Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:27 AM EDT

PDB ID	:	3FU9
Title	:	Melanocarpus albomyces laccase crystal soaked (20 min) with 2,6-dimethoxyphenol
Authors	:	Kallio, J.P.; Hakulinen, N.; Rouvinen, J.
Deposited on	:	2009-01-14
Resolution	:	2.00 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:

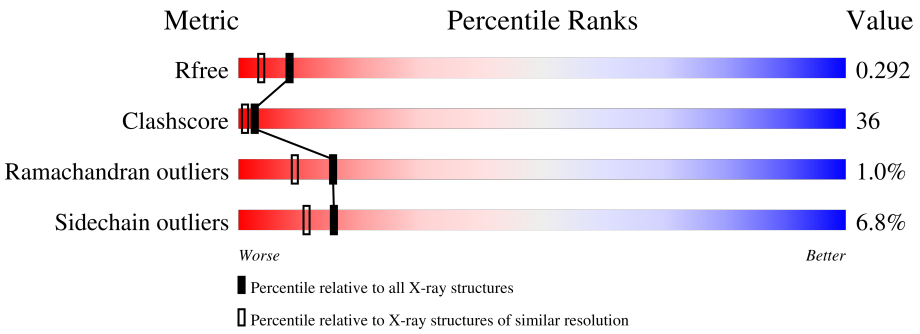
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Mol	Chain	Length	Quality of chain
1	A	559	52% 40% 7% •
1	B	559	48% 42% 9% •
2	C	2	100%
2	D	2	50% 50%
2	E	2	100%
2	F	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	610	-	-	X	-
7	KIB	B	2001	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9692 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 Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4369	2764	759	831	15	0	0	0
1	B	559	4369	2764	759	831	15	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	D	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0

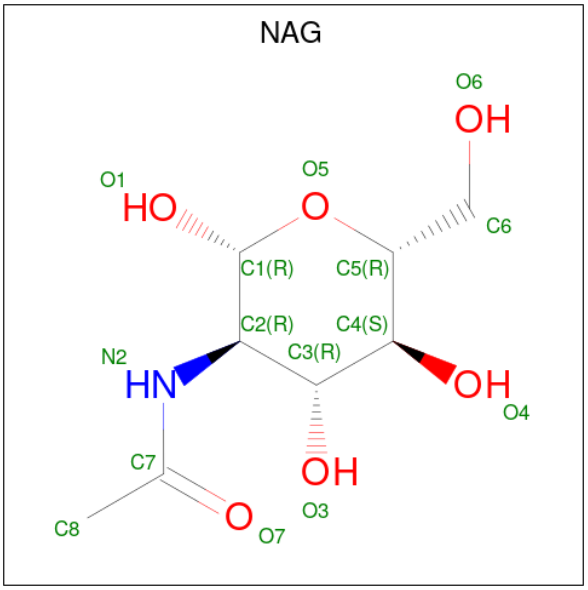
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

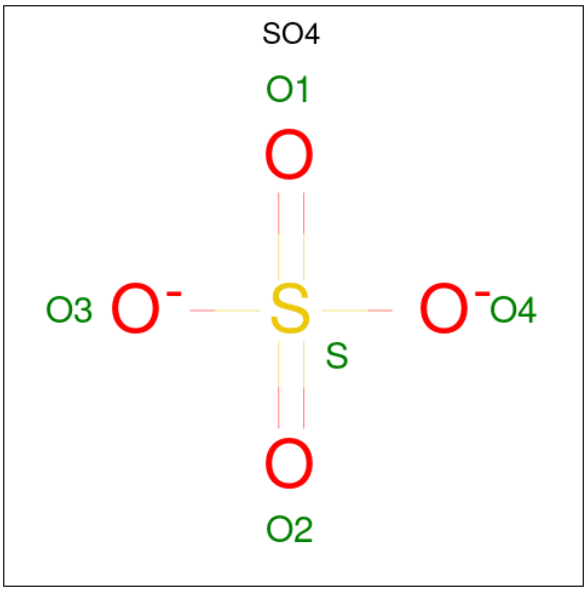
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	B	1	1	1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



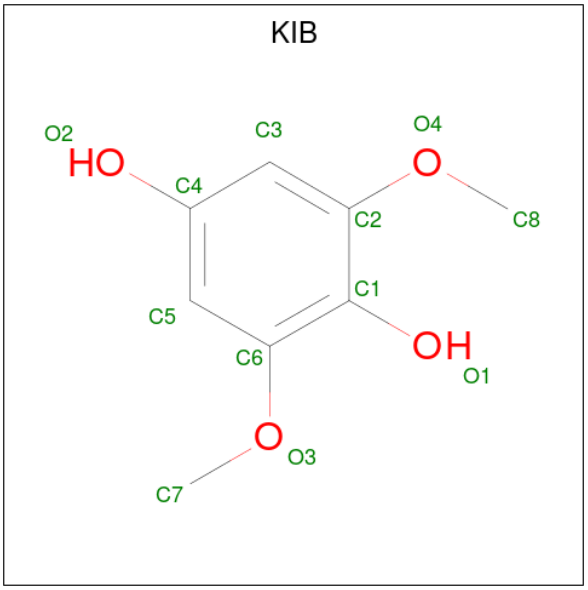
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is 2,6-dimethoxybenzene-1,4-diol (three-letter code: KIB) (formula: $C_8H_{10}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	12	8	4	0	0
			Total	C	O		
7	B	1	12	8	4	0	0

- Molecule 8 is water.

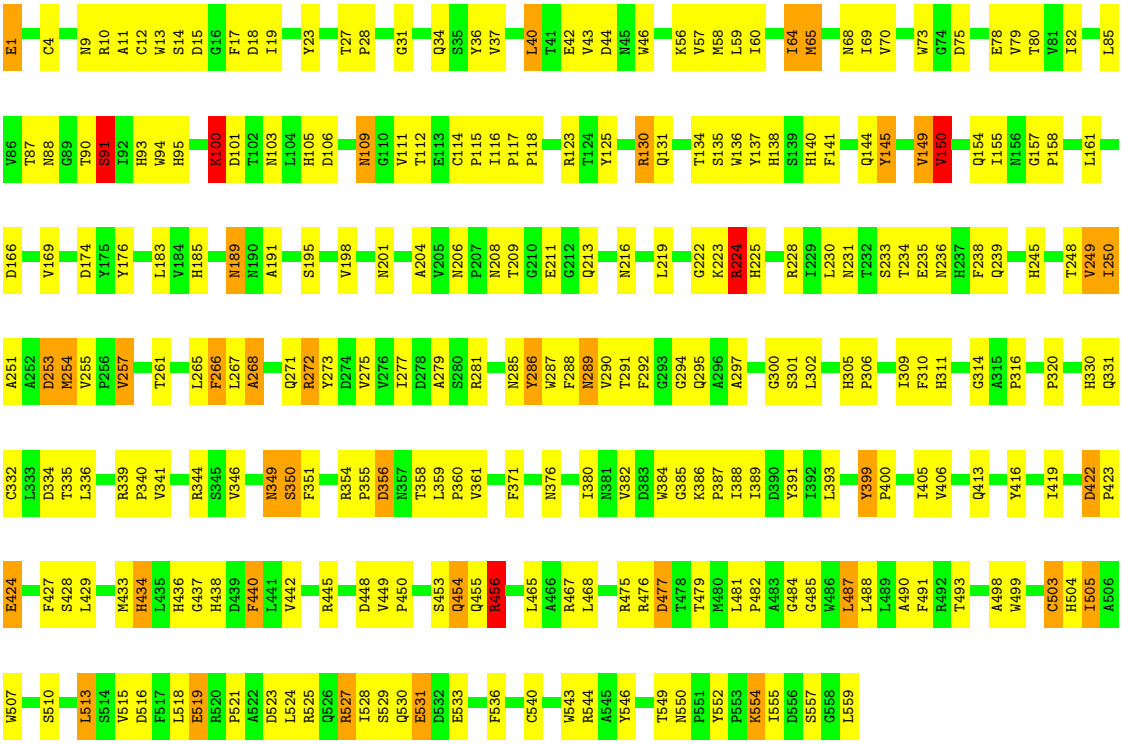
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	336	336	336	0	0
			Total	O		
8	B	364	364	364	0	0

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. 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. 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.

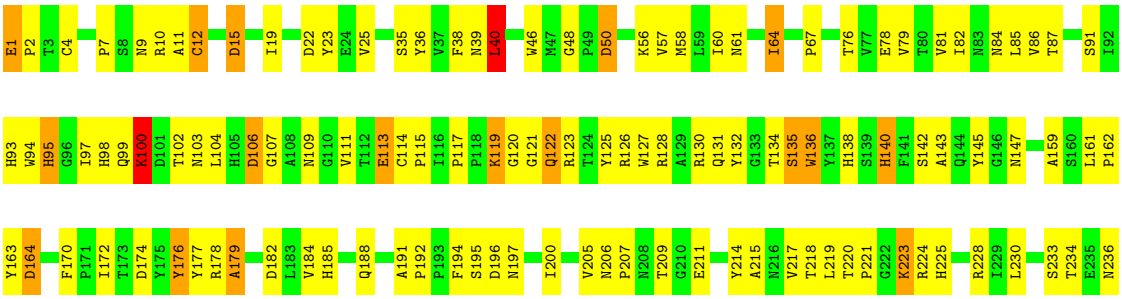
- Molecule 1: Laccase-1

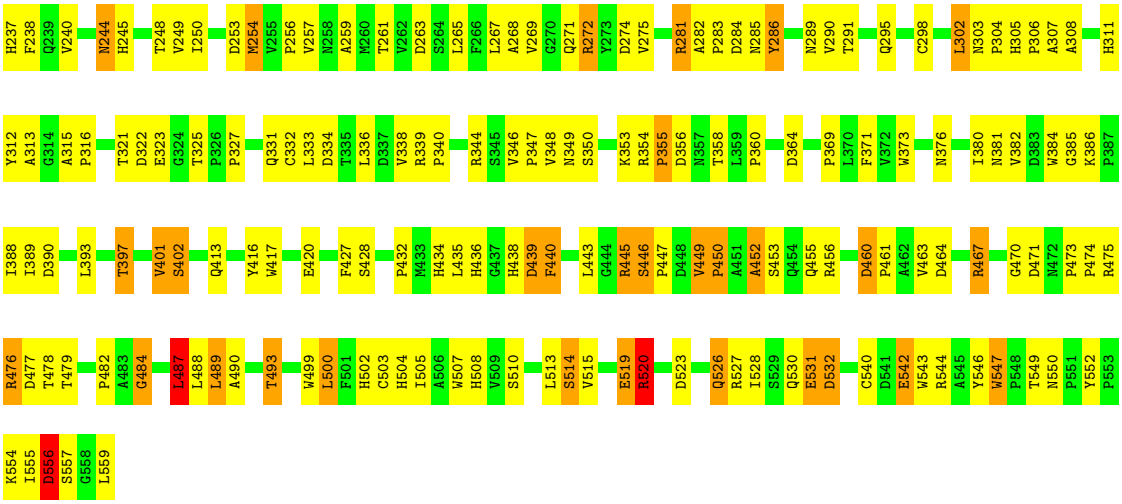
Chain A:



- Molecule 1: Laccase-1

Chain B:





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

Chain C: 100%

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

Chain D: 50% 50%

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

Chain E: 100%

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

Chain F: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.12Å 60.23Å 117.13Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	19.61 – 2.00 19.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.61-2.00) 96.4 (19.06-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.330 0.291 , 0.292	Depositor DCC
R_{free} test set	4595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	10.1	Xtriage
Anisotropy	1.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: CU, KIB, SO4, CL, NAG

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	1.44	29/4506 (0.6%)	1.26	22/6191 (0.4%)
1	B	1.40	20/4506 (0.4%)	1.33	37/6191 (0.6%)
All	All	1.42	49/9012 (0.5%)	1.30	59/12382 (0.5%)

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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	TYR	CD2-CE2	11.69	1.56	1.39
1	B	286	TYR	CD1-CE1	9.74	1.53	1.39
1	B	286	TYR	CD2-CE2	8.73	1.52	1.39
1	A	531	GLU	CG-CD	8.67	1.65	1.51
1	A	255	VAL	CB-CG2	8.35	1.70	1.52
1	A	503	CYS	CB-SG	-8.08	1.68	1.82
1	A	150	VAL	CB-CG2	7.15	1.67	1.52
1	A	154	GLN	C-O	-7.14	1.09	1.23
1	A	286	TYR	CD1-CE1	6.99	1.49	1.39
1	A	233	SER	CB-OG	6.76	1.51	1.42
1	B	257	VAL	CB-CG1	6.55	1.66	1.52
1	A	361	VAL	CA-CB	6.43	1.68	1.54
1	A	1	GLU	CG-CD	6.33	1.61	1.51
1	B	113	GLU	CG-CD	6.32	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	VAL	CB-CG1	6.16	1.65	1.52
1	B	519	GLU	CG-CD	6.06	1.61	1.51
1	A	145	TYR	CD1-CE1	6.04	1.48	1.39
1	A	356	ASP	CB-CG	6.03	1.64	1.51
1	A	257	VAL	CB-CG2	-5.98	1.40	1.52
1	B	531	GLU	CB-CG	5.94	1.63	1.52
1	B	452	ALA	CA-CB	5.86	1.64	1.52
1	A	250	ILE	CB-CG2	5.83	1.71	1.52
1	A	249	VAL	CB-CG1	5.75	1.65	1.52
1	B	445	ARG	CZ-NH2	5.70	1.40	1.33
1	A	399	TYR	CD2-CE2	5.68	1.47	1.39
1	A	266	PHE	CE1-CZ	5.64	1.48	1.37
1	A	136	TRP	CB-CG	5.63	1.60	1.50
1	B	499	TRP	CB-CG	5.61	1.60	1.50
1	A	288	PHE	CE2-CZ	5.51	1.47	1.37
1	A	505	ILE	C-O	5.50	1.33	1.23
1	A	78	GLU	CB-CG	5.47	1.62	1.52
1	B	446	SER	CB-OG	-5.43	1.35	1.42
1	A	339	ARG	CG-CD	5.40	1.65	1.51
1	B	136	TRP	CB-CG	5.38	1.59	1.50
1	A	519	GLU	CG-CD	5.30	1.59	1.51
1	A	191	ALA	CA-CB	5.28	1.63	1.52
1	B	257	VAL	CB-CG2	-5.26	1.41	1.52
1	A	440	PHE	CE2-CZ	5.26	1.47	1.37
1	B	179	ALA	CA-CB	5.25	1.63	1.52
1	B	531	GLU	CG-CD	5.24	1.59	1.51
1	B	542	GLU	CD-OE2	5.17	1.31	1.25
1	A	513	LEU	C-O	5.12	1.33	1.23
1	B	449	VAL	CB-CG2	5.10	1.63	1.52
1	A	482	PRO	C-O	5.09	1.33	1.23
1	B	176	TYR	CD2-CE2	-5.08	1.31	1.39
1	B	275	VAL	CA-CB	5.04	1.65	1.54
1	A	289	ASN	CG-ND2	5.03	1.45	1.32
1	B	547	TRP	CB-CG	-5.02	1.41	1.50
1	B	358	THR	CA-CB	5.01	1.66	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	40	LEU	CA-CB-CG	10.27	138.93	115.30
1	B	130	ARG	NE-CZ-NH1	9.37	124.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	520	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	554	LYS	CD-CE-NZ	-8.64	91.82	111.70
1	B	489	LEU	CA-CB-CG	7.78	133.19	115.30
1	A	527	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	439	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	520	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	75	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	B	350	SER	N-CA-C	7.01	129.93	111.00
1	A	101	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	A	467	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	10	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	467	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	B	50	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	B	500	LEU	CA-CB-CG	6.54	130.35	115.30
1	B	50	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	302	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	B	446	SER	C-N-CD	6.38	141.79	128.40
1	B	532	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	161	LEU	CB-CG-CD1	6.23	121.58	111.00
1	B	467	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	460	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	166	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	155	ILE	N-CA-C	-5.85	95.22	111.00
1	B	334	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	253	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	284	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	130	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	128	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	488	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	B	119	LYS	CD-CE-NZ	5.75	124.92	111.70
1	A	448	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	44	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	257	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	A	350	SER	N-CA-C	5.66	126.28	111.00
1	B	284	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	525	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	40	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	B	556	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	164	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	344	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	476	ARG	CA-CB-CG	5.43	125.34	113.40
1	A	70	VAL	N-CA-C	-5.40	96.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	364	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	106	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	249	VAL	CB-CA-C	-5.33	101.28	111.40
1	A	64	ILE	CG1-CB-CG2	5.30	123.06	111.40
1	B	298	CYS	CA-CB-SG	-5.27	104.51	114.00
1	A	253	ASP	CB-CA-C	5.27	120.93	110.40
1	B	120	GLY	N-CA-C	5.26	126.24	113.10
1	B	40	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	556	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	487	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	198	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	B	487	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	224	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	456	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLY	Peptide
1	B	514	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	4369	0	4114	252	0
1	B	4369	0	4114	365	1
2	C	28	0	24	5	0
2	D	28	0	24	3	0
2	E	28	0	25	8	0
2	F	28	0	25	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	3	0
4	B	1	0	0	0	0
5	A	42	0	39	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	56	0	52	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	12	0	8	1	0
7	B	12	0	8	7	0
8	A	336	0	0	108	0
8	B	364	0	0	182	0
All	All	9692	0	8433	630	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 36.

All (630) 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:261:THR:HG22	8:B:812:HOH:O	1.28	1.28
1:B:211:GLU:HB2	8:B:727:HOH:O	1.26	1.28
1:B:143:ALA:HA	8:B:868:HOH:O	1.29	1.27
1:B:230:LEU:HB3	8:B:907:HOH:O	1.34	1.27
1:A:510:SER:HB2	8:A:626:HOH:O	1.29	1.25
1:B:505:ILE:HD13	8:B:684:HOH:O	1.37	1.23
1:B:369:PRO:HB3	8:B:708:HOH:O	1.36	1.23
1:A:12:CYS:HB3	8:A:628:HOH:O	1.10	1.22
1:A:528:ILE:HD12	8:A:890:HOH:O	1.36	1.22
1:B:478:THR:HG22	8:B:916:HOH:O	1.36	1.21
1:B:134:THR:HG22	8:B:636:HOH:O	1.05	1.20
1:B:97:ILE:HD13	8:B:917:HOH:O	1.41	1.18
1:B:388:ILE:HG23	8:B:641:HOH:O	1.46	1.15
1:B:449:VAL:HG21	8:B:932:HOH:O	1.46	1.14
1:B:214:TYR:HA	8:B:723:HOH:O	1.44	1.13
1:B:140:HIS:CE1	8:B:623:HOH:O	1.99	1.12
1:B:217:VAL:HA	8:B:744:HOH:O	1.48	1.11
1:B:23:TYR:HB3	8:B:627:HOH:O	1.50	1.10
1:A:485:GLY:HA3	8:A:876:HOH:O	1.49	1.09
1:A:388:ILE:HD13	1:A:405:ILE:HD11	1.20	1.09
1:A:9:ASN:ND2	1:A:12:CYS:SG	2.25	1.07
1:B:447:PRO:HG2	8:B:656:HOH:O	1.55	1.06
1:B:440:PHE:HE1	8:B:668:HOH:O	1.35	1.05
1:A:64:ILE:HG13	8:A:667:HOH:O	1.55	1.04
1:B:178:ARG:HH21	1:B:182:ASP:HB3	1.23	1.03
1:B:463:VAL:HG23	8:B:650:HOH:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HA	8:B:833:HOH:O	1.58	1.03
1:A:285:ASN:OD1	1:A:311:HIS:HD2	1.41	1.02
1:B:38:PHE:CE1	1:B:67:PRO:HG2	1.94	1.01
1:B:178:ARG:NH2	1:B:182:ASP:HB3	1.76	1.00
1:B:322:ASP:HA	8:B:631:HOH:O	1.62	1.00
1:A:433:MET:HB2	8:A:895:HOH:O	1.62	1.00
1:A:271:GLN:HG2	1:A:476:ARG:NH2	1.77	0.99
1:B:57:VAL:HG22	8:B:634:HOH:O	1.62	0.99
1:A:382:VAL:HG13	8:A:690:HOH:O	1.63	0.98
1:B:172:ILE:HG13	8:B:643:HOH:O	1.63	0.97
1:B:417:TRP:HD1	8:B:895:HOH:O	1.48	0.97
1:A:141:PHE:CD1	8:A:642:HOH:O	2.19	0.96
1:B:46:TRP:HB2	8:B:634:HOH:O	1.66	0.96
1:A:115:PRO:HD2	8:A:792:HOH:O	1.64	0.96
1:A:309:ILE:HD12	5:A:720:NAG:H81	1.45	0.95
1:B:50:ASP:HB2	8:B:783:HOH:O	1.62	0.95
1:A:388:ILE:CD1	1:A:405:ILE:HD11	1.96	0.95
1:A:301:SER:HB3	8:A:597:HOH:O	1.66	0.94
1:B:19:ILE:HG13	8:B:911:HOH:O	1.65	0.94
1:B:308:ALA:HB2	8:B:923:HOH:O	1.67	0.94
1:B:82:ILE:HG12	1:B:122:GLN:HB2	1.48	0.93
8:A:696:HOH:O	1:B:191:ALA:HB3	1.69	0.92
1:B:140:HIS:ND1	8:B:623:HOH:O	1.96	0.92
1:B:461:PRO:HG3	8:B:652:HOH:O	1.69	0.92
1:A:510:SER:CB	8:A:626:HOH:O	1.96	0.92
1:B:46:TRP:CB	8:B:634:HOH:O	2.18	0.91
1:B:295:GLN:OE1	1:B:452:ALA:HB3	1.68	0.91
1:A:498:ALA:HB2	8:A:818:HOH:O	1.70	0.91
7:B:2001:KIB:H7	8:B:566:HOH:O	1.68	0.91
1:B:107:GLY:HA2	1:B:113:GLU:OE1	1.71	0.90
1:A:388:ILE:HD13	1:A:405:ILE:CD1	2.02	0.90
1:A:358:THR:O	5:A:740:NAG:H82	1.73	0.89
1:A:491:PHE:HB2	8:A:641:HOH:O	1.71	0.89
1:B:460:ASP:HB3	1:B:463:VAL:CG1	2.02	0.89
1:B:261:THR:CG2	8:B:812:HOH:O	1.95	0.87
1:A:438:HIS:NE2	1:A:519:GLU:OE1	2.06	0.87
1:B:428:SER:HB3	1:B:484:GLY:H	1.35	0.87
1:B:540:CYS:HB3	8:B:831:HOH:O	1.74	0.87
1:B:413:GLN:HG2	8:B:909:HOH:O	1.74	0.86
1:A:429:LEU:HD23	8:A:783:HOH:O	1.74	0.86
1:A:43:VAL:HB	1:A:57:VAL:HG23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HG	8:B:820:HOH:O	1.75	0.86
1:B:265:LEU:HB2	8:B:918:HOH:O	1.76	0.86
1:B:38:PHE:HE1	1:B:67:PRO:HG2	1.40	0.86
1:A:314:GLY:HA3	8:A:891:HOH:O	1.76	0.85
1:B:256:PRO:HB3	8:B:584:HOH:O	1.75	0.85
1:A:523:ASP:HA	8:A:902:HOH:O	1.75	0.85
1:B:381:ASN:OD1	1:B:554:LYS:NZ	2.10	0.85
1:A:273:TYR:CZ	8:A:791:HOH:O	2.28	0.84
1:B:267:LEU:HD11	8:B:918:HOH:O	1.77	0.84
1:B:347:PRO:HD3	8:B:897:HOH:O	1.76	0.84
1:B:295:GLN:HG2	8:B:611:HOH:O	1.78	0.84
1:B:228:ARG:HG2	1:B:274:ASP:OD2	1.78	0.84
1:B:61:ASN:HB3	8:B:884:HOH:O	1.79	0.83
1:B:455:GLN:HG2	8:B:766:HOH:O	1.77	0.83
1:A:518:LEU:HG	1:A:521:PRO:HG3	1.58	0.83
1:B:115:PRO:HA	8:B:747:HOH:O	1.78	0.83
1:B:145:TYR:CE2	8:B:599:HOH:O	2.31	0.83
1:A:271:GLN:HG2	1:A:476:ARG:HH21	1.40	0.83
1:B:479:THR:HB	8:B:668:HOH:O	1.79	0.82
1:B:244:ASN:ND2	1:B:281:ARG:HH12	1.78	0.82
1:A:285:ASN:OD1	1:A:311:HIS:CD2	2.31	0.82
1:B:206:ASN:HA	8:B:783:HOH:O	1.78	0.82
1:B:540:CYS:CB	8:B:831:HOH:O	2.28	0.82
1:A:95:HIS:O	1:A:135:SER:HB3	1.80	0.82
1:B:91:SER:HB3	8:B:747:HOH:O	1.79	0.81
7:B:2001:KIB:H7	8:B:819:HOH:O	1.79	0.81
1:B:523:ASP:HA	1:B:526:GLN:HE22	1.43	0.81
1:B:549:THR:HA	8:B:803:HOH:O	1.80	0.81
1:A:201:ASN:ND2	8:A:768:HOH:O	2.13	0.81
1:B:520:ARG:HH21	1:B:523:ASP:CG	1.85	0.80
1:A:306:PRO:CG	8:A:597:HOH:O	2.29	0.80
1:A:302:LEU:HD11	8:B:766:HOH:O	1.81	0.80
1:A:429:LEU:CD2	8:A:783:HOH:O	2.29	0.80
1:B:401:VAL:HG23	1:B:402:SER:H	1.47	0.80
1:A:438:HIS:HA	8:A:621:HOH:O	1.81	0.79
1:B:271:GLN:NE2	1:B:476:ARG:CZ	2.46	0.79
1:A:9:ASN:OD1	1:A:12:CYS:SG	2.41	0.79
1:A:189:ASN:ND2	8:A:632:HOH:O	2.13	0.79
1:B:114:CYS:SG	8:B:831:HOH:O	2.40	0.79
1:B:170:PHE:O	8:B:643:HOH:O	2.01	0.78
1:B:306:PRO:HG3	8:B:591:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:HB3	8:A:792:HOH:O	1.83	0.78
1:A:484:GLY:HA2	8:A:662:HOH:O	1.82	0.78
1:A:36:TYR:HB2	1:A:79:VAL:HG22	1.65	0.78
1:B:380:ILE:HG13	1:B:402:SER:O	1.83	0.78
1:A:456:ARG:HD2	8:A:742:HOH:O	1.83	0.78
1:B:440:PHE:CE1	8:B:668:HOH:O	2.17	0.78
1:B:95:HIS:CD2	1:B:272:ARG:HH12	2.02	0.77
1:B:267:LEU:CD1	8:B:918:HOH:O	2.32	0.77
1:B:95:HIS:O	1:B:135:SER:HB2	1.84	0.77
1:B:40:LEU:HD22	1:B:60:ILE:HG12	1.66	0.77
1:B:36:TYR:HB2	1:B:79:VAL:HG22	1.65	0.76
1:A:453:SER:HB2	8:A:653:HOH:O	1.84	0.76
1:B:479:THR:HG22	8:B:588:HOH:O	1.83	0.76
1:B:1:GLU:HG3	1:B:2:PRO:HD2	1.68	0.76
1:A:9:ASN:CG	1:A:12:CYS:SG	2.63	0.76
1:B:540:CYS:SG	8:B:831:HOH:O	2.44	0.76
1:B:476:ARG:HG3	8:B:668:HOH:O	1.85	0.75
1:B:290:VAL:HG23	8:B:772:HOH:O	1.87	0.75
1:B:303:ASN:O	8:B:664:HOH:O	2.03	0.75
1:A:249:VAL:HA	1:A:275:VAL:HG12	1.69	0.75
1:B:393:LEU:HD21	1:B:528:ILE:HD13	1.69	0.75
1:A:423:PRO:HA	8:A:662:HOH:O	1.85	0.75
1:A:65:MET:HB3	1:A:150:VAL:O	1.87	0.74
1:B:138:HIS:HE1	8:B:617:HOH:O	1.69	0.74
1:B:200:ILE:HD12	8:B:923:HOH:O	1.87	0.74
1:B:373:TRP:HZ3	8:B:586:HOH:O	1.70	0.74
1:A:505:ILE:HG23	8:A:665:HOH:O	1.86	0.73
1:B:4:CYS:HG	1:B:12:CYS:HG	1.31	0.73
1:B:393:LEU:HD21	1:B:528:ILE:CD1	2.18	0.73
1:A:118:PRO:HG3	1:A:546:TYR:CZ	2.22	0.73
1:B:447:PRO:HD2	8:B:869:HOH:O	1.88	0.73
1:B:138:HIS:CE1	8:B:617:HOH:O	2.42	0.73
1:A:109:ASN:HB2	1:A:115:PRO:HD3	1.71	0.72
1:B:447:PRO:CD	8:B:869:HOH:O	2.35	0.72
1:A:95:HIS:CD2	1:A:272:ARG:HH12	2.08	0.72
1:B:428:SER:CB	1:B:484:GLY:H	2.01	0.72
1:B:439:ASP:HB2	8:B:880:HOH:O	1.89	0.72
1:A:106:ASP:HB3	1:A:112:THR:HG21	1.69	0.72
8:B:937:HOH:O	2:E:1:NAG:H82	1.88	0.71
1:B:113:GLU:OE1	8:B:858:HOH:O	2.06	0.71
1:A:56:LYS:HE3	2:C:1:NAG:O6	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:THR:O	8:A:895:HOH:O	2.09	0.71
1:A:219:LEU:HD21	1:A:310:PHE:HD2	1.55	0.71
1:B:142:SER:OG	1:B:556:ASP:OD1	2.06	0.71
1:A:95:HIS:CD2	1:A:272:ARG:NH1	2.59	0.71
1:A:31:GLY:CA	8:A:901:HOH:O	2.40	0.70
1:A:115:PRO:CD	8:A:792:HOH:O	2.28	0.70
1:B:200:ILE:CD1	8:B:772:HOH:O	2.40	0.70
1:A:302:LEU:HD21	8:B:766:HOH:O	1.90	0.70
1:B:546:TYR:OH	1:B:550:ASN:ND2	2.25	0.70
1:A:42:GLU:OE1	8:A:615:HOH:O	2.08	0.70
1:B:446:SER:HB2	8:B:869:HOH:O	1.91	0.69
1:A:43:VAL:HB	1:A:57:VAL:CG2	2.21	0.69
1:A:176:TYR:CE2	1:A:195:SER:HA	2.26	0.69
1:B:50:ASP:CB	8:B:783:HOH:O	2.29	0.69
1:B:172:ILE:CG1	8:B:643:HOH:O	2.31	0.69
1:B:306:PRO:CG	8:B:591:HOH:O	2.39	0.69
1:B:285:ASN:OD1	1:B:311:HIS:HD2	1.76	0.68
1:B:520:ARG:NH2	1:B:523:ASP:OD2	2.17	0.68
1:B:244:ASN:O	1:B:281:ARG:NH1	2.24	0.68
1:A:131:GLN:HG2	1:A:254:MET:SD	2.33	0.68
1:A:297:ALA:HB1	8:A:783:HOH:O	1.93	0.68
1:A:445:ARG:HD3	8:A:666:HOH:O	1.93	0.68
1:B:436:HIS:O	8:B:717:HOH:O	2.12	0.68
1:B:554:LYS:NZ	1:B:557:SER:O	2.27	0.68
1:B:254:MET:SD	8:B:917:HOH:O	2.51	0.67
1:B:460:ASP:HB3	1:B:463:VAL:HG12	1.75	0.67
1:B:97:ILE:HA	8:B:917:HOH:O	1.93	0.67
7:B:2001:KIB:C7	7:B:2001:KIB:O1	2.43	0.67
1:B:380:ILE:HD12	8:B:689:HOH:O	1.93	0.67
1:A:23:TYR:O	8:A:620:HOH:O	2.11	0.67
1:A:224:ARG:HG3	8:A:588:HOH:O	1.94	0.67
1:B:515:VAL:C	8:B:689:HOH:O	2.31	0.67
1:B:291:THR:HG21	8:B:762:HOH:O	1.95	0.67
1:A:309:ILE:HD12	5:A:720:NAG:C8	2.22	0.67
1:A:389:ILE:CG2	1:A:389:ILE:O	2.43	0.67
1:A:389:ILE:O	1:A:389:ILE:HG22	1.95	0.67
1:A:306:PRO:HG3	8:A:597:HOH:O	1.89	0.66
1:B:307:ALA:HB2	2:F:1:NAG:H62	1.77	0.66
1:A:219:LEU:HD21	1:A:310:PHE:CD2	2.30	0.66
1:B:196:ASP:OD1	8:B:658:HOH:O	2.13	0.66
1:B:135:SER:N	8:B:636:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:610:CL:CL	8:A:715:HOH:O	2.51	0.65
1:A:37:VAL:CG1	1:A:82:ILE:HD12	2.26	0.65
1:A:311:HIS:CE1	5:A:720:NAG:O4	2.49	0.65
1:A:301:SER:CB	8:A:597:HOH:O	2.35	0.65
1:B:438:HIS:N	8:B:717:HOH:O	2.18	0.65
1:B:117:PRO:HG2	1:B:542:GLU:HB2	1.78	0.65
1:B:200:ILE:HD11	8:B:772:HOH:O	1.96	0.65
1:B:520:ARG:O	1:B:523:ASP:HB2	1.95	0.65
1:B:107:GLY:CA	1:B:113:GLU:OE1	2.45	0.65
1:A:236:ASN:HB3	1:A:238:PHE:CE1	2.31	0.65
1:B:240:VAL:HG22	8:B:918:HOH:O	1.96	0.64
1:A:543:TRP:CD1	8:A:792:HOH:O	2.49	0.64
1:A:468:LEU:HD13	1:A:488:LEU:CD2	2.27	0.64
1:B:420:GLU:OE2	8:B:633:HOH:O	2.15	0.64
1:A:13:TRP:HB2	1:A:158:PRO:HG3	1.78	0.64
1:B:371:PHE:CG	8:B:819:HOH:O	2.50	0.64
1:A:31:GLY:HA3	8:A:901:HOH:O	1.97	0.64
1:A:222:GLY:N	1:A:279:ALA:O	2.31	0.64
1:A:349:ASN:O	1:A:351:PHE:N	2.25	0.64
1:A:559:LEU:CD1	8:A:690:HOH:O	2.45	0.64
1:A:235:GLU:HB2	8:A:665:HOH:O	1.98	0.64
1:A:289:ASN:HB2	8:A:785:HOH:O	1.97	0.63
1:B:455:GLN:CD	8:B:932:HOH:O	2.35	0.63
1:B:178:ARG:NH2	1:B:182:ASP:CB	2.59	0.63
1:B:179:ALA:CB	2:E:2:NAG:H81	2.28	0.63
1:B:303:ASN:HB3	8:B:591:HOH:O	1.97	0.63
1:B:332:CYS:O	1:B:333:LEU:HD23	1.98	0.63
1:A:68:ASN:OD1	8:A:907:HOH:O	2.15	0.63
1:B:455:GLN:HB2	8:B:932:HOH:O	1.97	0.63
1:A:204:ALA:HB1	8:A:625:HOH:O	1.98	0.62
1:B:523:ASP:HA	1:B:526:GLN:NE2	2.12	0.62
7:B:2001:KIB:O1	7:B:2001:KIB:H7B	1.99	0.62
1:B:347:PRO:HA	8:B:930:HOH:O	1.98	0.62
1:B:500:LEU:HD11	8:B:623:HOH:O	1.99	0.62
1:B:523:ASP:O	1:B:527:ARG:HD2	1.98	0.62
1:A:540:CYS:O	1:A:544:ARG:HG3	1.99	0.62
1:B:179:ALA:HB3	2:E:2:NAG:H81	1.82	0.62
1:B:382:VAL:HG13	1:B:559:LEU:HD11	1.81	0.62
1:B:449:VAL:HG11	8:B:932:HOH:O	1.98	0.61
1:A:484:GLY:C	8:A:662:HOH:O	2.39	0.61
1:B:436:HIS:C	8:B:717:HOH:O	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CE1	8:A:791:HOH:O	2.49	0.61
1:B:131:GLN:HE21	1:B:254:MET:HB3	1.65	0.61
1:A:31:GLY:N	8:A:901:HOH:O	2.33	0.61
1:B:286:TYR:HA	8:B:630:HOH:O	1.99	0.61
1:B:455:GLN:CB	8:B:932:HOH:O	2.49	0.60
1:B:209:THR:OG1	1:B:211:GLU:OE2	2.17	0.60
1:B:327:PRO:HA	8:B:685:HOH:O	2.00	0.60
1:B:502:HIS:HB3	1:B:514:SER:OG	2.01	0.60
1:B:95:HIS:CD2	1:B:272:ARG:NH1	2.69	0.60
1:B:382:VAL:CG1	1:B:559:LEU:HD11	2.31	0.60
1:B:371:PHE:HB3	8:B:819:HOH:O	2.01	0.60
1:B:219:LEU:O	1:B:221:PRO:HD3	2.02	0.60
1:B:38:PHE:CE1	1:B:67:PRO:CG	2.80	0.59
1:B:307:ALA:CB	2:F:1:NAG:H62	2.32	0.59
1:B:323:GLU:O	2:F:1:NAG:H83	2.03	0.59
1:B:302:LEU:HD11	8:B:658:HOH:O	2.03	0.59
1:A:286:TYR:OH	8:A:811:HOH:O	2.16	0.59
8:A:721:HOH:O	2:C:2:NAG:H61	2.02	0.59
1:B:196:ASP:O	1:B:197:ASN:HB2	2.03	0.59
1:A:116:ILE:HG22	1:A:117:PRO:O	2.03	0.58
1:B:206:ASN:CA	8:B:783:HOH:O	2.44	0.58
1:B:432:PRO:O	1:B:503:CYS:HA	2.02	0.58
1:A:185:HIS:CD2	8:A:632:HOH:O	2.56	0.58
1:A:546:TYR:OH	1:A:550:ASN:ND2	2.36	0.58
1:B:176:TYR:CE2	1:B:195:SER:HA	2.39	0.58
1:A:231:ASN:HB3	1:A:268:ALA:O	2.03	0.58
1:B:417:TRP:CD1	8:B:895:HOH:O	2.34	0.58
1:B:447:PRO:CG	8:B:656:HOH:O	2.26	0.58
1:A:453:SER:OG	1:A:455:GLN:HG3	2.04	0.57
1:B:353:LYS:HD2	8:B:633:HOH:O	2.03	0.57
1:A:294:GLY:CA	1:A:331:GLN:HA	2.34	0.57
1:B:46:TRP:HH2	1:B:64:ILE:HD12	1.70	0.57
1:B:174:ASP:HB3	1:B:236:ASN:HB2	1.86	0.57
1:B:230:LEU:HD21	8:B:636:HOH:O	2.04	0.57
1:B:380:ILE:CD1	8:B:689:HOH:O	2.50	0.57
1:B:446:SER:CB	8:B:869:HOH:O	2.48	0.57
1:B:46:TRP:HB3	8:B:634:HOH:O	1.98	0.57
1:B:87:THR:HG21	1:B:552:TYR:HE2	1.70	0.57
1:A:436:HIS:HA	4:A:610:CL:CL	2.42	0.57
1:A:174:ASP:HB3	1:A:236:ASN:HB2	1.87	0.57
1:B:174:ASP:HB2	1:B:195:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TYR:CD1	1:B:416:TYR:N	2.73	0.57
1:A:141:PHE:HA	8:A:642:HOH:O	2.04	0.57
1:B:87:THR:HG21	1:B:552:TYR:CE2	2.39	0.57
8:A:653:HOH:O	1:B:194:PHE:CD2	2.52	0.56
1:A:60:ILE:HD11	1:A:149:VAL:HG13	1.88	0.56
1:A:216:ASN:CG	5:A:720:NAG:H82	2.24	0.56
1:A:479:THR:HG22	8:A:895:HOH:O	2.04	0.56
1:B:95:HIS:CD2	1:B:95:HIS:C	2.79	0.56
1:B:385:GLY:O	1:B:544:ARG:NH1	2.31	0.56
1:A:100:LYS:HG3	8:A:680:HOH:O	2.05	0.56
1:A:103:ASN:HB2	8:A:635:HOH:O	2.05	0.56
1:A:117:PRO:HG3	1:A:543:TRP:HA	1.88	0.56
1:A:42:GLU:OE2	1:A:56:LYS:NZ	2.33	0.55
1:B:184:VAL:O	1:B:188:GLN:HG3	2.05	0.55
1:B:220:THR:HB	1:B:223:LYS:HG3	1.88	0.55
1:B:249:VAL:HG21	1:B:265:LEU:HD21	1.88	0.55
1:B:360:PRO:HG2	1:B:376:ASN:HA	1.88	0.55
1:B:237:HIS:HE1	1:B:505:ILE:HD11	1.71	0.55
1:B:464:ASP:OD1	1:B:467:ARG:HD3	2.06	0.55
8:B:734:HOH:O	2:E:2:NAG:H61	2.06	0.55
1:A:555:ILE:HD11	8:A:571:HOH:O	2.06	0.55
1:B:145:TYR:CD2	8:B:599:HOH:O	2.57	0.55
1:A:90:THR:O	1:A:91:SER:HB3	2.07	0.55
1:B:302:LEU:CD1	8:B:658:HOH:O	2.55	0.55
1:B:373:TRP:CZ3	8:B:586:HOH:O	2.53	0.55
1:B:162:PRO:HG2	8:B:820:HOH:O	2.07	0.55
1:A:388:ILE:HD12	1:A:516:ASP:OD2	2.08	0.54
1:B:35:SER:HB3	8:B:764:HOH:O	2.07	0.54
1:A:34:GLN:HA	8:A:593:HOH:O	2.06	0.54
1:B:315:ALA:HB1	1:B:316:PRO:HD2	1.90	0.54
1:B:427:PHE:HA	1:B:456:ARG:HH22	1.73	0.54
1:B:100:LYS:HE3	8:B:576:HOH:O	2.07	0.54
1:A:27:THR:OG1	1:A:130:ARG:NH1	2.40	0.54
1:A:223:LYS:O	1:A:225:HIS:CE1	2.60	0.54
1:A:290:VAL:HB	1:A:306:PRO:HB2	1.89	0.54
1:A:306:PRO:HG2	8:A:597:HOH:O	2.00	0.54
1:B:348:VAL:HG21	1:B:470:GLY:H	1.72	0.54
1:A:422:ASP:N	1:A:423:PRO:CD	2.69	0.54
1:B:36:TYR:O	1:B:79:VAL:HA	2.08	0.54
8:B:560:HOH:O	2:E:1:NAG:H62	2.07	0.54
1:A:292:PHE:CE1	1:A:300:GLY:HA2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HD11	8:A:690:HOH:O	2.04	0.54
1:B:559:LEU:HD22	8:B:623:HOH:O	2.08	0.54
7:B:2001:KIB:C7	8:B:819:HOH:O	2.45	0.54
1:B:104:LEU:HD22	1:B:532:ASP:HB3	1.89	0.53
1:B:117:PRO:O	1:B:121:GLY:HA3	2.08	0.53
1:B:371:PHE:CB	8:B:819:HOH:O	2.55	0.53
1:A:384:TRP:NE1	8:A:642:HOH:O	2.39	0.53
1:B:64:ILE:HG13	1:B:64:ILE:O	2.08	0.53
1:A:311:HIS:NE2	1:A:316:PRO:O	2.40	0.53
1:A:413:GLN:NE2	8:A:806:HOH:O	2.39	0.53
1:B:354:ARG:CB	1:B:356:ASP:OD1	2.57	0.53
1:A:419:ILE:N	1:A:419:ILE:HD12	2.23	0.53
1:A:424:GLU:HB3	8:A:904:HOH:O	2.08	0.53
1:B:163:TYR:HA	1:B:224:ARG:HB2	1.91	0.53
1:A:302:LEU:CD1	8:B:766:HOH:O	2.47	0.53
1:B:217:VAL:HG13	8:B:744:HOH:O	2.09	0.53
1:B:104:LEU:CD2	1:B:528:ILE:HG23	2.39	0.52
1:B:82:ILE:CD1	1:B:122:GLN:NE2	2.72	0.52
1:B:263:ASP:HB2	8:B:805:HOH:O	2.09	0.52
1:B:520:ARG:NH2	1:B:523:ASP:CG	2.59	0.52
1:B:438:HIS:NE2	1:B:519:GLU:OE1	2.34	0.52
1:B:308:ALA:CA	8:B:923:HOH:O	2.58	0.52
1:A:19:ILE:HG13	1:A:341:VAL:HG11	1.92	0.52
1:B:87:THR:HG23	8:B:560:HOH:O	2.09	0.52
1:B:355:PRO:HB3	8:B:622:HOH:O	2.09	0.52
1:B:384:TRP:HH2	8:B:937:HOH:O	1.93	0.52
1:A:406:VAL:HB	8:A:888:HOH:O	2.10	0.52
1:B:39:ASN:OD1	1:B:84:ASN:ND2	2.39	0.52
1:A:344:ARG:NH2	8:A:605:HOH:O	2.42	0.51
1:B:450:PRO:HB2	1:B:453:SER:HB3	1.91	0.51
1:A:384:TRP:CZ2	8:A:642:HOH:O	2.62	0.51
1:B:249:VAL:CG2	1:B:265:LEU:HD21	2.41	0.51
1:B:487:LEU:HD21	8:B:588:HOH:O	2.09	0.51
1:A:423:PRO:CA	8:A:662:HOH:O	2.49	0.51
1:B:200:ILE:HD13	8:B:772:HOH:O	2.04	0.51
8:A:721:HOH:O	2:C:2:NAG:C6	2.58	0.51
1:B:321:THR:HG21	8:B:933:HOH:O	2.11	0.51
1:B:174:ASP:CG	1:B:233:SER:HB3	2.30	0.51
1:A:58:MET:HG2	1:A:85:LEU:HD22	1.92	0.51
1:B:104:LEU:HD22	1:B:528:ILE:HG23	1.93	0.51
1:B:493:THR:O	1:B:520:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:CD2	8:B:766:HOH:O	2.56	0.50
1:A:371:PHE:CD1	7:A:1001:KIB:C8	2.95	0.50
1:A:46:TRP:CE3	1:A:57:VAL:HG11	2.46	0.50
1:B:82:ILE:HD11	1:B:122:GLN:NE2	2.26	0.50
1:B:267:LEU:HD12	1:B:267:LEU:N	2.26	0.50
1:A:416:TYR:HD1	8:A:787:HOH:O	1.94	0.50
1:A:440:PHE:O	1:A:475:ARG:HA	2.12	0.50
1:B:346:VAL:O	8:B:698:HOH:O	2.19	0.50
1:B:393:LEU:HD21	1:B:528:ILE:HD12	1.93	0.50
1:B:23:TYR:CD2	1:B:23:TYR:N	2.78	0.50
1:B:552:TYR:OH	8:B:692:HOH:O	2.15	0.50
8:A:786:HOH:O	2:C:1:NAG:H61	2.11	0.50
1:B:271:GLN:HE21	1:B:476:ARG:NE	2.09	0.50
1:B:559:LEU:O	8:B:921:HOH:O	2.19	0.50
1:A:250:ILE:O	1:A:251:ALA:HB2	2.12	0.50
1:A:490:ALA:CB	8:A:852:HOH:O	2.60	0.50
1:B:99:GLN:HB3	1:B:102:THR:O	2.12	0.50
1:A:239:GLN:HG2	1:A:330:HIS:CD2	2.47	0.50
1:B:245:HIS:CE1	1:B:281:ARG:HG3	2.47	0.50
1:B:295:GLN:CD	8:B:769:HOH:O	2.49	0.50
1:B:46:TRP:CE3	1:B:57:VAL:HG11	2.47	0.50
1:B:98:HIS:NE2	1:B:131:GLN:OE1	2.45	0.50
1:A:141:PHE:CG	8:A:642:HOH:O	2.58	0.49
1:A:428:SER:CB	1:A:484:GLY:H	2.24	0.49
1:B:234:THR:O	1:B:505:ILE:HA	2.12	0.49
1:A:131:GLN:HB2	8:A:561:HOH:O	2.11	0.49
1:B:473:PRO:O	1:B:474:PRO:C	2.47	0.49
1:A:543:TRP:CG	8:A:792:HOH:O	2.65	0.49
1:A:169:VAL:HA	1:A:228:ARG:HB2	1.94	0.49
1:A:546:TYR:O	1:A:549:THR:OG1	2.26	0.49
1:B:95:HIS:O	1:B:135:SER:CB	2.58	0.49
1:B:331:GLN:O	1:B:332:CYS:HB2	2.11	0.49
1:B:122:GLN:CG	8:B:832:HOH:O	2.61	0.49
1:B:285:ASN:OD1	1:B:311:HIS:CD2	2.62	0.49
1:A:134:THR:HG21	1:A:228:ARG:HB3	1.94	0.49
1:B:355:PRO:CB	8:B:622:HOH:O	2.60	0.49
1:A:287:TRP:CE2	1:A:320:PRO:HB2	2.48	0.49
1:A:552:TYR:CD1	2:C:2:NAG:H62	2.48	0.49
1:A:64:ILE:CG2	8:A:821:HOH:O	2.61	0.49
1:B:209:THR:CB	1:B:211:GLU:OE2	2.61	0.49
1:A:454:GLN:HG2	8:B:660:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LEU:HG	8:B:717:HOH:O	2.13	0.49
1:B:237:HIS:NE2	1:B:432:PRO:HD3	2.28	0.48
1:B:530:GLN:N	1:B:531:GLU:OE1	2.46	0.48
1:A:427:PHE:HA	1:A:456:ARG:HH12	1.78	0.48
1:A:523:ASP:O	1:A:527:ARG:HG3	2.13	0.48
1:A:393:LEU:CD2	8:A:890:HOH:O	2.62	0.48
1:B:200:ILE:CD1	8:B:923:HOH:O	2.54	0.48
1:B:428:SER:HB3	1:B:484:GLY:N	2.16	0.48
1:B:467:ARG:NH2	8:B:900:HOH:O	2.34	0.48
1:B:544:ARG:NH1	8:B:831:HOH:O	2.46	0.48
1:B:103:ASN:HB2	8:B:748:HOH:O	2.12	0.48
1:A:103:ASN:N	8:A:635:HOH:O	2.46	0.48
1:B:447:PRO:CB	8:B:656:HOH:O	2.57	0.48
1:B:76:THR:CG2	1:B:126:ARG:HG3	2.43	0.48
1:A:484:GLY:CA	8:A:662:HOH:O	2.46	0.48
1:B:479:THR:CG2	8:B:588:HOH:O	2.54	0.48
1:B:543:TRP:CZ2	1:B:547:TRP:CE3	3.02	0.48
1:A:266:PHE:CE1	1:A:332:CYS:HA	2.49	0.48
1:A:331:GLN:OE1	1:A:450:PRO:HA	2.13	0.48
1:A:449:VAL:HB	1:A:455:GLN:NE2	2.29	0.48
1:A:434:HIS:CD2	1:A:504:HIS:HD2	2.32	0.47
1:A:529:SER:OG	1:A:531:GLU:HG2	2.14	0.47
1:B:97:ILE:CD1	8:B:917:HOH:O	2.23	0.47
1:B:174:ASP:OD1	1:B:233:SER:HB3	2.14	0.47
1:B:308:ALA:CB	8:B:923:HOH:O	2.40	0.47
1:A:530:GLN:HA	1:A:530:GLN:OE1	2.14	0.47
1:B:184:VAL:HG12	1:B:185:HIS:N	2.29	0.47
1:B:304:PRO:O	8:B:914:HOH:O	2.20	0.47
1:A:267:LEU:HG	1:A:273:TYR:HD2	1.79	0.47
1:A:384:TRP:CZ3	1:A:554:LYS:HD2	2.49	0.47
1:B:268:ALA:O	1:B:269:VAL:C	2.50	0.47
1:B:445:ARG:HD3	8:B:582:HOH:O	2.13	0.47
1:B:7:PRO:HB3	1:B:164:ASP:HA	1.95	0.47
1:B:336:LEU:HD22	1:B:474:PRO:HG2	1.96	0.47
1:B:476:ARG:CG	8:B:668:HOH:O	2.55	0.47
1:A:1:GLU:HG3	8:A:777:HOH:O	2.13	0.47
1:A:95:HIS:O	1:A:135:SER:CB	2.56	0.47
8:B:734:HOH:O	2:E:2:NAG:C6	2.63	0.47
1:A:245:HIS:CE1	1:A:281:ARG:HG3	2.49	0.47
1:A:336:LEU:HD21	1:A:442:VAL:HG11	1.96	0.47
1:B:381:ASN:O	1:B:402:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HB2	1:A:100:LYS:HE3	1.82	0.47
1:A:305:HIS:O	1:A:306:PRO:C	2.53	0.47
1:A:449:VAL:HG21	8:A:796:HOH:O	2.14	0.47
1:B:79:VAL:CG2	8:B:756:HOH:O	2.63	0.47
1:B:248:THR:CG2	1:B:259:ALA:HB1	2.44	0.47
1:B:354:ARG:HB3	1:B:356:ASP:OD1	2.14	0.47
1:B:449:VAL:CG2	8:B:932:HOH:O	2.28	0.47
1:A:4:CYS:SG	8:A:628:HOH:O	2.11	0.47
1:A:115:PRO:HG2	8:A:792:HOH:O	2.14	0.47
1:A:434:HIS:HD2	1:A:504:HIS:HD2	1.63	0.47
1:B:228:ARG:O	1:B:230:LEU:HD12	2.14	0.47
1:A:251:ALA:HA	1:A:257:VAL:HG22	1.95	0.47
1:B:22:ASP:HB3	1:B:25:VAL:HG22	1.96	0.47
1:B:111:VAL:HG21	1:B:500:LEU:HD21	1.97	0.47
1:A:64:ILE:HA	8:A:667:HOH:O	2.15	0.46
1:B:500:LEU:CD1	8:B:623:HOH:O	2.60	0.46
1:A:359:LEU:HD22	1:A:515:VAL:HG11	1.97	0.46
1:A:434:HIS:HE1	4:A:610:CL:CL	2.35	0.46
1:B:93:HIS:HA	1:B:106:ASP:O	2.15	0.46
1:B:306:PRO:O	8:B:624:HOH:O	2.20	0.46
1:B:104:LEU:CD2	1:B:532:ASP:HB3	2.45	0.46
1:B:58:MET:HG3	1:B:147:ASN:HB3	1.97	0.46
1:B:100:LYS:HA	1:B:100:LYS:HD3	1.52	0.46
1:A:434:HIS:HA	1:A:477:ASP:O	2.15	0.46
1:A:533:GLU:O	1:A:536:PHE:HB3	2.16	0.46
1:B:142:SER:HG	1:B:556:ASP:CG	2.14	0.46
1:A:354:ARG:NH1	1:A:356:ASP:OD1	2.49	0.46
1:B:91:SER:O	1:B:91:SER:OG	2.33	0.46
1:B:122:GLN:HG2	8:B:832:HOH:O	2.15	0.46
1:B:131:GLN:O	1:B:254:MET:CE	2.64	0.46
1:B:386:LYS:HE3	1:B:390:ASP:OD2	2.15	0.46
1:A:253:ASP:OD2	1:A:476:ARG:HB2	2.15	0.46
1:B:19:ILE:CG1	8:B:911:HOH:O	2.44	0.46
1:B:332:CYS:C	1:B:333:LEU:HD23	2.35	0.46
1:B:349:ASN:HB3	8:B:661:HOH:O	2.16	0.46
1:A:138:HIS:HB2	1:A:145:TYR:CB	2.46	0.46
1:B:91:SER:CB	8:B:747:HOH:O	2.52	0.46
1:B:315:ALA:HB1	1:B:316:PRO:CD	2.46	0.46
1:B:131:GLN:HB3	8:B:629:HOH:O	2.16	0.45
1:B:215:ALA:HB3	1:B:308:ALA:HB2	1.97	0.45
1:A:145:TYR:OH	1:A:234:THR:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:CG2	8:A:791:HOH:O	2.65	0.45
1:A:344:ARG:CZ	8:A:605:HOH:O	2.63	0.45
1:A:454:GLN:HB3	8:A:645:HOH:O	2.16	0.45
1:B:348:VAL:HG21	1:B:470:GLY:N	2.31	0.45
1:B:1:GLU:HG3	1:B:2:PRO:CD	2.42	0.45
1:A:138:HIS:HE1	8:A:568:HOH:O	1.99	0.45
1:A:468:LEU:CD1	1:A:488:LEU:CD2	2.94	0.45
1:B:23:TYR:CB	8:B:627:HOH:O	2.32	0.45
1:A:13:TRP:CE3	1:A:157:GLY:HA2	2.52	0.45
1:A:111:VAL:HG13	1:A:516:ASP:OD2	2.17	0.45
1:A:248:THR:HA	1:A:261:THR:HA	1.98	0.45
1:B:223:LYS:O	1:B:225:HIS:CE1	2.70	0.45
1:B:244:ASN:HD22	1:B:244:ASN:HA	1.59	0.45
1:A:271:GLN:CG	1:A:476:ARG:NH2	2.66	0.45
1:A:384:TRP:CE2	8:A:642:HOH:O	2.55	0.45
1:B:76:THR:HG21	1:B:126:ARG:HG3	1.98	0.45
1:A:118:PRO:CG	1:A:546:TYR:CE1	2.99	0.45
1:A:384:TRP:CE3	1:A:554:LYS:HD2	2.52	0.45
1:B:432:PRO:O	1:B:504:HIS:N	2.45	0.45
1:A:64:ILE:HG21	8:A:821:HOH:O	2.16	0.44
1:A:118:PRO:HG3	1:A:546:TYR:CE1	2.52	0.44
1:A:391:TYR:OH	1:A:400:PRO:HD3	2.17	0.44
1:B:122:GLN:NE2	8:B:832:HOH:O	2.50	0.44
1:B:132:TYR:CD1	1:B:132:TYR:N	2.85	0.44
1:B:215:ALA:HB3	1:B:308:ALA:CB	2.47	0.44
1:A:206:ASN:C	1:A:208:ASN:H	2.20	0.44
1:A:386:LYS:N	1:A:387:PRO:HD3	2.32	0.44
1:A:468:LEU:HD13	1:A:488:LEU:HD23	1.99	0.44
1:B:86:VAL:O	1:B:119:LYS:HE2	2.18	0.44
1:B:192:PRO:HD3	7:B:2001:KIB:C1	2.47	0.44
1:B:19:ILE:CD1	8:B:911:HOH:O	2.64	0.44
1:B:325:THR:HG23	8:B:859:HOH:O	2.17	0.44
1:A:94:TRP:O	8:A:782:HOH:O	2.21	0.44
1:B:136:TRP:CZ3	1:B:138:HIS:CD2	3.05	0.44
1:A:287:TRP:CH2	2:D:1:NAG:H62	2.52	0.44
1:A:427:PHE:HB3	8:A:696:HOH:O	2.17	0.44
1:B:111:VAL:HG21	1:B:500:LEU:CD2	2.48	0.44
1:B:440:PHE:O	1:B:475:ARG:HA	2.18	0.44
1:A:518:LEU:CG	1:A:521:PRO:HG3	2.41	0.44
1:B:136:TRP:CH2	1:B:138:HIS:CD2	3.06	0.44
1:B:209:THR:HG21	1:B:211:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TYR:CE2	1:B:196:ASP:HB3	2.53	0.44
1:B:182:ASP:OD1	8:B:841:HOH:O	2.21	0.44
1:B:333:LEU:CD2	8:B:835:HOH:O	2.66	0.43
1:B:443:LEU:HD11	1:B:490:ALA:HB2	1.99	0.43
1:B:482:PRO:HA	8:B:835:HOH:O	2.16	0.43
1:B:552:TYR:CD1	2:E:2:NAG:H62	2.52	0.43
1:A:287:TRP:CZ2	2:D:1:NAG:H62	2.53	0.43
1:B:230:LEU:HG	1:B:272:ARG:HG2	2.00	0.43
1:B:449:VAL:HB	1:B:455:GLN:NE2	2.33	0.43
1:A:490:ALA:HB1	8:A:852:HOH:O	2.18	0.43
1:A:292:PHE:CD1	1:A:300:GLY:HA2	2.53	0.43
1:A:427:PHE:CA	1:A:456:ARG:HH12	2.31	0.43
1:A:453:SER:CB	8:A:653:HOH:O	2.55	0.43
1:A:58:MET:HG2	1:A:85:LEU:CD2	2.47	0.43
1:B:15:ASP:HA	8:B:929:HOH:O	2.19	0.43
1:A:37:VAL:CG1	1:A:82:ILE:CD1	2.95	0.43
1:A:213:GLN:NE2	8:A:708:HOH:O	2.35	0.43
1:A:393:LEU:HD23	8:A:890:HOH:O	2.19	0.43
1:B:218:THR:CG2	1:B:313:ALA:HB2	2.48	0.43
1:B:253:ASP:OD2	1:B:476:ARG:HB2	2.19	0.43
1:B:389:ILE:O	1:B:393:LEU:HG	2.18	0.43
1:A:37:VAL:HG13	1:A:82:ILE:HD12	1.97	0.43
1:B:354:ARG:HB2	1:B:356:ASP:OD1	2.18	0.43
1:A:103:ASN:ND2	1:A:499:TRP:CZ3	2.82	0.43
1:A:479:THR:HG23	1:A:487:LEU:HD21	2.00	0.43
1:B:446:SER:OG	1:B:482:PRO:HG2	2.18	0.43
1:A:10:ARG:O	1:A:158:PRO:HA	2.19	0.43
1:B:440:PHE:CD1	1:B:489:LEU:HD22	2.53	0.43
1:B:339:ARG:HG3	8:B:706:HOH:O	2.17	0.42
1:B:531:GLU:OE1	1:B:531:GLU:N	2.48	0.42
1:A:105:HIS:ND1	1:A:125:TYR:HA	2.34	0.42
1:B:271:GLN:NE2	1:B:476:ARG:NE	2.65	0.42
1:B:446:SER:CA	8:B:869:HOH:O	2.67	0.42
1:A:11:ALA:O	1:A:158:PRO:HB3	2.20	0.42
1:A:36:TYR:O	1:A:79:VAL:HA	2.19	0.42
1:B:131:GLN:O	1:B:254:MET:HE2	2.18	0.42
1:B:244:ASN:ND2	1:B:281:ARG:NH1	2.58	0.42
1:A:93:HIS:O	1:A:137:TYR:HA	2.20	0.42
1:A:206:ASN:OD1	1:A:208:ASN:HB2	2.19	0.42
1:A:334:ASP:OD1	1:A:334:ASP:N	2.51	0.42
1:B:38:PHE:HE1	1:B:67:PRO:CG	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:O	1:B:215:ALA:HB2	2.18	0.42
1:A:385:GLY:N	8:A:853:HOH:O	2.52	0.42
1:B:48:GLY:HA3	8:B:567:HOH:O	2.19	0.42
1:B:434:HIS:HA	1:B:477:ASP:O	2.20	0.42
1:B:526:GLN:HE21	1:B:526:GLN:HB2	1.65	0.42
1:B:185:HIS:CD2	1:B:185:HIS:C	2.93	0.42
1:B:197:ASN:ND2	8:B:783:HOH:O	2.48	0.42
1:B:244:ASN:OD1	8:B:826:HOH:O	2.22	0.42
1:B:283:PRO:HA	1:B:312:TYR:CD2	2.54	0.42
1:B:295:GLN:CG	8:B:611:HOH:O	2.48	0.42
1:B:311:HIS:NE2	1:B:316:PRO:O	2.53	0.42
1:B:353:LYS:CD	8:B:633:HOH:O	2.65	0.42
1:A:95:HIS:HD2	1:A:272:ARG:HH12	1.61	0.42
8:A:653:HOH:O	1:B:194:PHE:HD2	1.95	0.42
1:A:100:LYS:CG	8:A:680:HOH:O	2.68	0.42
1:A:380:ILE:HG23	1:A:557:SER:HB2	2.01	0.42
1:B:11:ALA:HB2	8:B:777:HOH:O	2.20	0.42
1:B:456:ARG:CG	8:B:881:HOH:O	2.67	0.42
1:B:461:PRO:HG2	8:B:824:HOH:O	2.20	0.41
1:A:46:TRP:CG	1:A:57:VAL:HG21	2.55	0.41
1:A:360:PRO:HG2	1:A:376:ASN:HA	2.02	0.41
1:B:233:SER:O	1:B:269:VAL:HG13	2.20	0.41
1:B:508:HIS:NE2	7:B:2001:KIB:H7B	2.36	0.41
1:A:340:PRO:HG2	8:A:631:HOH:O	2.19	0.41
1:A:346:VAL:HG21	8:A:852:HOH:O	2.21	0.41
1:B:56:LYS:HE3	2:E:1:NAG:O6	2.20	0.41
1:B:104:LEU:HD21	1:B:528:ILE:CG2	2.50	0.41
1:B:135:SER:HB2	1:B:136:TRP:H	1.68	0.41
1:A:36:TYR:CB	1:A:79:VAL:HG22	2.43	0.41
1:A:423:PRO:HG3	8:A:765:HOH:O	2.20	0.41
1:B:471:ASP:OD2	8:B:872:HOH:O	2.20	0.41
1:B:289:ASN:OD1	2:F:1:NAG:H82	2.20	0.41
1:A:12:CYS:CB	8:A:628:HOH:O	1.97	0.41
1:B:81:VAL:HG21	1:B:125:TYR:HE1	1.85	0.41
1:A:87:THR:O	1:A:550:ASN:ND2	2.53	0.41
1:B:305:HIS:O	1:B:306:PRO:C	2.59	0.41
1:A:428:SER:OG	1:A:484:GLY:N	2.44	0.41
1:B:197:ASN:ND2	1:B:205:VAL:O	2.51	0.41
1:A:36:TYR:CE1	1:A:69:ILE:HG23	2.56	0.41
1:A:454:GLN:NE2	8:A:884:HOH:O	2.53	0.41
1:A:481:LEU:HA	1:A:487:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ILE:CA	8:B:917:HOH:O	2.60	0.41
1:B:99:GLN:OE1	1:B:127:TRP:HB3	2.21	0.41
1:B:237:HIS:CD2	1:B:268:ALA:CB	3.03	0.41
1:B:282:ALA:HA	1:B:283:PRO:HD3	1.77	0.41
1:B:401:VAL:HG23	1:B:402:SER:N	2.26	0.41
1:B:505:ILE:CD1	8:B:684:HOH:O	2.22	0.41
1:B:555:ILE:HD13	8:B:608:HOH:O	2.20	0.41
1:A:14:SER:OG	1:A:17:PHE:HB2	2.21	0.41
1:A:291:THR:HG23	8:A:596:HOH:O	2.21	0.41
1:A:521:PRO:HA	1:A:524:LEU:HD23	2.03	0.41
1:B:94:TRP:CD1	1:B:94:TRP:N	2.86	0.41
1:B:401:VAL:CG2	1:B:402:SER:H	2.22	0.41
1:B:460:ASP:HA	1:B:461:PRO:HD2	1.88	0.41
1:A:28:PRO:HD3	1:A:73:TRP:CE2	2.56	0.40
1:B:78:GLU:HA	1:B:125:TYR:O	2.21	0.40
1:B:94:TRP:O	1:B:97:ILE:HB	2.21	0.40
1:B:159:ALA:HB1	1:B:250:ILE:HD12	2.03	0.40
1:B:397:THR:O	1:B:397:THR:OG1	2.34	0.40
1:A:176:TYR:CB	1:A:183:LEU:HD11	2.52	0.40
1:B:207:PRO:HG3	1:B:303:ASN:HA	2.04	0.40
1:A:521:PRO:O	1:A:524:LEU:HB3	2.21	0.40
1:B:131:GLN:NE2	1:B:254:MET:HB3	2.35	0.40
1:A:206:ASN:HB3	1:A:209:THR:OG1	2.21	0.40
1:A:265:LEU:CD2	8:A:791:HOH:O	2.70	0.40
1:B:479:THR:HG21	1:B:489:LEU:HD21	2.03	0.40
1:A:18:ASP:HB2	1:A:19:ILE:H	1.67	0.40
1:A:287:TRP:CE2	2:D:1:NAG:H5	2.57	0.40
1:A:399:TYR:CZ	1:A:518:LEU:CD2	3.04	0.40
1:A:555:ILE:HG12	8:A:867:HOH:O	2.21	0.40
1:B:236:ASN:HB3	1:B:238:PHE:CE1	2.55	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:78:GLU:OE2	5:A:700:NAG:O7[3_545]	2.04	0.16

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	557/559 (100%)	504 (90%)	47 (8%)	6 (1%)	14 8
1	B	557/559 (100%)	502 (90%)	50 (9%)	5 (1%)	17 11
All	All	1114/1118 (100%)	1006 (90%)	97 (9%)	11 (1%)	15 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	SER
1	B	402	SER
1	A	91	SER
1	A	493	THR
1	B	15	ASP
1	B	100	LYS
1	B	484	GLY
1	A	268	ALA
1	B	401	VAL
1	A	100	LYS
1	A	149	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	478/478 (100%)	444 (93%)	34 (7%)	14 10
1	B	478/478 (100%)	447 (94%)	31 (6%)	17 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	956/956 (100%)	891 (93%)	65 (7%)	16 11

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	40	LEU
1	A	59	LEU
1	A	65	MET
1	A	80	THR
1	A	88	ASN
1	A	91	SER
1	A	100	LYS
1	A	109	ASN
1	A	123	ARG
1	A	140	HIS
1	A	144	GLN
1	A	150	VAL
1	A	189	ASN
1	A	211	GLU
1	A	224	ARG
1	A	230	LEU
1	A	254	MET
1	A	272	ARG
1	A	277	ILE
1	A	295	GLN
1	A	349	ASN
1	A	355	PRO
1	A	422	ASP
1	A	424	GLU
1	A	434	HIS
1	A	454	GLN
1	A	456	ARG
1	A	465	LEU
1	A	477	ASP
1	A	487	LEU
1	A	503	CYS
1	A	507	TRP
1	A	513	LEU
1	B	1	GLU
1	B	9	ASN
1	B	12	CYS

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Mol	Chain	Res	Type
1	B	40	LEU
1	B	64	ILE
1	B	95	HIS
1	B	100	LYS
1	B	109	ASN
1	B	122	GLN
1	B	123	ARG
1	B	135	SER
1	B	140	HIS
1	B	223	LYS
1	B	244	ASN
1	B	254	MET
1	B	272	ARG
1	B	281	ARG
1	B	338	VAL
1	B	340	PRO
1	B	355	PRO
1	B	397	THR
1	B	440	PHE
1	B	450	PRO
1	B	487	LEU
1	B	493	THR
1	B	507	TRP
1	B	510	SER
1	B	513	LEU
1	B	520	ARG
1	B	526	GLN
1	B	556	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	95	HIS
1	A	122	GLN
1	A	154	GLN
1	A	156	ASN
1	A	185	HIS
1	A	236	ASN
1	A	295	GLN
1	A	311	HIS
1	A	349	ASN

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Mol	Chain	Res	Type
1	B	63	ASN
1	B	122	GLN
1	B	131	GLN
1	B	185	HIS
1	B	244	ASN
1	B	271	GLN
1	B	311	HIS
1	B	455	GLN
1	B	526	GLN
1	B	550	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	1.23	1 (7%)	17,19,21	3.08	5 (29%)
2	NAG	C	2	2	14,14,15	0.98	1 (7%)	17,19,21	2.17	5 (29%)
2	NAG	D	1	1,2	14,14,15	1.41	2 (14%)	17,19,21	3.74	10 (58%)
2	NAG	D	2	2	14,14,15	1.65	5 (35%)	17,19,21	2.75	7 (41%)
2	NAG	E	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	2.37	7 (41%)
2	NAG	E	2	2	14,14,15	0.88	0	17,19,21	1.35	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.71	3 (21%)	17,19,21	4.75	13 (76%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	F	2	2	14,14,15	1.53	2 (14%)	17,19,21	3.91	12 (70%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	6/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C5	-4.05	1.35	1.43
2	D	1	NAG	C2-N2	3.92	1.52	1.46
2	F	2	NAG	O5-C5	-3.55	1.36	1.43
2	D	2	NAG	C1-C2	-3.36	1.47	1.52
2	F	1	NAG	C3-C2	-3.11	1.46	1.52
2	F	2	NAG	O5-C1	-3.07	1.38	1.43
2	D	1	NAG	O5-C1	-2.83	1.38	1.43
2	F	1	NAG	O5-C1	-2.77	1.39	1.43
2	D	2	NAG	C2-N2	-2.60	1.42	1.46
2	E	1	NAG	C1-C2	2.55	1.55	1.52
2	C	1	NAG	C1-C2	2.45	1.55	1.52
2	D	2	NAG	O5-C1	-2.44	1.39	1.43
2	D	2	NAG	O7-C7	2.24	1.28	1.23
2	D	2	NAG	O5-C5	-2.14	1.39	1.43
2	C	2	NAG	O3-C3	-2.02	1.38	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C1-O5-C5	11.20	127.20	112.19
2	D	1	NAG	C1-C2-N2	9.73	125.77	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	C1-O5-C5	-9.42	99.56	112.19
2	C	1	NAG	C1-O5-C5	9.29	124.64	112.19
2	F	1	NAG	C2-N2-C7	7.87	133.44	122.90
2	F	1	NAG	O4-C4-C3	-7.67	92.31	110.38
2	F	2	NAG	C1-C2-N2	-7.13	99.20	110.43
2	D	2	NAG	C2-N2-C7	-6.94	113.59	122.90
2	D	1	NAG	C8-C7-N2	6.45	126.81	116.12
2	D	2	NAG	O5-C1-C2	-5.50	102.79	111.29
2	D	1	NAG	C2-N2-C7	-5.10	116.07	122.90
2	F	1	NAG	O7-C7-C8	-5.06	113.05	122.05
2	F	2	NAG	O6-C6-C5	-5.02	94.24	111.33
2	D	2	NAG	O5-C5-C4	-4.68	99.44	110.83
2	F	1	NAG	O5-C5-C6	-4.58	98.75	107.66
2	E	1	NAG	O5-C5-C6	-4.57	98.77	107.66
2	C	1	NAG	C2-N2-C7	-4.51	116.86	122.90
2	F	2	NAG	C6-C5-C4	4.49	124.05	113.02
2	C	2	NAG	C1-C2-N2	4.39	117.35	110.43
2	F	1	NAG	O7-C7-N2	4.04	129.12	121.98
2	F	1	NAG	C6-C5-C4	3.94	122.69	113.02
2	C	2	NAG	C3-C4-C5	-3.91	103.14	110.23
2	D	1	NAG	O7-C7-C8	-3.84	115.21	122.05
2	E	1	NAG	C1-O5-C5	3.82	117.31	112.19
2	C	2	NAG	O4-C4-C5	3.81	118.71	109.32
2	D	1	NAG	O3-C3-C2	3.75	117.19	109.40
2	F	1	NAG	C1-C2-N2	3.69	116.25	110.43
2	E	1	NAG	C1-C2-N2	3.66	116.19	110.43
2	F	2	NAG	C4-C3-C2	3.63	116.34	111.02
2	E	1	NAG	C4-C3-C2	-3.58	105.77	111.02
2	F	2	NAG	O4-C4-C3	-3.57	101.95	110.38
2	C	1	NAG	O7-C7-C8	-3.45	115.91	122.05
2	D	1	NAG	O5-C5-C6	3.43	114.35	107.66
2	F	1	NAG	C4-C3-C2	3.43	116.05	111.02
2	F	2	NAG	O5-C5-C4	-3.41	102.52	110.83
2	C	1	NAG	C3-C4-C5	3.29	116.19	110.23
2	D	1	NAG	C1-O5-C5	-3.27	107.80	112.19
2	C	1	NAG	O5-C5-C4	3.22	118.66	110.83
2	C	2	NAG	O3-C3-C2	-3.22	102.72	109.40
2	F	1	NAG	O5-C5-C4	-3.09	103.32	110.83
2	F	2	NAG	C2-N2-C7	3.06	127.00	122.90
2	F	2	NAG	C8-C7-N2	3.01	121.12	116.12
2	F	1	NAG	O3-C3-C4	2.92	117.25	110.38
2	E	1	NAG	C8-C7-N2	-2.84	111.40	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	O5-C1-C2	-2.75	107.04	111.29
2	D	2	NAG	C3-C4-C5	-2.73	105.29	110.23
2	D	2	NAG	C6-C5-C4	2.71	119.68	113.02
2	D	1	NAG	C4-C3-C2	2.68	114.94	111.02
2	F	2	NAG	O3-C3-C2	2.64	114.88	109.40
2	E	2	NAG	C1-C2-N2	2.56	114.46	110.43
2	E	1	NAG	O5-C5-C4	2.47	116.85	110.83
2	F	2	NAG	O5-C5-C6	-2.37	103.04	107.66
2	D	1	NAG	O7-C7-N2	-2.32	117.87	121.98
2	D	2	NAG	C8-C7-N2	-2.32	112.27	116.12
2	D	1	NAG	O5-C5-C4	-2.22	105.44	110.83
2	F	1	NAG	O3-C3-C2	-2.18	104.86	109.40
2	F	1	NAG	O4-C4-C5	-2.12	104.09	109.32
2	E	1	NAG	O7-C7-N2	2.07	125.64	121.98
2	D	2	NAG	O4-C4-C5	2.02	114.31	109.32
2	C	2	NAG	O5-C1-C2	-2.01	108.19	111.29
2	F	2	NAG	O7-C7-C8	-2.00	118.48	122.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6

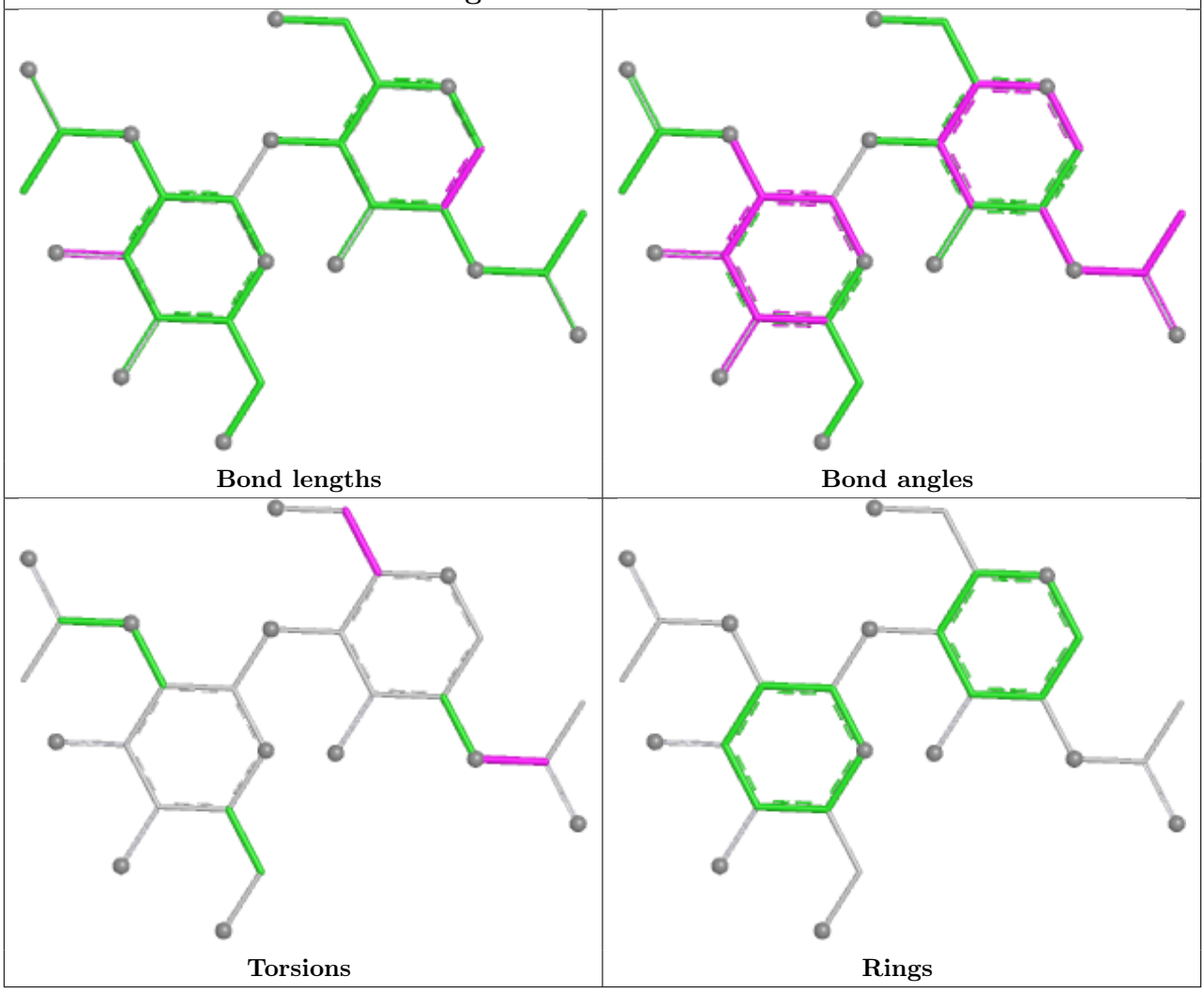
There are no ring outliers.

6 monomers are involved in 20 short contacts:

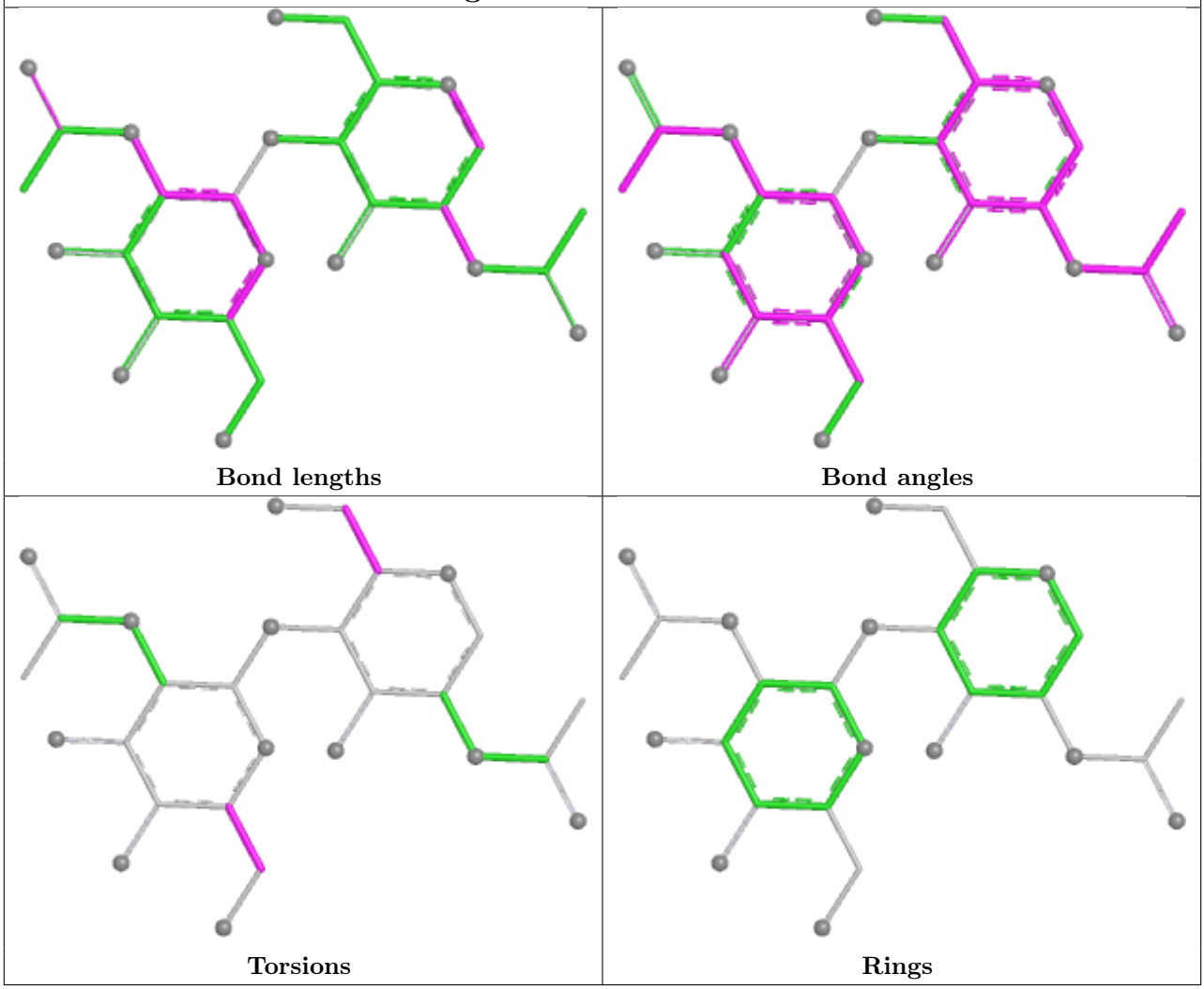
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	C	2	NAG	3	0
2	E	1	NAG	3	0
2	D	1	NAG	3	0
2	E	2	NAG	5	0
2	F	1	NAG	4	0

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

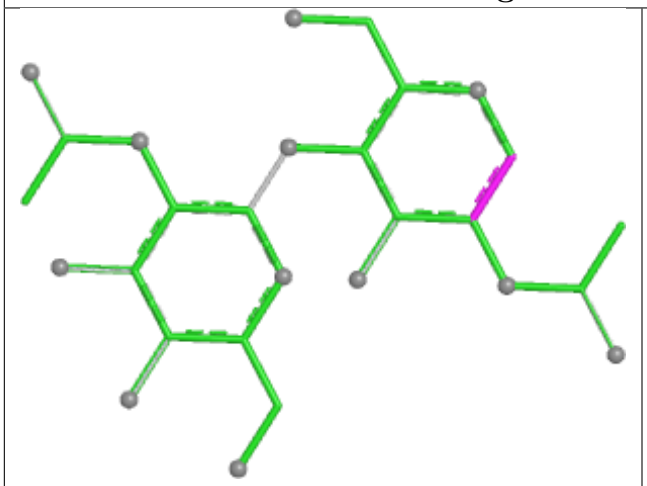
Oligosaccharide Chain C



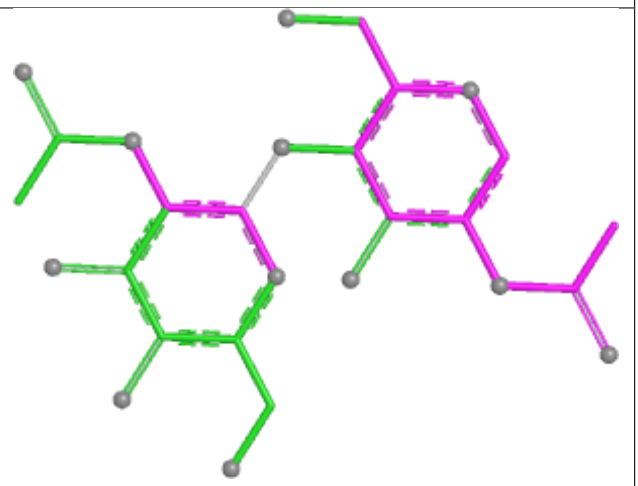
Oligosaccharide Chain D



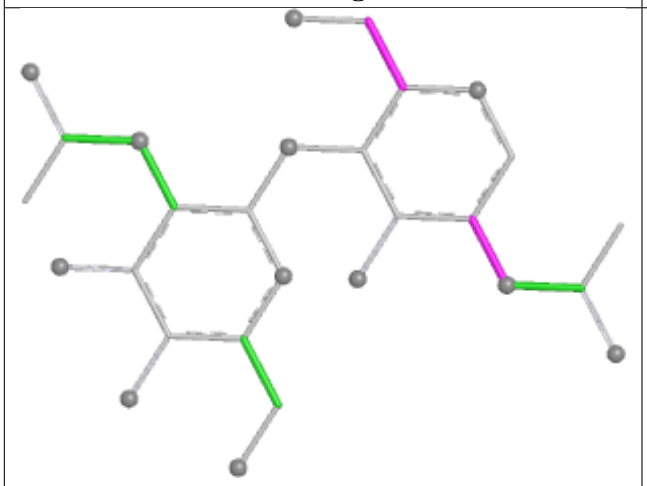
Oligosaccharide Chain E



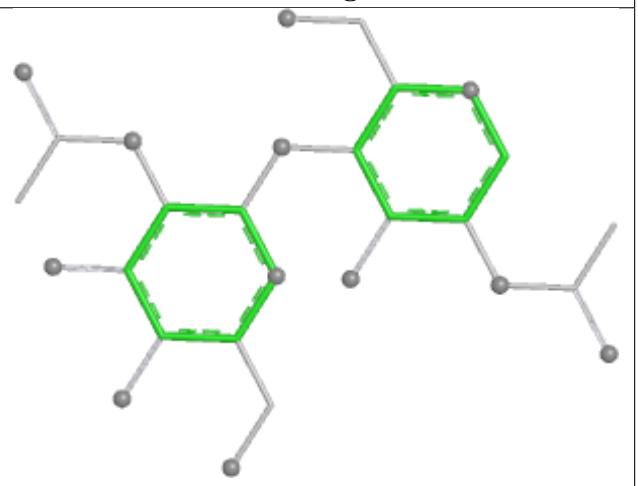
Bond lengths



Bond angles

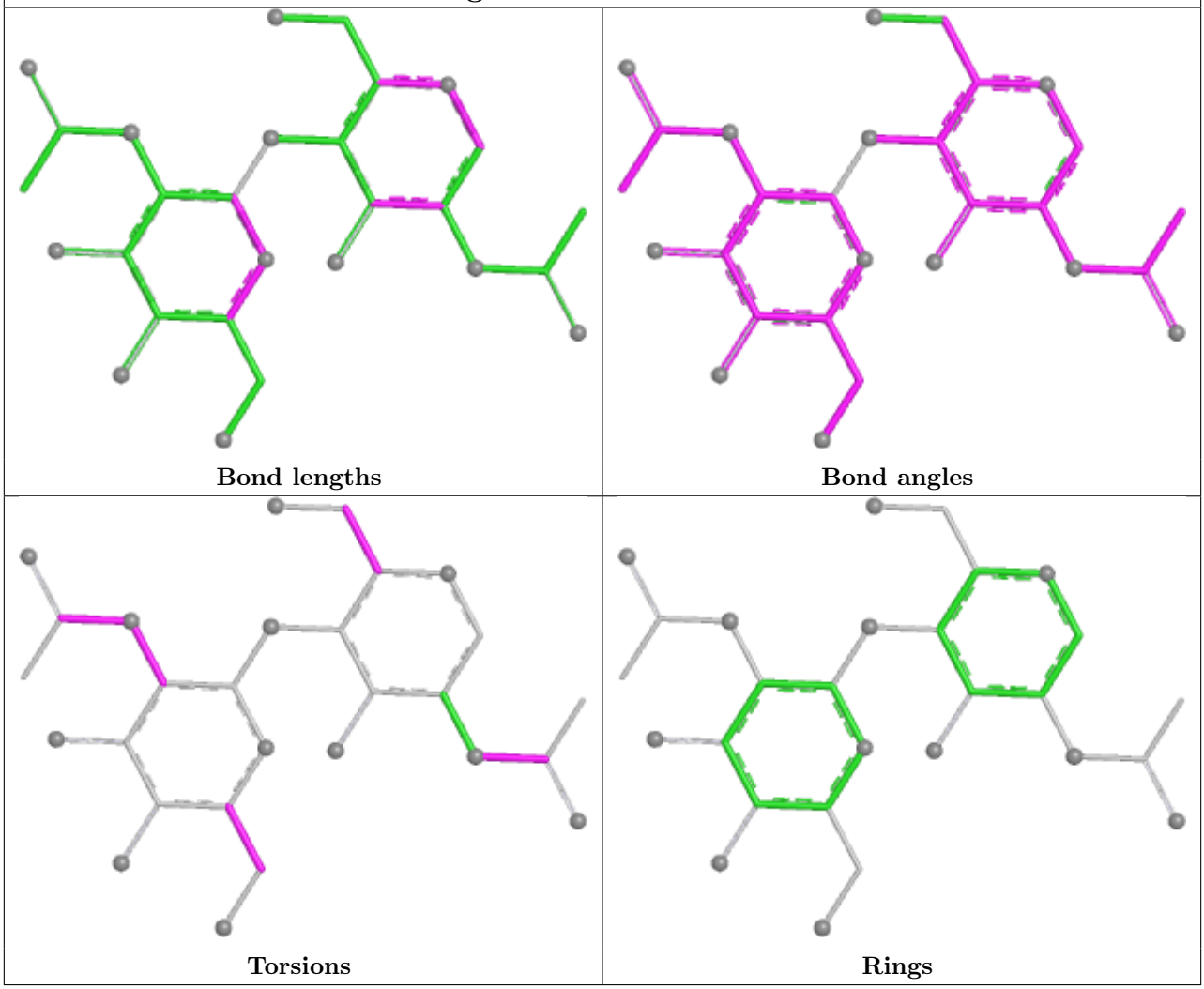


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	SO4	A	8002	-	4,4,4	0.37	0	6,6,6	0.53	0
7	KIB	B	2001	-	12,12,12	3.64	6 (50%)	16,16,16	2.07	5 (31%)
5	NAG	A	740	1	14,14,15	0.78	0	17,19,21	2.48	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	B	8001	-	4,4,4	0.36	0	6,6,6	1.08	0
5	NAG	B	760	1	14,14,15	0.95	1 (7%)	17,19,21	2.03	6 (35%)
5	NAG	B	720	1	14,14,15	0.74	0	17,19,21	1.45	2 (11%)
5	NAG	A	720	1	14,14,15	1.08	0	17,19,21	2.62	8 (47%)
5	NAG	B	700	1	14,14,15	1.00	1 (7%)	17,19,21	2.54	6 (35%)
5	NAG	A	700	1	14,14,15	1.07	1 (7%)	17,19,21	1.48	3 (17%)
5	NAG	B	740	1	14,14,15	0.85	1 (7%)	17,19,21	2.26	5 (29%)
7	KIB	A	1001	-	12,12,12	3.08	4 (33%)	16,16,16	2.12	7 (43%)

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
7	KIB	B	2001	-	-	2/4/4/4	0/1/1/1
5	NAG	A	740	1	-	0/6/23/26	0/1/1/1
5	NAG	B	760	1	-	2/6/23/26	0/1/1/1
5	NAG	B	720	1	-	0/6/23/26	0/1/1/1
5	NAG	A	720	1	-	2/6/23/26	0/1/1/1
5	NAG	B	700	1	-	0/6/23/26	0/1/1/1
5	NAG	A	700	1	-	4/6/23/26	0/1/1/1
5	NAG	B	740	1	-	2/6/23/26	0/1/1/1
7	KIB	A	1001	-	-	0/4/4/4	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2001	KIB	C6-C1	8.18	1.51	1.40
7	A	1001	KIB	C2-C1	7.48	1.50	1.40
7	B	2001	KIB	C2-C1	5.80	1.48	1.40
7	A	1001	KIB	O1-C1	-4.41	1.26	1.36
7	B	2001	KIB	C5-C4	4.17	1.45	1.39
7	A	1001	KIB	O2-C4	-3.93	1.28	1.37
7	A	1001	KIB	C6-C1	3.82	1.45	1.40
7	B	2001	KIB	O4-C2	3.55	1.42	1.37
7	B	2001	KIB	C3-C4	3.16	1.43	1.39
7	B	2001	KIB	O2-C4	-3.07	1.30	1.37
5	A	700	NAG	O5-C1	-3.00	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	760	NAG	C1-C2	2.45	1.55	1.52
5	B	700	NAG	C4-C3	-2.15	1.46	1.52
5	B	740	NAG	C1-C2	2.12	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	700	NAG	O4-C4-C3	-6.66	94.67	110.38
5	A	740	NAG	C3-C4-C5	-5.71	99.88	110.23
5	B	740	NAG	C2-N2-C7	-5.41	115.65	122.90
5	B	760	NAG	O5-C1-C2	-4.93	103.66	111.29
7	B	2001	KIB	C3-C2-C1	-4.69	116.13	120.59
5	A	720	NAG	C4-C3-C2	4.56	117.70	111.02
5	A	720	NAG	C1-C2-N2	4.48	117.49	110.43
5	A	740	NAG	O5-C1-C2	-4.45	104.41	111.29
5	A	720	NAG	O7-C7-C8	-4.33	114.34	122.05
5	B	740	NAG	C8-C7-N2	4.24	123.15	116.12
5	B	700	NAG	C1-C2-N2	-3.98	104.16	110.43
5	B	720	NAG	O5-C1-C2	-3.81	105.39	111.29
7	A	1001	KIB	C5-C6-C1	-3.77	117.01	120.59
5	A	720	NAG	O7-C7-N2	3.64	128.41	121.98
5	A	740	NAG	C1-O5-C5	-3.60	107.36	112.19
7	A	1001	KIB	C7-O3-C6	3.50	122.65	117.51
7	A	1001	KIB	O4-C2-C1	3.47	118.16	114.53
5	B	740	NAG	C3-C4-C5	3.42	116.43	110.23
5	A	740	NAG	C2-N2-C7	3.41	127.47	122.90
7	B	2001	KIB	O4-C2-C1	3.37	118.06	114.53
5	A	720	NAG	O5-C5-C6	3.30	114.08	107.66
7	B	2001	KIB	C2-C3-C4	3.27	124.13	118.98
7	A	1001	KIB	C8-O4-C2	3.26	122.29	117.51
5	A	700	NAG	O5-C1-C2	-3.23	106.29	111.29
5	B	700	NAG	O3-C3-C4	-3.22	102.78	110.38
5	B	700	NAG	O3-C3-C2	3.05	115.73	109.40
5	B	760	NAG	O3-C3-C2	2.99	115.61	109.40
5	A	720	NAG	C3-C4-C5	2.90	115.48	110.23
5	B	760	NAG	C2-N2-C7	-2.89	119.03	122.90
5	A	720	NAG	C2-N2-C7	2.76	126.59	122.90
5	B	760	NAG	O5-C5-C6	2.74	112.99	107.66
5	B	760	NAG	C1-O5-C5	-2.71	108.55	112.19
5	A	720	NAG	O3-C3-C2	-2.68	103.84	109.40
5	B	700	NAG	O6-C6-C5	-2.67	102.23	111.33
5	B	740	NAG	O7-C7-N2	-2.57	117.43	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1001	KIB	O1-C1-C2	2.45	124.47	119.21
5	A	700	NAG	C1-C2-N2	-2.44	106.58	110.43
7	B	2001	KIB	C7-O3-C6	2.42	121.07	117.51
7	A	1001	KIB	C6-C5-C4	2.38	122.73	118.98
5	A	740	NAG	C6-C5-C4	2.36	118.83	113.02
5	B	760	NAG	C1-C2-N2	-2.35	106.73	110.43
5	B	700	NAG	C3-C4-C5	-2.35	105.97	110.23
5	A	700	NAG	C8-C7-N2	2.31	119.95	116.12
5	B	720	NAG	O7-C7-C8	-2.29	117.98	122.05
5	A	740	NAG	O7-C7-N2	2.26	125.97	121.98
7	B	2001	KIB	C5-C6-C1	2.21	122.69	120.59
7	A	1001	KIB	O3-C6-C1	2.18	116.81	114.53
5	B	740	NAG	O5-C5-C4	2.01	115.73	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	720	NAG	C8-C7-N2-C2
5	A	720	NAG	O7-C7-N2-C2
7	B	2001	KIB	C1-C6-O3-C7
7	B	2001	KIB	C5-C6-O3-C7
5	A	700	NAG	C8-C7-N2-C2
5	A	700	NAG	C4-C5-C6-O6
5	B	760	NAG	C4-C5-C6-O6
5	B	740	NAG	C4-C5-C6-O6
5	A	700	NAG	O5-C5-C6-O6
5	A	700	NAG	O7-C7-N2-C2
5	B	740	NAG	O5-C5-C6-O6
5	B	760	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2001	KIB	7	0
5	A	740	NAG	1	0
5	A	720	NAG	4	0
5	A	700	NAG	0	1
7	A	1001	KIB	1	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

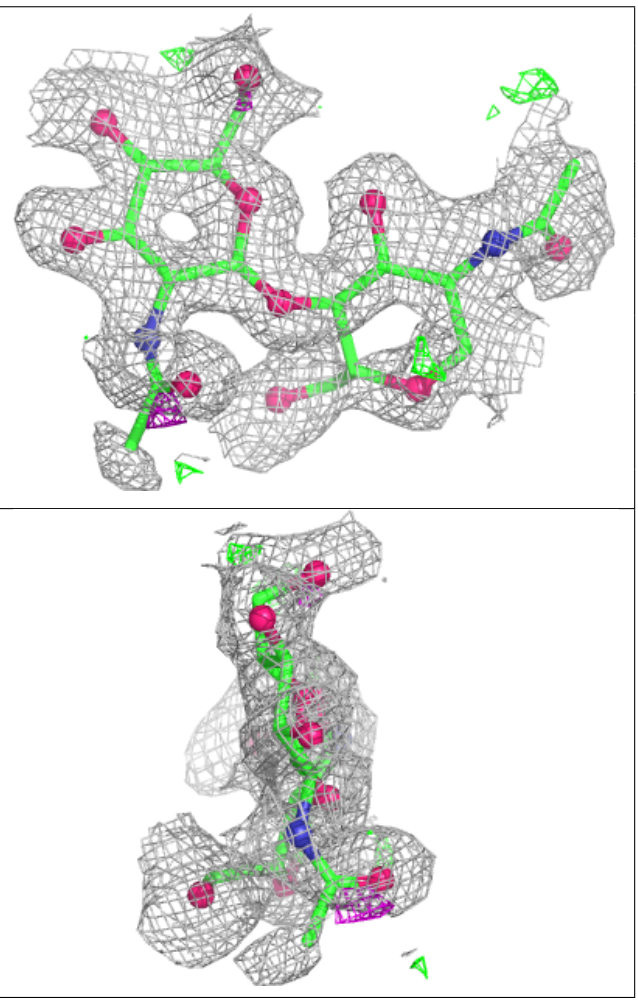
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

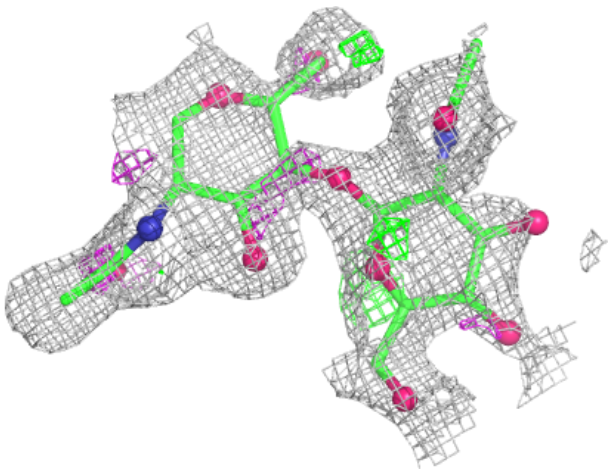
Electron density around Chain C:

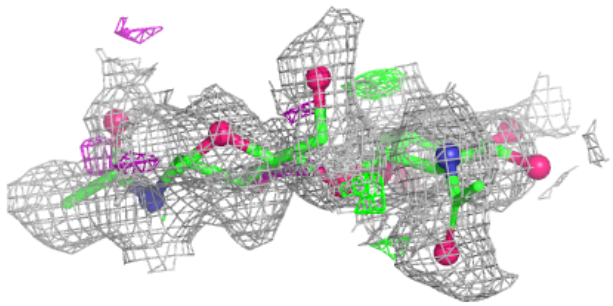
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

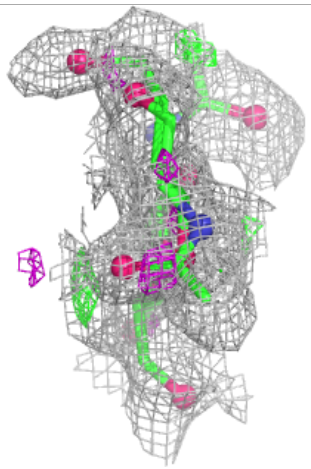


Electron density around Chain D:

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

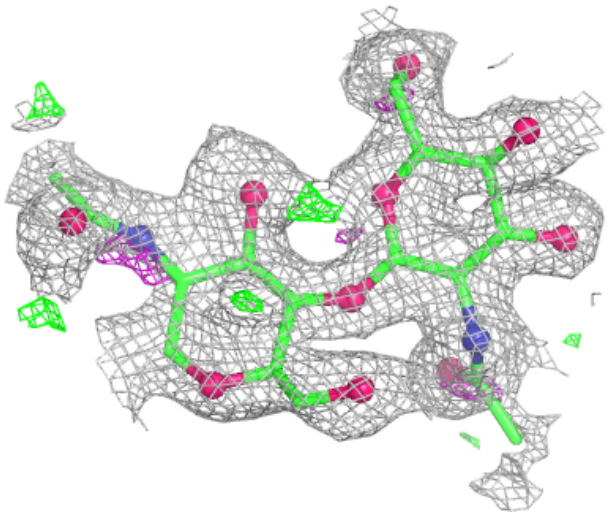


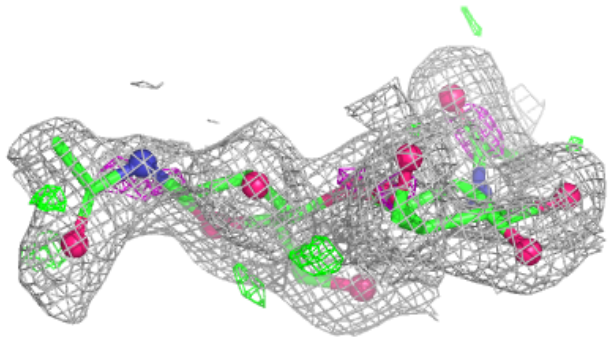


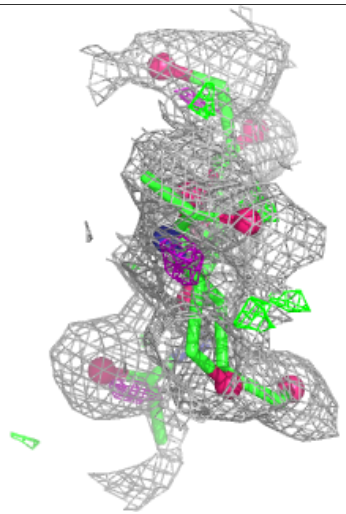


Electron density around Chain E:

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

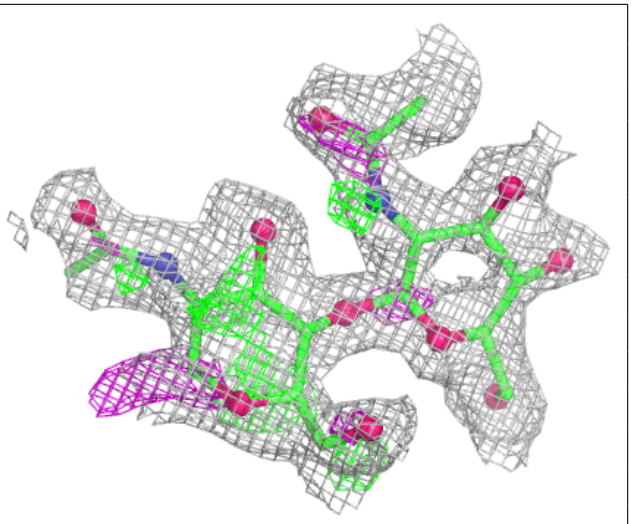


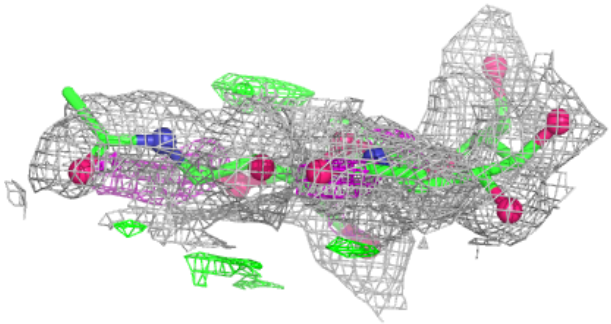


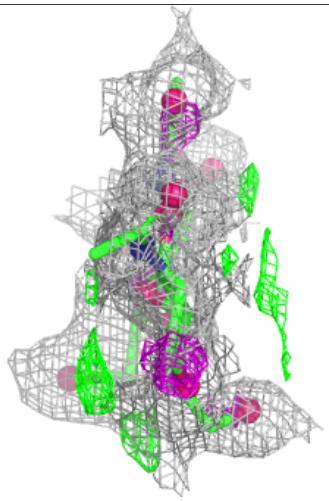


Electron density around Chain F:

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







6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.