125:LEU:HD23	1:B:126:ALA:N	2.34	0.43
1:B:217:GLY:HA3	1:B:222:ASP:CB	2.48	0.43
1:B:739:LEU:HD23	1:B:742:LEU:HD11	2.01	0.43
1:A:403:ASP:HB3	1:A:465:MET:CE	2.49	0.42
1:A:613:GLU:HG3	1:A:614:PRO:CD	2.48	0.42
1:A:650:GLN:OE1	1:A:650:GLN:HA	2.19	0.42
1:B:411:VAL:HG12	1:B:412:ASP:N	2.34	0.42
1:A:465:MET:SD	1:B:442:ARG:CD	3.07	0.42
1:A:748:CYS:H	1:B:749:ALA:HB3	1.84	0.42
1:A:459:VAL:HG23	1:A:480:HIS:HA	2.01	0.42
1:A:553:TRP:CZ3	1:B:377:PRO:HB3	2.55	0.42
1:A:559:LEU:HD23	1:A:559:LEU:O	2.18	0.42
1:B:187:GLU:HB3	1:B:274:LEU:HD12	2.01	0.42
1:B:382:THR:C	1:B:383:ARG:HD3	2.40	0.42
1:B:405:PRO:HG2	1:B:432:PHE:CD1	2.55	0.42
1:B:568:LEU:HG	1:B:569:LEU:N	2.34	0.42
1:A:282:GLU:C	1:A:284:GLY:H	2.22	0.42
1:A:500:LEU:CD2	1:A:510:GLN:HG3	2.49	0.42
1:B:282:GLU:C	1:B:284:GLY:H	2.22	0.42
1:B:389:PHE:CE1	7:B:2000:JWF:HAD	2.54	0.42
1:A:359:LEU:N	1:A:359:LEU:HD23	2.35	0.42
1:A:585:ARG:CG	1:A:585:ARG:NH1	2.82	0.42
1:B:539:VAL:HG13	1:B:569:LEU:HB2	2.02	0.42
1:A:203:HIS:O	1:A:204:ARG:HB2	2.19	0.42
1:B:187:GLU:HG3	1:B:261:ILE:HD11	2.02	0.42
1:B:271:TYR:CE1	1:B:277:LEU:HD13	2.55	0.42
1:B:620:SER:OG	1:B:654:TRP:HD1	2.03	0.42
1:A:212:THR:OG1	1:A:216:ARG:NH2	2.49	0.42
1:B:188:LEU:N	1:B:189:PRO:CD	2.83	0.42
1:B:723:ILE:HD11	1:B:739:LEU:HG	2.01	0.42
7:B:2000:JWF:HAU	7:B:2000:JWF:HAS	1.66	0.42
1:A:220:SER:HB2	1:A:654:TRP:HB2	2.02	0.42
1:B:339:PHE:HB3	1:B:349:ILE:HG22	2.01	0.42
1:B:382:THR:O	1:B:383:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:PHE:HB3	1:B:394:TYR:CE2	2.54	0.42
1:A:383:ARG:NH2	1:B:560:GLN:O	2.44	0.41
1:A:606:GLN:HB3	1:A:704:PHE:HB2	2.02	0.41
1:A:735:GLU:CD	1:A:735:GLU:N	2.73	0.41
1:B:166:TYR:O	1:B:169:ARG:HD3	2.19	0.41
1:A:386:ASP:HB3	1:A:468:LEU:CD2	2.50	0.41
1:A:445:SER:CB	1:A:451:TYR:CE2	3.03	0.41
1:A:509:ASN:O	1:A:516:LEU:HD12	2.20	0.41
1:B:177:LEU:HD12	7:B:2000:JWF:CAI	2.50	0.41
1:B:278:GLU:O	1:B:282:GLU:HG3	2.20	0.41
1:A:225:THR:HB	1:A:227:PHE:CE2	2.54	0.41
1:A:383:ARG:HD3	1:A:383:ARG:N	2.35	0.41
1:B:69:THR:HG23	1:B:422:PRO:HG3	2.02	0.41
1:B:750:PRO:HB3	1:B:752:LEU:HD21	2.03	0.41
1:A:144:GLY:C	1:A:151:TYR:CE1	2.94	0.41
1:B:366:GLN:HG3	1:B:644:SER:OG	2.21	0.41
1:B:212:THR:HG21	1:B:216:ARG:NH2	2.34	0.41
1:A:110:LEU:O	1:A:111:ALA:C	2.59	0.41
1:B:460:LEU:HB3	1:B:479:PHE:HB2	2.02	0.41
1:A:73:ARG:O	1:A:76:THR:HB	2.20	0.41
1:A:246:GLU:OE1	1:A:376:SER:HB2	2.21	0.41
1:B:469:LEU:HD23	1:B:469:LEU:HA	1.90	0.41
1:A:188:LEU:HB2	1:A:189:PRO:HD2	2.02	0.41
1:A:308:PRO:HA	1:B:720:ALA:O	2.21	0.41
1:A:359:LEU:HD13	1:A:603:TYR:CZ	2.56	0.41
1:A:476:ASP:O	1:A:477:THR:CB	2.69	0.41
1:A:638:LYS:HD2	1:A:641:GLU:CD	2.41	0.41
1:A:246:GLU:C	1:A:247:LEU:HD12	2.40	0.41
1:A:465:MET:SD	1:B:442:ARG:HD2	2.61	0.41
1:B:74:PHE:CD1	1:B:74:PHE:C	2.94	0.41
1:B:211:MET:HA	8:B:2002:HOH:O	2.21	0.41
1:B:436:GLN:HB2	1:B:438:LEU:HB2	2.02	0.41
1:A:71:VAL:HG13	1:A:143:VAL:HG11	2.03	0.40
1:A:144:GLY:O	1:A:151:TYR:CD1	2.74	0.40
1:A:344:PHE:HA	1:A:390:GLY:HA2	2.03	0.40
1:A:695:VAL:CG1	1:B:440:LEU:HG	2.50	0.40
1:B:174:GLN:HA	1:B:174:GLN:NE2	2.35	0.40
1:B:341:LEU:HD12	1:B:347:PRO:N	2.35	0.40
1:A:245:LEU:HG	1:A:247:LEU:CD1	2.52	0.40
1:A:344:PHE:HA	1:A:390:GLY:CA	2.51	0.40
1:B:84:VAL:HG21	1:B:93:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:C	1:A:209:VAL:HG23	2.41	0.40
1:A:213:THR:HG21	1:A:226:TRP:H	1.87	0.40
1:A:341:LEU:HB2	1:A:429:PHE:CZ	2.56	0.40
7:A:2000:JWF:HAH	7:A:2000:JWF:HAQ2	1.94	0.40
1:B:260:THR:HG22	1:B:261:ILE:N	2.36	0.40
1:B:325:VAL:HG22	1:B:330:VAL:HG22	2.03	0.40
1:A:476:ASP:O	1:A:477:THR:OG1	2.34	0.40
1:B:760:PHE:O	1:B:761:SER:C	2.60	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	708/737 (96%)	596 (84%)	73 (10%)	39 (6%)	2 11
1	B	704/737 (96%)	593 (84%)	79 (11%)	32 (4%)	2 15
All	All	1412/1474 (96%)	1189 (84%)	152 (11%)	71 (5%)	2 13

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	116	GLY
1	A	203	HIS
1	A	204	ARG
1	A	206	ARG
1	A	214	ALA
1	A	219	GLN
1	A	310	PRO
1	A	477	THR
1	A	642	PRO

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Mol	Chain	Res	Type
1	B	116	GLY
1	B	181	GLN
1	B	201	TYR
1	B	202	LYS
1	B	214	ALA
1	B	297	GLY
1	B	320	GLY
1	B	481	PRO
1	B	504	THR
1	B	618	ASN
1	B	622	ALA
1	B	667	GLU
1	B	742	LEU
1	A	81	PRO
1	A	253	ALA
1	A	284	GLY
1	A	298	GLY
1	A	320	GLY
1	A	593	HIS
1	B	133	GLN
1	B	501	PHE
1	B	749	ALA
1	A	283	ALA
1	A	292	PRO
1	A	347	PRO
1	A	502	GLY
1	A	584	PRO
1	B	283	ALA
1	B	448	TYR
1	B	557	HIS
1	B	743	PRO
1	B	761	SER
1	A	55	GLY
1	A	76	THR
1	A	183	ILE
1	A	439	PRO
1	A	504	THR
1	A	623	ARG
1	A	647	VAL
1	A	761	SER
1	B	81	PRO
1	B	132	ARG

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Mol	Chain	Res	Type
1	B	199	CYS
1	B	442	ARG
1	B	555	PRO
1	B	665	ASN
1	A	232	ASN
1	A	280	GLN
1	A	697	VAL
1	A	743	PRO
1	B	405	PRO
1	B	746	ALA
1	A	612	GLY
1	A	742	LEU
1	B	666	ASN
1	A	54	PRO
1	A	80	GLY
1	A	205	GLY
1	B	163	PRO
1	A	145	PRO
1	B	692	PRO

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	588/610 (96%)	527 (90%)	61 (10%)	7 27
1	B	584/610 (96%)	524 (90%)	60 (10%)	7 27
All	All	1172/1220 (96%)	1051 (90%)	121 (10%)	7 27

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	62	ASP
1	A	64	SER
1	A	69	THR

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Mol	Chain	Res	Type
1	A	78	ARG
1	A	90	ARG
1	A	95	CYS
1	A	103	LEU
1	A	117	SER
1	A	174	GLN
1	A	192	SER
1	A	210	THR
1	A	213	THR
1	A	216	ARG
1	A	218	LEU
1	A	229	LEU
1	A	230	TYR
1	A	240	LEU
1	A	254	LEU
1	A	285	LEU
1	A	290	LEU
1	A	291	ILE
1	A	299	SER
1	A	302	LEU
1	A	310	PRO
1	A	319	GLN
1	A	329	ARG
1	A	334	LEU
1	A	336	THR
1	A	338	SER
1	A	345	SER
1	A	359	LEU
1	A	360	VAL
1	A	376	SER
1	A	383	ARG
1	A	389	PHE
1	A	446	ASP
1	A	464	SER
1	A	489	PHE
1	A	492	THR
1	A	497	SER
1	A	506	LYS
1	A	510	GLN
1	A	518	THR
1	A	558	GLN
1	A	559	LEU

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Mol	Chain	Res	Type
1	A	567	LYS
1	A	570	GLU
1	A	573	GLU
1	A	583	THR
1	A	585	ARG
1	A	587	LEU
1	A	621	MET
1	A	632	LEU
1	A	635	THR
1	A	645	SER
1	A	713	GLU
1	A	726	ARG
1	A	742	LEU
1	A	756	SER
1	A	763	ASN
1	B	58	GLN
1	B	59	LEU
1	B	73	ARG
1	B	88	GLN
1	B	90	ARG
1	B	92	SER
1	B	98	SER
1	B	100	GLU
1	B	155	VAL
1	B	177	LEU
1	B	192	SER
1	B	198	CYS
1	B	199	CYS
1	B	209	VAL
1	B	216	ARG
1	B	218	LEU
1	B	238	PHE
1	B	272	ASP
1	B	292	PRO
1	B	319	GLN
1	B	324	SER
1	B	336	THR
1	B	338	SER
1	B	345	SER
1	B	358	ARG
1	B	360	VAL
1	B	380	MET

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Mol	Chain	Res	Type
1	B	383	ARG
1	B	391	MET
1	B	395	THR
1	B	409	THR
1	B	426	ARG
1	B	442	ARG
1	B	449	SER
1	B	450	HIS
1	B	458	THR
1	B	464	SER
1	B	481	PRO
1	B	489	PHE
1	B	515	THR
1	B	518	THR
1	B	559	LEU
1	B	561	ARG
1	B	573	GLU
1	B	603	TYR
1	B	607	MET
1	B	608	LEU
1	B	613	GLU
1	B	620	SER
1	B	621	MET
1	B	634	VAL
1	B	637	ARG
1	B	645	SER
1	B	647	VAL
1	B	666	ASN
1	B	669	ILE
1	B	694	THR
1	B	701	VAL
1	B	714	ASP
1	B	734	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	592	ASN
1	B	593	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPQ	A	471	1	13,14,15	1.38	4 (30%)	15,19,21	1.53	3 (20%)
1	TPQ	B	471	1	13,14,15	1.37	2 (15%)	15,19,21	1.77	3 (20%)

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
1	TPQ	A	471	1	-	1/5/22/24	0/1/1/1
1	TPQ	B	471	1	-	2/5/22/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	TPQ	C3-C4	2.84	1.40	1.35
1	A	471	TPQ	C3-C4	2.53	1.39	1.35
1	A	471	TPQ	C6-C5	-2.45	1.38	1.44
1	A	471	TPQ	C3-C2	-2.17	1.38	1.44
1	B	471	TPQ	C3-C2	-2.11	1.39	1.44
1	A	471	TPQ	C6-C1	2.01	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	471	TPQ	CB-CA-C	-4.28	103.45	111.47
1	B	471	TPQ	C6-C1-C2	4.08	121.78	118.64
1	A	471	TPQ	C6-C1-C2	3.49	121.32	118.64
1	A	471	TPQ	CB-CA-C	-3.11	105.64	111.47
1	A	471	TPQ	O5-C5-C4	2.58	123.60	119.38
1	B	471	TPQ	O5-C5-C4	2.19	122.97	119.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	471	TPQ	N-CA-CB-C1
1	B	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

9 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	0.58	0	17,19,21	1.39	2 (11%)
2	NAG	C	2	2	14,14,15	0.70	0	17,19,21	1.24	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.69	0	17,19,21	2.01	4 (23%)
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	1.69	1 (5%)
3	BMA	D	3	3	11,11,12	1.31	2 (18%)	15,15,17	2.45	7 (46%)
3	MAN	D	4	3	11,11,12	1.69	3 (27%)	15,15,17	1.87	5 (33%)
3	MAN	D	5	3	11,11,12	0.26	0	15,15,17	0.64	0
2	NAG	E	1	2,1	14,14,15	0.81	0	17,19,21	1.57	4 (23%)
2	NAG	E	2	2	14,14,15	0.71	0	17,19,21	2.76	7 (41%)

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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	D	5	3	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	C1-C2	3.46	1.60	1.52
3	D	4	MAN	C2-C3	3.27	1.57	1.52
3	D	3	BMA	O3-C3	2.80	1.49	1.43
3	D	4	MAN	C4-C3	2.41	1.58	1.52
3	D	3	BMA	O6-C6	2.11	1.51	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	O5-C1-C2	6.19	121.06	111.29
3	D	3	BMA	O3-C3-C2	5.82	121.15	109.99
2	E	2	NAG	C1-O5-C5	5.60	119.78	112.19
3	D	2	NAG	C1-O5-C5	5.27	119.33	112.19
3	D	1	NAG	O4-C4-C3	-4.56	99.80	110.35
3	D	3	BMA	O2-C2-C1	4.16	117.67	109.15
2	E	2	NAG	C2-N2-C7	4.13	128.79	122.90
2	E	1	NAG	C2-N2-C7	3.65	128.10	122.90
3	D	4	MAN	O5-C5-C6	3.64	112.91	107.20
3	D	3	BMA	O5-C5-C6	3.39	112.52	107.20
2	E	2	NAG	O7-C7-C8	-3.33	115.87	122.06
3	D	1	NAG	C3-C4-C5	-3.26	104.43	110.24
2	E	1	NAG	O3-C3-C2	3.01	115.70	109.47
3	D	4	MAN	C1-O5-C5	-3.00	108.12	112.19
2	C	2	NAG	C1-O5-C5	2.99	116.24	112.19
3	D	4	MAN	O2-C2-C1	2.92	115.12	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-C2-N2	-2.91	105.51	110.49
2	C	1	NAG	O3-C3-C2	2.78	115.22	109.47
2	C	1	NAG	C1-O5-C5	2.63	115.75	112.19
3	D	1	NAG	O4-C4-C5	2.59	115.73	109.30
2	E	1	NAG	C4-C3-C2	-2.55	107.28	111.02
3	D	3	BMA	O5-C1-C2	2.47	114.59	110.77
3	D	3	BMA	C3-C4-C5	2.46	114.64	110.24
3	D	4	MAN	O4-C4-C3	2.45	116.01	110.35
2	C	2	NAG	O4-C4-C5	2.42	115.30	109.30
2	E	2	NAG	O3-C3-C2	2.35	114.33	109.47
3	D	1	NAG	O3-C3-C4	-2.30	105.02	110.35
3	D	3	BMA	O6-C6-C5	2.28	119.11	111.29
2	E	1	NAG	O4-C4-C5	2.28	114.95	109.30
2	E	2	NAG	O7-C7-N2	2.12	125.84	121.95
3	D	3	BMA	O3-C3-C4	2.07	115.13	110.35
3	D	4	MAN	C1-C2-C3	-2.03	107.17	109.67

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	NAG	C1
3	D	1	NAG	C1
3	D	4	MAN	C1
3	D	5	MAN	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

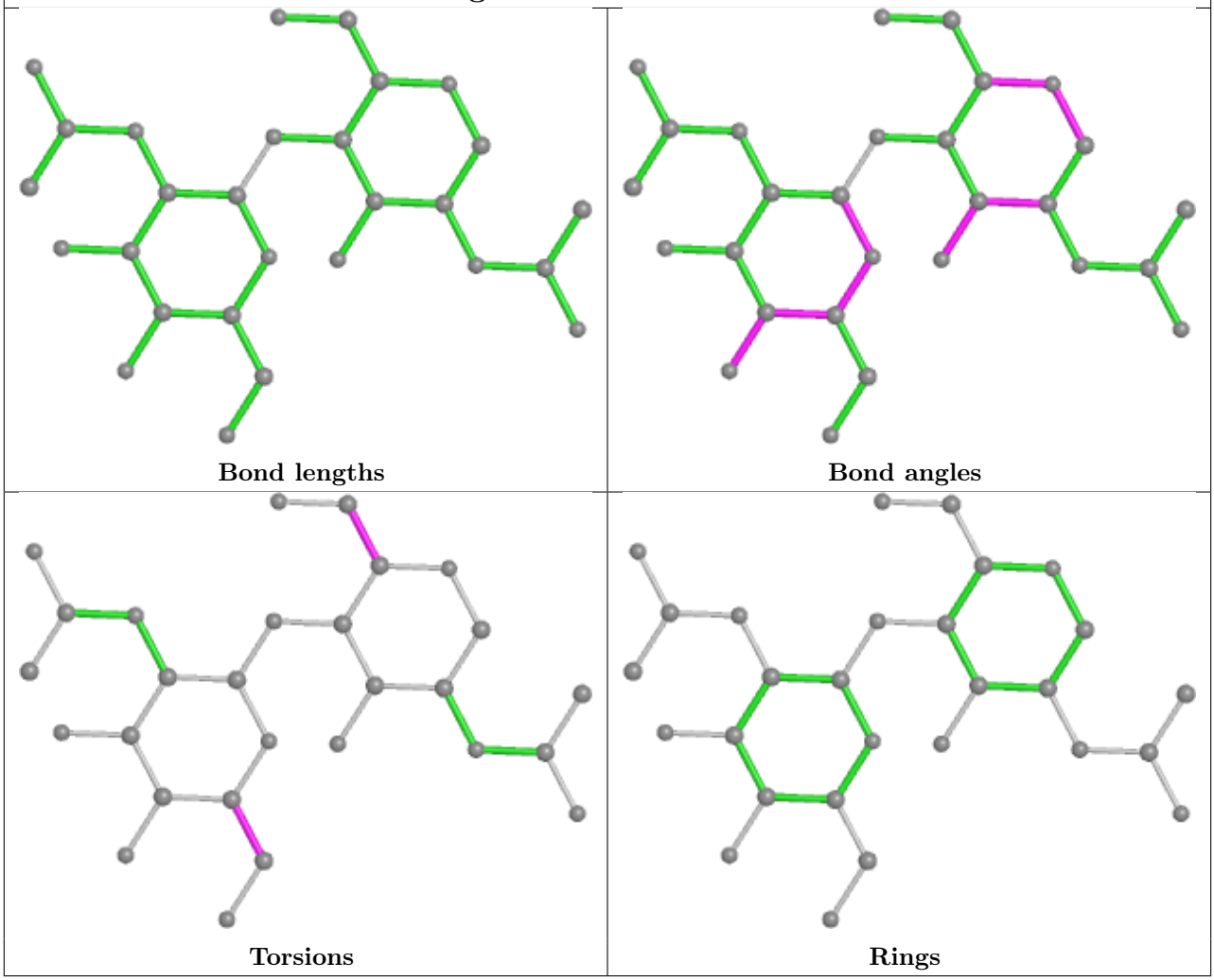
There are no ring outliers.

6 monomers are involved in 11 short contacts:

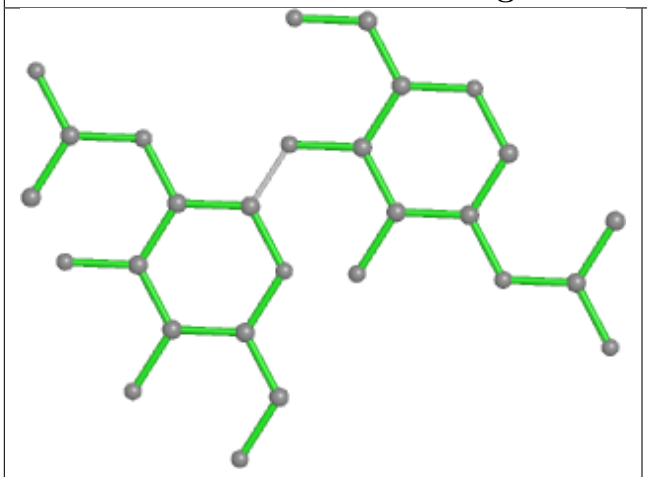
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
2	C	1	NAG	1	0
3	D	5	MAN	8	0
3	D	3	BMA	8	0
2	E	1	NAG	1	0
2	E	2	NAG	1	0

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

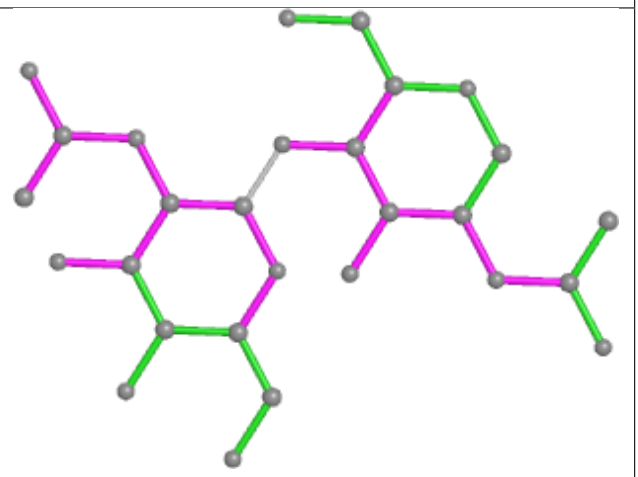
Oligosaccharide Chain C



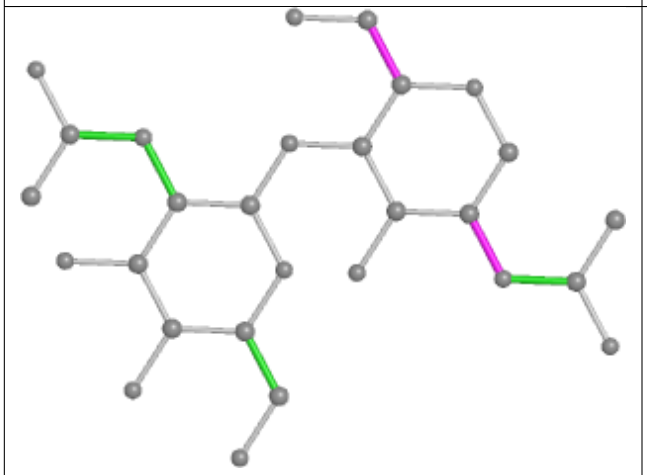
Oligosaccharide Chain E



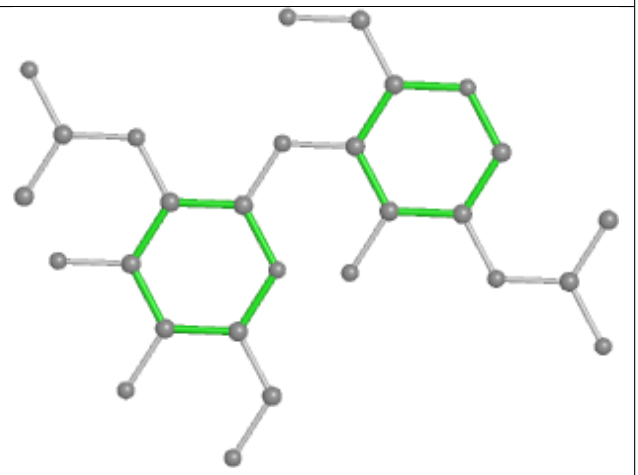
Bond lengths



Bond angles

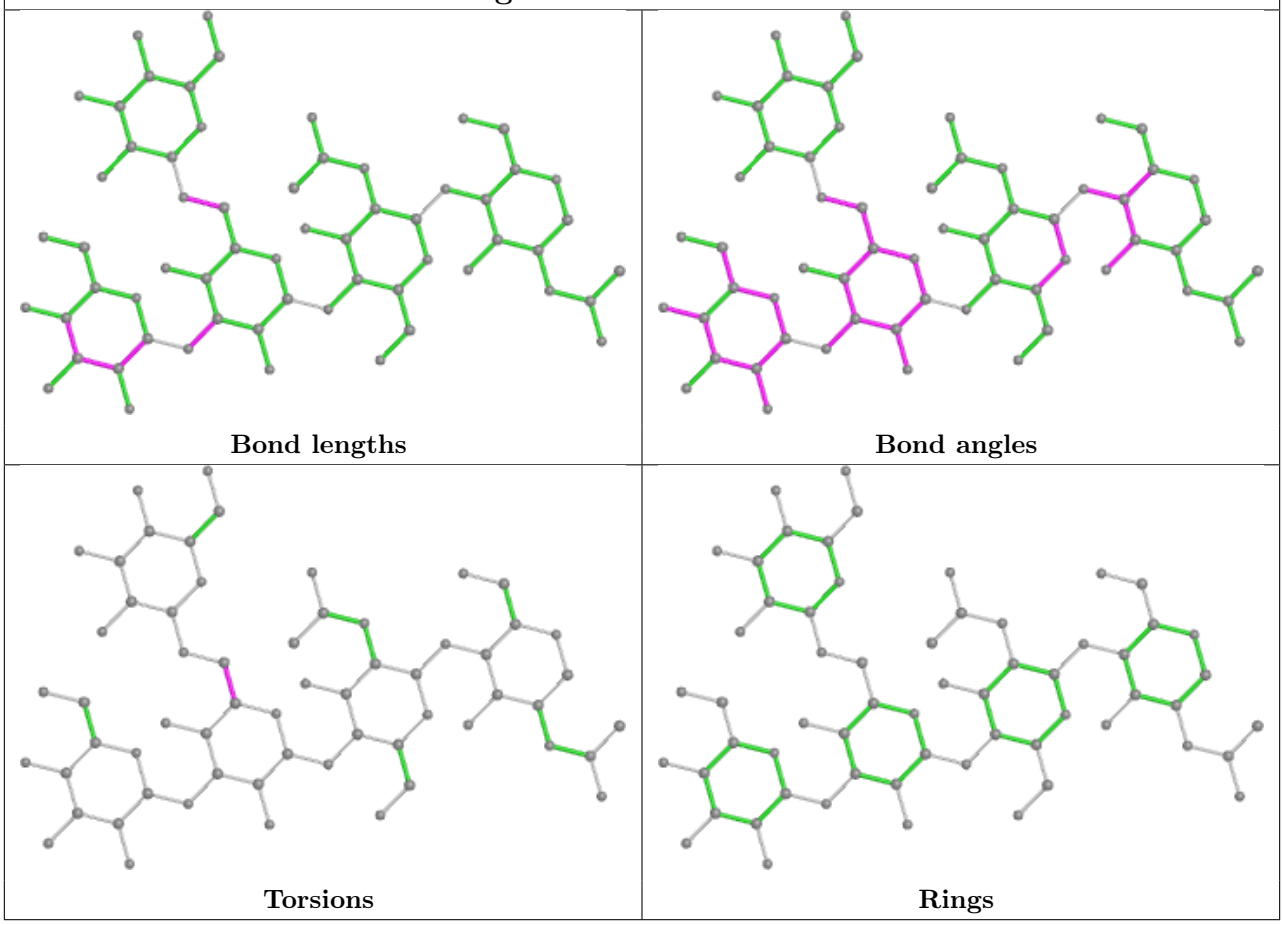


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	1772	-	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	A	1770	1	14,14,15	2.67	3 (21%)	17,19,21	3.97	9 (52%)
7	JWF	B	2000	-	34,37,37	2.16	6 (17%)	44,52,52	2.51	14 (31%)
6	NAG	A	1768	1	14,14,15	1.00	1 (7%)	17,19,21	2.65	6 (35%)
6	NAG	A	1767	1	14,14,15	0.83	0	17,19,21	2.28	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	JWF	A	2000	-	34,37,37	2.51	8 (23%)	44,52,52	2.30	17 (38%)
6	NAG	B	1773	1	14,14,15	1.62	2 (14%)	17,19,21	2.69	4 (23%)
6	NAG	A	1769	1	14,14,15	0.79	0	17,19,21	1.98	4 (23%)

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
6	NAG	B	1772	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1770	1	-	2/6/23/26	0/1/1/1
7	JWF	B	2000	-	-	2/12/26/26	0/5/5/5
6	NAG	A	1768	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	1767	1	-	3/6/23/26	0/1/1/1
7	JWF	A	2000	-	-	2/12/26/26	0/5/5/5
6	NAG	B	1773	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1769	1	-	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2000	JWF	NAV-NAS	-8.93	1.18	1.37
6	A	1770	NAG	C1-C2	7.85	1.64	1.52
7	B	2000	JWF	NAV-NAS	-7.46	1.21	1.37
7	A	2000	JWF	NBG-NAT	-6.75	1.19	1.38
7	B	2000	JWF	NBG-NAT	-6.21	1.21	1.38
6	A	1770	NAG	C2-N2	4.51	1.54	1.46
6	B	1773	NAG	C1-C2	4.41	1.58	1.52
7	A	2000	JWF	CAZ-NBG	-4.16	1.35	1.43
6	B	1773	NAG	O5-C1	3.57	1.49	1.43
7	B	2000	JWF	CAZ-NBG	-3.49	1.36	1.43
7	A	2000	JWF	CAX-NAU	-3.17	1.35	1.41
7	B	2000	JWF	CAW-CLAC	3.16	1.81	1.74
7	A	2000	JWF	CAP-NBF	2.95	1.51	1.46
7	A	2000	JWF	CAQ-NBF	2.90	1.51	1.46
7	B	2000	JWF	CAX-NAU	-2.86	1.35	1.41
7	A	2000	JWF	CBD-NBG	-2.70	1.34	1.41
6	A	1770	NAG	C3-C2	2.64	1.58	1.52
7	A	2000	JWF	CBC-NAT	2.48	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2000	JWF	CBC-NAT	2.48	1.35	1.31
6	A	1768	NAG	C2-N2	2.27	1.50	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1770	NAG	O5-C1-C2	-9.25	96.69	111.29
7	A	2000	JWF	NAR-CBB-NAS	-9.08	107.20	114.72
6	B	1773	NAG	C1-O5-C5	9.02	124.41	112.19
6	A	1770	NAG	C2-N2-C7	8.46	134.96	122.90
7	B	2000	JWF	NAR-CBB-NAS	-7.99	108.09	114.72
6	A	1768	NAG	C2-N2-C7	6.50	132.16	122.90
6	A	1769	NAG	C1-O5-C5	6.26	120.68	112.19
7	B	2000	JWF	CAO-NBE-CAN	5.93	117.81	109.52
6	A	1770	NAG	C1-O5-C5	5.60	119.78	112.19
6	A	1768	NAG	O5-C5-C6	5.51	115.84	107.20
6	A	1767	NAG	O5-C5-C6	5.15	115.27	107.20
7	B	2000	JWF	OAB-CBD-CAM	-4.85	113.30	125.72
7	B	2000	JWF	CAM-CBD-NBG	4.77	120.00	111.83
7	B	2000	JWF	OAB-CBD-NBG	4.54	126.69	119.76
6	A	1770	NAG	O7-C7-C8	-4.50	113.70	122.06
6	B	1773	NAG	O5-C1-C2	-4.01	104.96	111.29
6	A	1767	NAG	C3-C4-C5	-3.90	103.28	110.24
7	A	2000	JWF	CAM-CBD-NBG	3.89	118.49	111.83
6	A	1770	NAG	O7-C7-N2	3.74	128.82	121.95
6	A	1770	NAG	O3-C3-C2	3.69	117.11	109.47
6	A	1770	NAG	C1-C2-N2	3.41	116.31	110.49
6	A	1767	NAG	O4-C4-C5	3.35	117.62	109.30
6	B	1773	NAG	O5-C5-C6	3.30	112.38	107.20
7	A	2000	JWF	CAZ-NBG-NAT	3.20	119.10	113.53
7	A	2000	JWF	OAB-CBD-CAM	-3.15	117.66	125.72
7	A	2000	JWF	CBC-CBA-NAU	3.00	121.03	115.97
7	A	2000	JWF	CAK-CAE-CAW	2.99	122.39	119.24
7	A	2000	JWF	CAP-CAN-NBE	-2.96	107.46	110.80
6	A	1767	NAG	C2-N2-C7	2.96	127.11	122.90
7	B	2000	JWF	CAP-CAN-NBE	-2.93	107.50	110.80
6	A	1768	NAG	C4-C3-C2	-2.87	106.81	111.02
6	A	1767	NAG	O3-C3-C2	2.82	115.31	109.47
7	B	2000	JWF	CBC-CBA-NAU	2.80	120.70	115.97
6	A	1768	NAG	O7-C7-C8	-2.77	116.90	122.06
7	B	2000	JWF	CAH-CAY-NBF	2.73	125.14	121.38
7	B	2000	JWF	CAM-CBA-CBC	-2.72	116.79	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2000	JWF	CAQ-NBF-CAY	2.72	125.44	118.09
7	A	2000	JWF	OAB-CBD-NBG	2.68	123.85	119.76
6	B	1773	NAG	C3-C4-C5	-2.61	105.58	110.24
6	A	1767	NAG	O5-C1-C2	-2.58	107.22	111.29
7	B	2000	JWF	CBC-CBB-NAS	2.55	130.87	123.28
6	A	1768	NAG	O5-C1-C2	2.54	115.30	111.29
6	A	1769	NAG	O7-C7-C8	-2.53	117.36	122.06
7	A	2000	JWF	CAQ-NBF-CAP	2.52	117.07	111.52
7	A	2000	JWF	CBC-CBB-NAS	2.51	130.74	123.28
6	A	1769	NAG	C2-N2-C7	2.51	126.47	122.90
7	A	2000	JWF	CAO-NBE-CAN	2.42	112.91	109.52
7	B	2000	JWF	CAD-CAW-CLAC	2.41	123.12	119.35
7	A	2000	JWF	CAX-NAU-CBA	-2.39	121.80	127.86
7	A	2000	JWF	CAJ-CAZ-NBG	2.39	123.46	119.73
6	A	1769	NAG	O7-C7-N2	2.33	126.23	121.95
7	A	2000	JWF	CAM-CBA-CBC	-2.32	117.24	119.86
6	A	1767	NAG	C4-C3-C2	-2.24	107.74	111.02
7	A	2000	JWF	CAM-CBA-NAU	-2.22	121.71	125.96
7	B	2000	JWF	CAE-CAW-CAD	-2.20	118.39	121.24
7	A	2000	JWF	CBB-NAS-NAV	2.19	110.11	104.86
7	B	2000	JWF	CAI-CAY-NBF	-2.17	118.39	121.38
6	A	1770	NAG	C6-C5-C4	2.15	118.03	113.00
6	A	1768	NAG	O3-C3-C2	2.14	113.90	109.47
6	A	1770	NAG	O4-C4-C5	2.08	114.46	109.30
7	A	2000	JWF	CAA-NBE-CAO	-2.06	107.58	110.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1768	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1767	NAG	C3-C2-N2-C7
6	A	1768	NAG	C3-C2-N2-C7
6	A	1770	NAG	C3-C2-N2-C7
6	B	1773	NAG	O5-C5-C6-O6
6	B	1773	NAG	C4-C5-C6-O6
6	A	1769	NAG	O5-C5-C6-O6
6	A	1767	NAG	O5-C5-C6-O6
6	A	1769	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1767	NAG	C4-C5-C6-O6
6	A	1770	NAG	C1-C2-N2-C7
6	B	1772	NAG	C4-C5-C6-O6
6	A	1768	NAG	C1-C2-N2-C7
6	B	1772	NAG	O5-C5-C6-O6
7	B	2000	JWF	CAF-CAX-NAU-CBA
7	B	2000	JWF	CAG-CAX-NAU-CBA
7	A	2000	JWF	CAG-CAX-NAU-CBA
7	A	2000	JWF	CAF-CAX-NAU-CBA

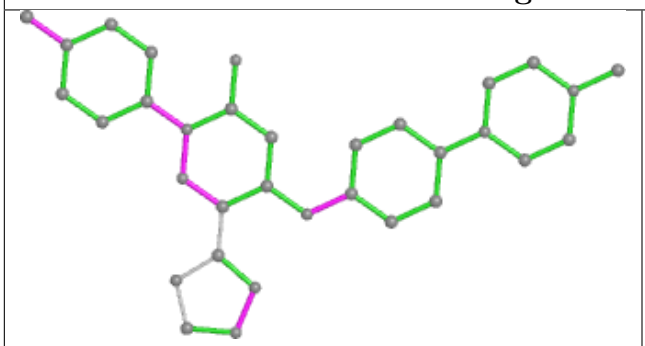
There are no ring outliers.

4 monomers are involved in 13 short contacts:

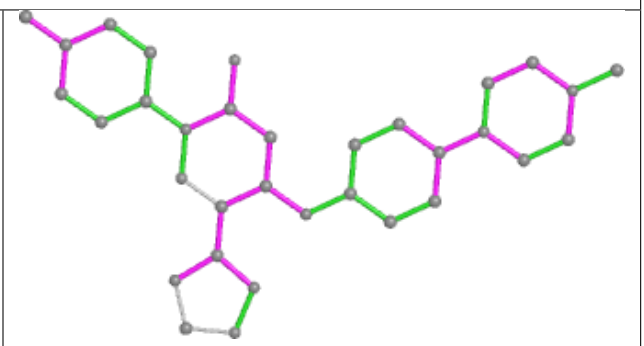
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1772	NAG	4	0
7	B	2000	JWF	3	0
6	A	1768	NAG	1	0
7	A	2000	JWF	5	0

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 then 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.

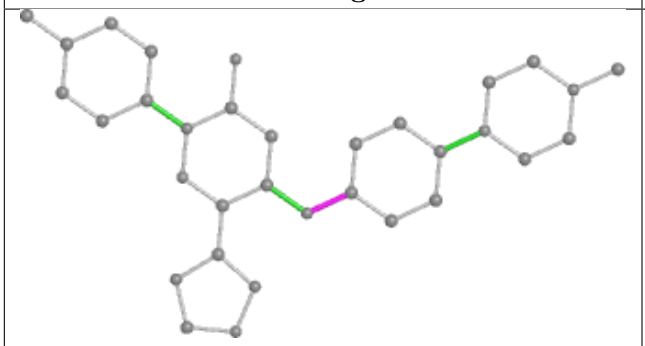
Ligand JWF B 2000



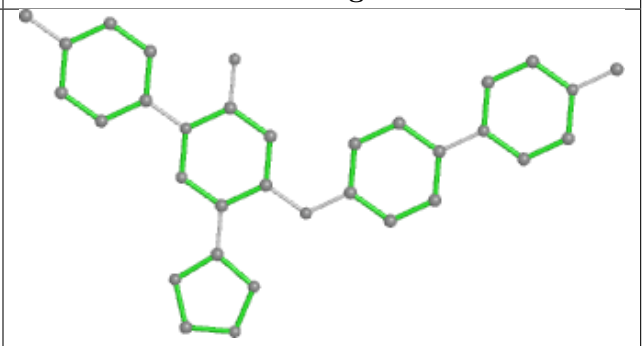
Bond lengths



Bond angles

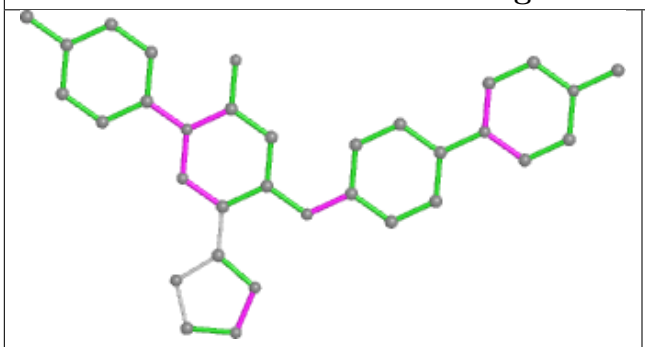


Torsions

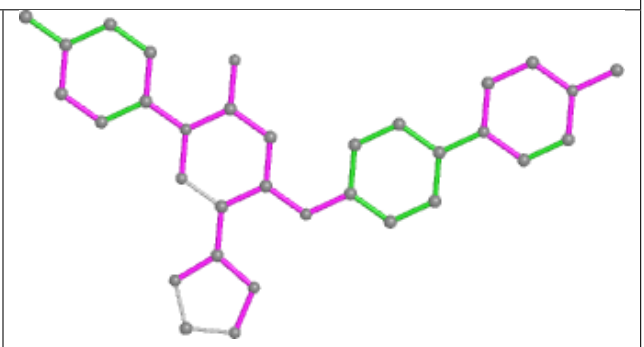


Rings

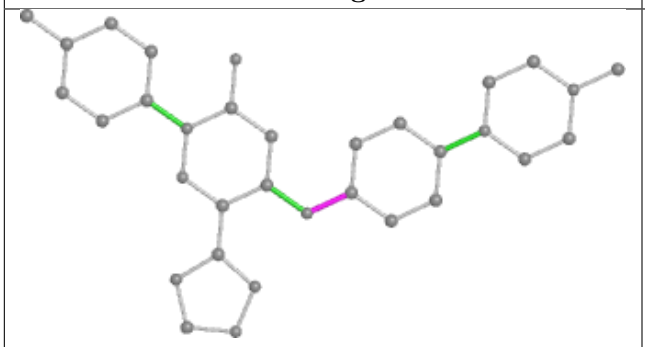
Ligand JWF A 2000



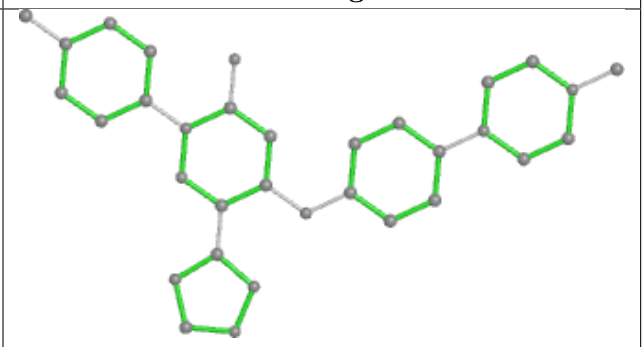
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	710/737 (96%)	-0.26	3 (0%)	92	84	58, 83, 112, 163	0
1	B	706/737 (95%)	-0.16	7 (0%)	82	67	63, 84, 115, 180	0
All	All	1416/1474 (96%)	-0.21	10 (0%)	87	75	58, 83, 115, 180	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	746	ALA	4.0
1	B	744	GLN	3.9
1	B	745	ALA	3.9
1	A	203	HIS	3.4
1	A	763	ASN	3.2
1	A	746	ALA	3.0
1	B	748	CYS	2.8
1	B	731	ALA	2.6
1	B	747	ALA	2.5
1	B	698	GLY	2.5

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPQ	A	471	14/15	0.94	0.24	68,74,80,80	0
1	TPQ	B	471	14/15	0.97	0.31	68,76,90,94	0

6.3 Carbohydrates (i)

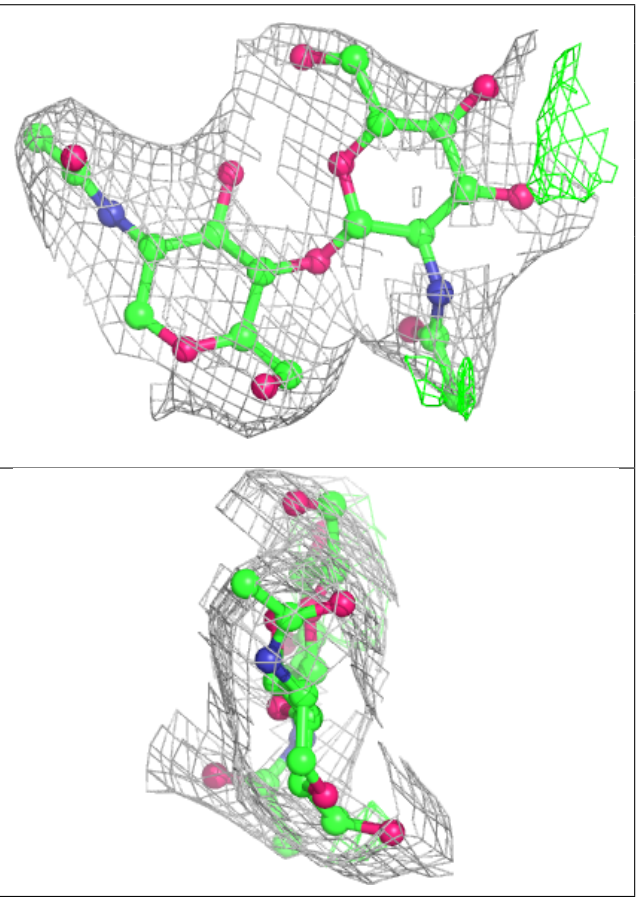
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	D	5	11/12	0.56	0.36	89,129,154,162	0
3	BMA	D	3	11/12	0.80	0.30	113,133,158,163	0
3	MAN	D	4	11/12	0.81	0.49	87,119,138,139	0
2	NAG	C	2	14/15	0.85	0.24	101,123,145,157	0
3	NAG	D	1	14/15	0.90	0.16	74,82,91,94	0
2	NAG	E	2	14/15	0.90	0.23	106,130,141,143	0
3	NAG	D	2	14/15	0.94	0.17	100,110,119,123	0
2	NAG	E	1	14/15	0.94	0.14	97,105,126,137	0
2	NAG	C	1	14/15	0.96	0.17	78,83,93,101	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.

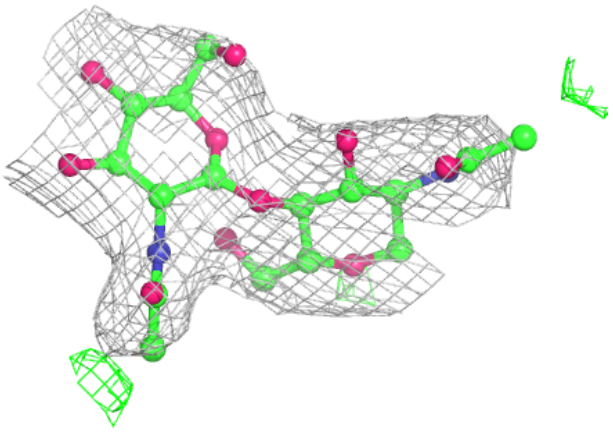
Electron density around Chain C:

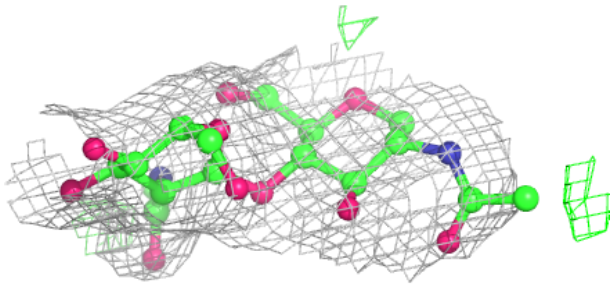
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

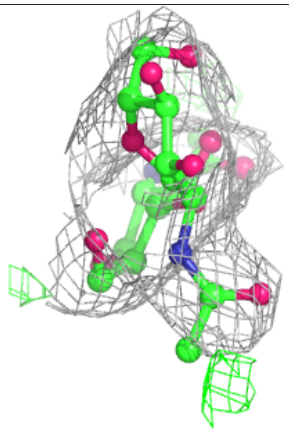


Electron density around Chain E:

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

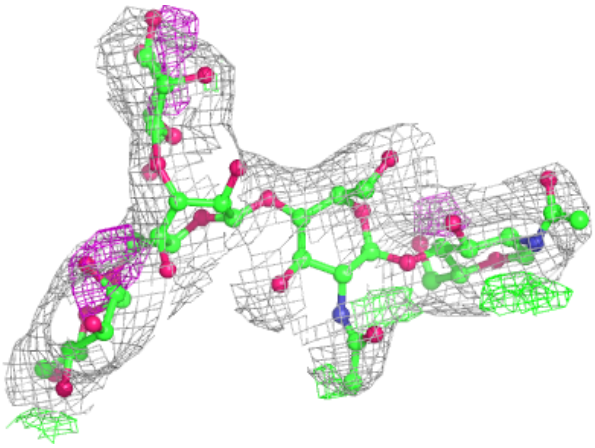


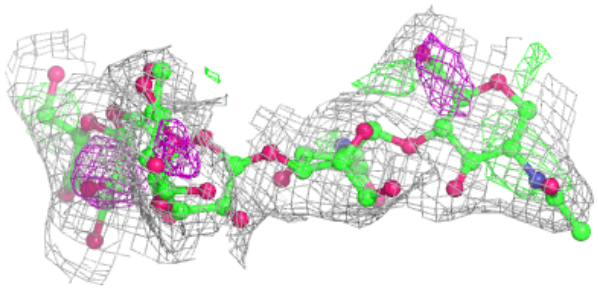


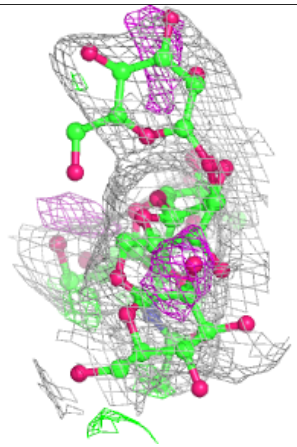


Electron density around Chain D:

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







6.4 Ligands (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
6	NAG	A	1770	14/15	0.54	0.61	114,149,166,170	0
6	NAG	A	1769	14/15	0.63	0.56	127,148,167,183	0
6	NAG	B	1772	14/15	0.64	0.21	98,134,157,157	0
6	NAG	A	1768	14/15	0.67	0.28	121,169,177,179	0
6	NAG	B	1773	14/15	0.76	0.46	118,149,156,156	0
5	CA	A	1764	1/1	0.77	0.13	94,94,94,94	0
6	NAG	A	1767	14/15	0.87	0.20	93,104,130,130	0
4	CU	A	1762	1/1	0.89	0.20	85,85,85,85	0
4	CU	B	1762	1/1	0.90	0.24	74,74,74,74	0
7	JWF	B	2000	33/33	0.91	0.21	71,78,101,108	0
5	CA	B	1764	1/1	0.93	0.11	81,81,81,81	0
5	CA	B	1763	1/1	0.95	0.05	72,72,72,72	0

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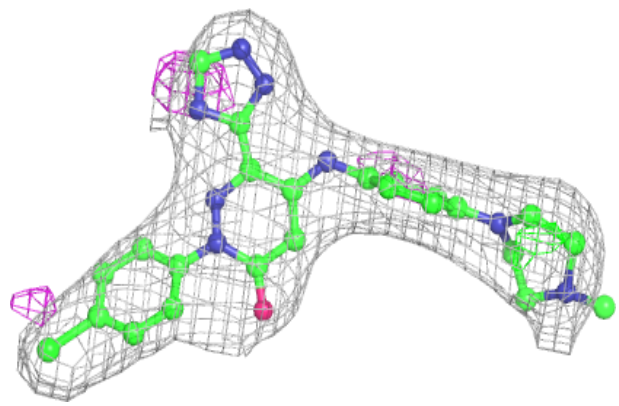
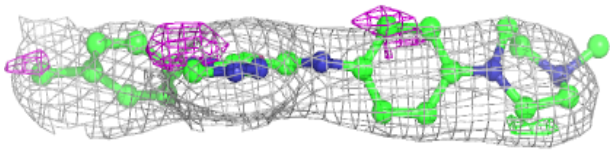
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	JWF	A	2000	33/33	0.96	0.18	71,90,120,127	0
5	CA	A	1763	1/1	0.96	0.05	71,71,71,71	0

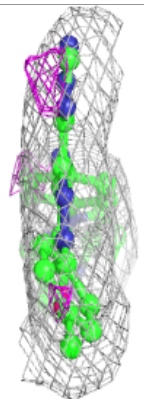
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JWF B 2000:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

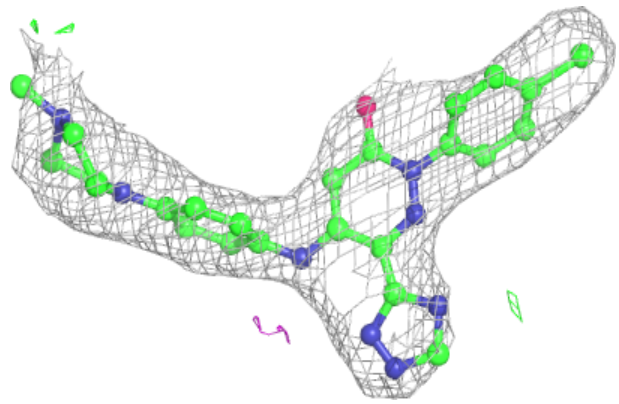


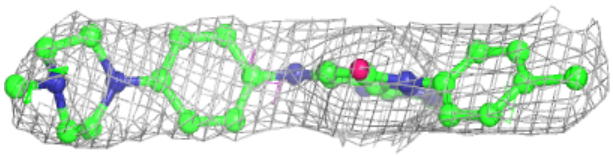


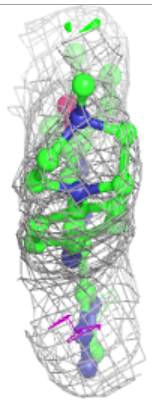


Electron density around JWF A 2000:

$2mF_o$-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.