



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:59 PM UTC

PDB ID : 5CU5 / pdb_00005cu5
Title : Crystal structure of ERAP2 without catalytic Zn(II) atom
Authors : Saridakis, E.; Mathioudakis, N.; Giastas, P.; Mavridis, I.M.; Stratikos, E.
Deposited on : 2015-07-24
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

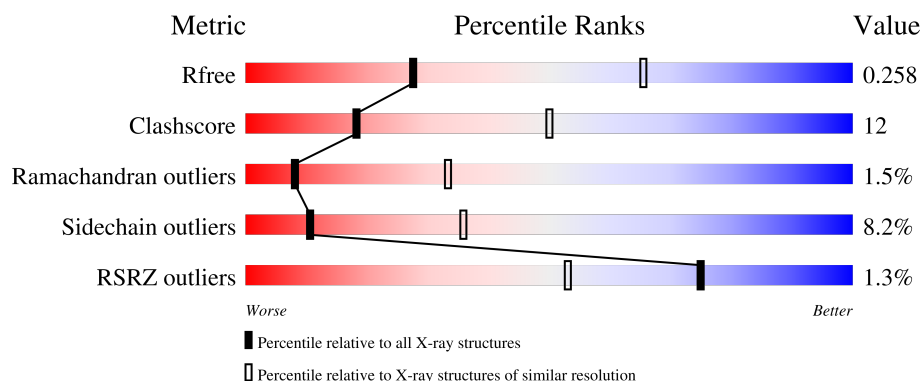
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	967	68% 18% • 10%
1	B	967	67% 20% • 11%
2	C	3	67% 33%
3	D	2	50% 50%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
4	E	4	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14562 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.

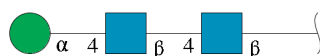
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	1	0
			7089	4576	1176	1309	28			
1	B	862	Total	C	N	O	S	0	0	0
			7009	4523	1164	1295	27			

There are 16 discrepancies between the modelled and reference sequences:

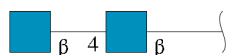
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	conflict	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	2	VAL	PHE	conflict	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

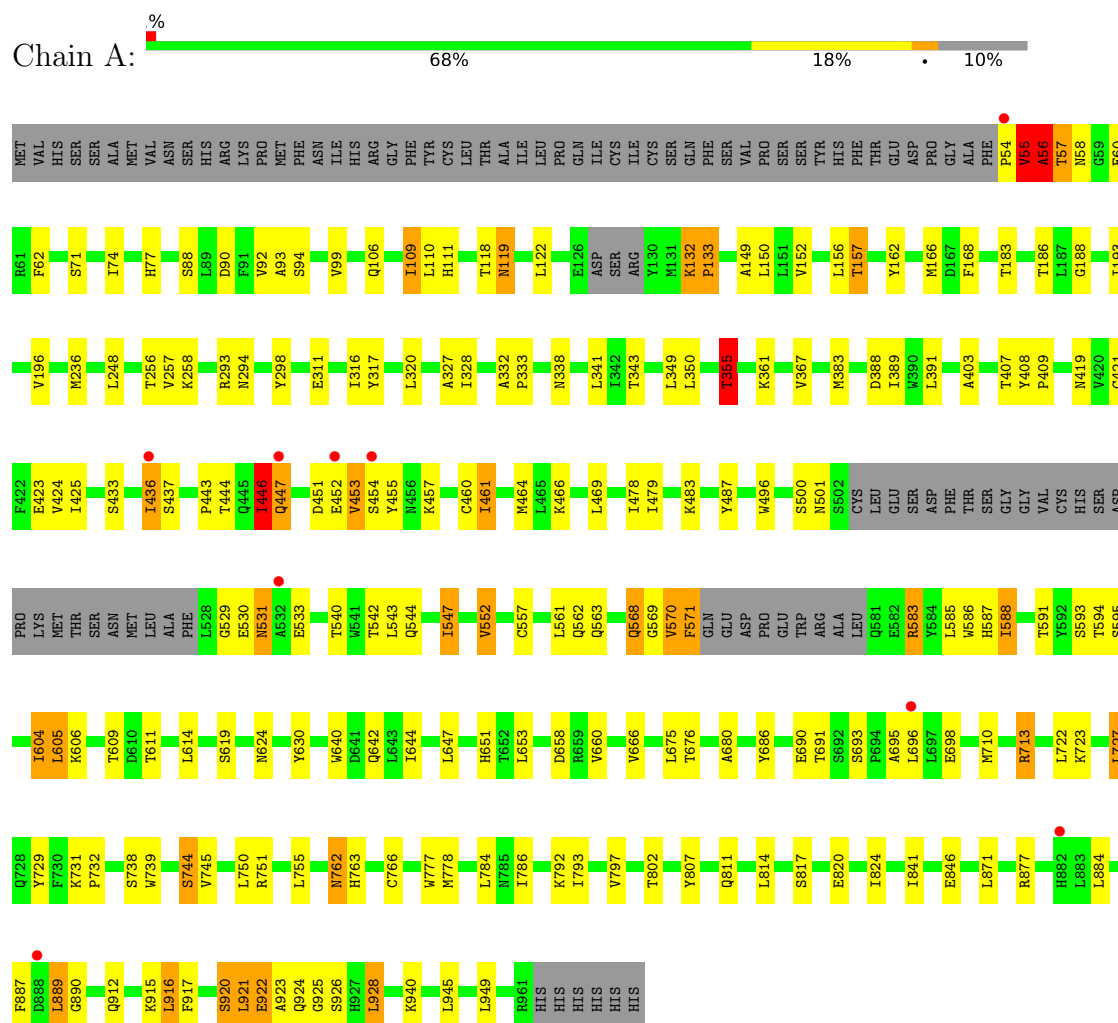
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	109	Total	O	0	0
			109	109		
6	B	84	Total	O	0	0
			84	84		

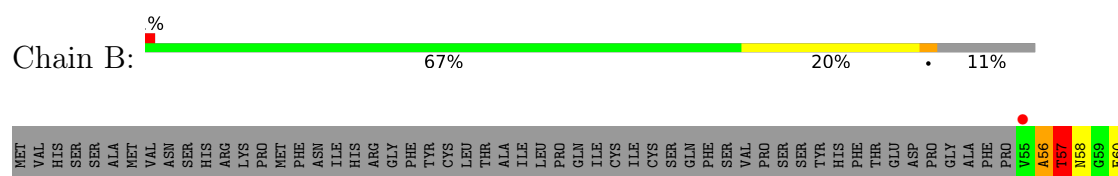
3 Residue-property plots

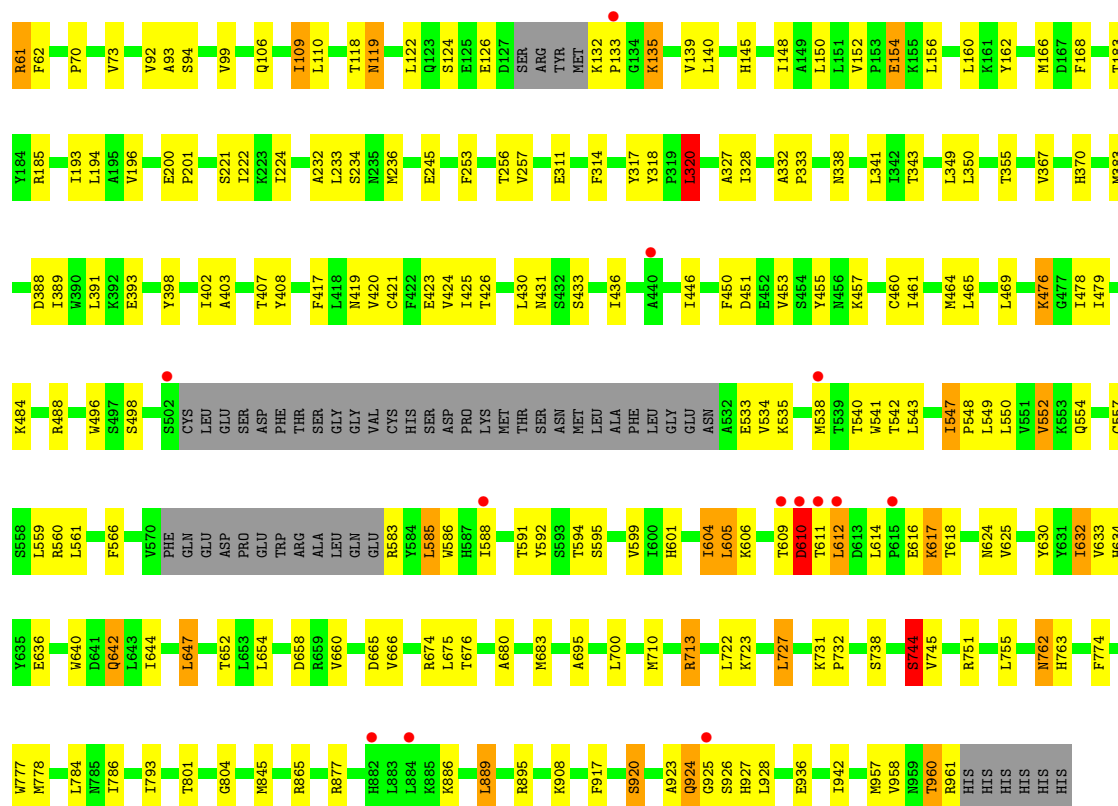
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Endoplasmic reticulum aminopeptidase 2



• Molecule 1: Endoplasmic reticulum aminopeptidase 2





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

Chain C: 67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50% 50%

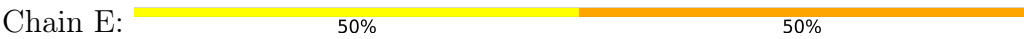


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



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



HA01
HA02
HA03
HA04

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.65Å 135.17Å 126.49Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	48.56 – 3.02 48.56 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.56-3.02) 100.0 (48.56-3.02)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.210 , 0.263 0.211 , 0.258	Depositor DCC
R_{free} test set	2497 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14562	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.63	1/7266 (0.0%)	0.94	8/9844 (0.1%)
1	B	0.64	0/7179	0.95	8/9726 (0.1%)
All	All	0.64	1/14445 (0.0%)	0.94	16/19570 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	ALA	CA-C	5.32	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ALA	N-CA-C	9.37	122.28	108.60
1	B	713	ARG	N-CA-C	-6.93	101.38	110.53
1	A	713	ARG	N-CA-C	-6.93	101.38	110.53
1	A	367	VAL	CB-CA-C	-6.87	103.03	112.24
1	A	55	VAL	N-CA-C	6.82	123.53	109.34
1	B	57	THR	CB-CA-C	6.81	125.42	111.11
1	A	446	ILE	N-CA-CB	6.71	120.64	110.58
1	B	320	LEU	CB-CG-CD2	6.13	129.08	110.70
1	A	157	THR	CB-CA-C	5.79	116.44	109.31
1	A	797	VAL	CB-CA-C	-5.68	104.48	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	762	ASN	N-CA-C	5.54	119.61	112.86
1	A	729	TYR	N-CA-C	-5.20	102.69	110.23
1	B	642	GLN	N-CA-CB	5.16	117.71	110.12
1	B	762	ASN	N-CA-C	5.10	119.08	112.86
1	B	73	VAL	CB-CA-C	5.08	117.03	110.12
1	B	647	LEU	CA-CB-CG	5.03	133.90	116.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	530	GLU	Peptide
1	A	531	ASN	Peptide
1	A	56	ALA	Peptide
1	A	921	LEU	Peptide
1	A	922	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7089	0	7041	149	1
1	B	7009	0	6979	189	1
2	C	39	0	34	1	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
4	E	50	0	43	2	0
5	A	98	0	90	9	0
5	B	28	0	26	1	0
6	A	109	0	0	11	0
6	B	84	0	0	39	0
All	All	14562	0	14263	342	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 12.

All (342) 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:224:ILE:CD1	1:B:232:ALA:HB1	1.38	1.49
1:B:224:ILE:CD1	1:B:232:ALA:CB	1.96	1.41
1:B:224:ILE:HD12	1:B:232:ALA:CB	1.53	1.37
1:B:610:ASP:O	1:B:611:THR:HG22	1.09	1.22
1:B:611:THR:OG1	1:B:612:LEU:CB	1.91	1.18
1:A:690:GLU:HB3	1:A:696:LEU:HD21	1.19	1.16
1:B:801:THR:HG23	6:B:1101:HOH:O	1.42	1.14
1:B:611:THR:OG1	1:B:612:LEU:HB3	1.41	1.13
1:B:548:PRO:HG3	1:B:588:ILE:HD11	1.25	1.13
1:B:224:ILE:HD11	1:B:232:ALA:CB	1.73	1.12
1:B:561:LEU:HG	1:B:611:THR:HG21	1.24	1.11
1:A:690:GLU:HB3	1:A:696:LEU:CD2	1.82	1.09
1:B:610:ASP:O	1:B:611:THR:CG2	2.00	1.09
1:B:224:ILE:HD11	1:B:232:ALA:HB3	1.30	1.05
1:A:619:SER:O	1:A:642:GLN:NE2	1.90	1.04
1:A:619:SER:O	1:A:642:GLN:CD	2.01	1.03
1:B:548:PRO:CG	1:B:588:ILE:HD11	1.94	0.98
1:B:314:PHE:HB2	6:B:1109:HOH:O	1.61	0.98
1:B:561:LEU:CG	1:B:611:THR:HG21	1.93	0.97
1:B:224:ILE:HD12	1:B:232:ALA:HB1	1.04	0.96
1:A:570:VAL:HG12	1:A:571:PHE:H	1.32	0.95
1:B:801:THR:O	6:B:1101:HOH:O	1.86	0.92
1:A:294:ASN:H	5:A:1011:NAG:H82	1.35	0.91
1:B:611:THR:OG1	1:B:612:LEU:HB2	1.68	0.91
1:A:690:GLU:CB	1:A:696:LEU:HD21	1.99	0.91
1:B:548:PRO:CG	1:B:588:ILE:CD1	2.49	0.91
1:B:957:MET:O	6:B:1102:HOH:O	1.88	0.90
1:A:606:LYS:HA	6:A:1101:HOH:O	1.72	0.89
1:B:611:THR:HG1	1:B:612:LEU:HB3	1.35	0.89
1:A:690:GLU:O	1:A:696:LEU:HD11	1.74	0.88
1:B:957:MET:SD	6:B:1105:HOH:O	2.31	0.88
1:A:54:PRO:C	1:A:55:VAL:HG12	1.98	0.88
1:B:804:GLY:N	6:B:1101:HOH:O	2.06	0.88
1:B:541:TRP:CZ2	1:B:588:ILE:HG12	2.10	0.85
1:B:636:GLU:HB3	6:B:1119:HOH:O	1.75	0.85
1:A:605:LEU:HD23	6:A:1101:HOH:O	1.77	0.84
1:B:804:GLY:CA	6:B:1101:HOH:O	2.28	0.82
1:B:224:ILE:HD12	1:B:232:ALA:HB2	1.61	0.82
1:B:611:THR:HA	1:B:612:LEU:HB2	1.61	0.80
1:B:611:THR:CA	1:B:612:LEU:HB2	2.11	0.79
1:A:55:VAL:HG21	1:A:62:PHE:HB2	1.64	0.79
1:B:612:LEU:O	6:B:1103:HOH:O	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:THR:OG1	6:B:1104:HOH:O	2.01	0.78
1:B:224:ILE:HD13	1:B:232:ALA:HB1	1.62	0.77
1:A:454:SER:HB2	6:A:1104:HOH:O	1.84	0.76
1:B:633:VAL:HG12	6:B:1110:HOH:O	1.86	0.75
1:A:56:ALA:HB1	1:A:57:THR:HA	1.68	0.75
1:A:587:HIS:HA	6:A:1101:HOH:O	1.86	0.75
1:B:586:TRP:HB3	1:B:588:ILE:HG13	1.67	0.75
1:B:421:CYS:HG	1:B:460:CYS:HG	0.76	0.75
1:A:619:SER:O	1:A:642:GLN:OE1	2.05	0.73
1:B:960:THR:OG1	6:B:1105:HOH:O	2.07	0.73
1:A:236:MET:HE3	1:A:256:THR:HA	1.71	0.72
1:B:465:LEU:HD11	1:B:538:MET:CE	2.19	0.72
1:B:559:LEU:O	1:B:611:THR:HG23	1.88	0.72
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.71	0.72
1:B:957:MET:HA	6:B:1105:HOH:O	1.88	0.72
1:B:236:MET:HE3	1:B:256:THR:HA	1.71	0.72
1:B:561:LEU:HD12	1:B:611:THR:HB	1.70	0.72
1:A:690:GLU:HG3	1:A:696:LEU:HG	1.72	0.71
1:A:388:ASP:HB3	1:A:391:LEU:HD12	1.72	0.71
1:B:611:THR:CB	1:B:612:LEU:HB2	2.19	0.71
1:B:549:LEU:HD13	1:B:632:ILE:HD12	1.72	0.71
1:A:586:TRP:O	6:A:1101:HOH:O	2.07	0.70
1:A:921:LEU:O	1:A:926:SER:N	2.24	0.70
4:E:3:MAN:O3	4:E:4:MAN:H5	1.92	0.70
1:A:403:ALA:O	1:A:407:THR:HG23	1.93	0.69
1:B:610:ASP:C	1:B:611:THR:HG22	2.11	0.68
1:A:570:VAL:HG12	1:A:571:PHE:N	2.08	0.68
1:B:548:PRO:HG3	1:B:588:ILE:CD1	2.08	0.68
1:A:55:VAL:HG11	1:A:62:PHE:N	2.08	0.67
1:B:774:PHE:CE1	1:B:778:MET:HE3	2.30	0.67
1:B:804:GLY:HA3	6:B:1101:HOH:O	1.90	0.66
1:A:55:VAL:HG11	1:A:62:PHE:H	1.61	0.66
1:A:54:PRO:C	1:A:55:VAL:CG1	2.67	0.66
1:B:548:PRO:CG	1:B:588:ILE:HD13	2.24	0.66
1:A:563:GLN:NE2	1:A:605:LEU:HD21	2.12	0.65
1:A:436:ILE:HD11	1:A:542:THR:HB	1.78	0.65
1:A:466:LYS:NZ	5:A:1006:NAG:H81	2.12	0.65
1:A:257:VAL:HG11	1:A:487:TYR:CE1	2.32	0.64
1:B:958:VAL:C	6:B:1102:HOH:O	2.40	0.64
1:B:56:ALA:HB3	1:B:61:ARG:HA	1.79	0.64
1:B:58:ASN:O	6:B:1106:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:HD11	1:B:538:MET:HE1	1.79	0.64
1:B:548:PRO:HG2	1:B:588:ILE:HD13	1.78	0.64
1:A:443:PRO:HA	1:A:446:ILE:CD1	2.28	0.64
1:A:778:MET:HE3	1:A:807:TYR:HB2	1.79	0.63
1:B:224:ILE:HG12	1:B:253:PHE:HE2	1.63	0.62
1:A:690:GLU:HB3	1:A:696:LEU:HD23	1.79	0.62
1:A:436:ILE:HD12	1:A:437:SER:N	2.14	0.62
1:B:62:PHE:HB3	6:B:1130:HOH:O	1.98	0.62
1:A:571:PHE:N	1:A:571:PHE:CD1	2.66	0.62
1:A:294:ASN:CG	5:A:1011:NAG:N2	2.58	0.62
1:B:561:LEU:CB	1:B:611:THR:HG21	2.30	0.61
1:B:586:TRP:CB	1:B:588:ILE:HG13	2.30	0.61
1:A:690:GLU:CB	1:A:696:LEU:CD2	2.66	0.61
1:A:409:PRO:HB3	6:A:1105:HOH:O	2.00	0.60
1:A:444:THR:HA	1:A:447:GLN:CD	2.27	0.60
1:A:186:THR:HG22	1:A:188:GLY:H	1.67	0.59
1:B:124:SER:OG	1:B:132:LYS:HG2	2.02	0.59
1:B:586:TRP:HB2	1:B:588:ILE:CD1	2.32	0.59
1:B:548:PRO:HG2	1:B:588:ILE:CD1	2.30	0.59
1:B:550:LEU:HD23	6:B:1110:HOH:O	2.02	0.59
1:A:338:ASN:HB2	1:A:341:LEU:O	2.02	0.58
1:A:55:VAL:HG23	1:A:56:ALA:N	2.18	0.58
1:B:407:THR:HG23	1:B:408:TYR:CD2	2.38	0.57
1:B:407:THR:HG23	1:B:408:TYR:HD2	1.69	0.57
1:B:957:MET:CE	6:B:1105:HOH:O	2.52	0.57
1:B:461:ILE:O	1:B:465:LEU:HD13	2.04	0.57
1:B:338:ASN:HB2	1:B:341:LEU:O	2.04	0.57
1:B:222:ILE:HD12	1:B:234:SER:OG	2.05	0.56
1:A:119:ASN:OD1	5:A:1012:NAG:N2	2.38	0.56
1:A:332:ALA:HB3	1:A:333:PRO:HD3	1.88	0.56
1:A:588:ILE:HG23	1:A:605:LEU:HD22	1.87	0.56
1:B:660:VAL:HG12	1:B:695:ALA:HA	1.88	0.56
1:B:632:ILE:HG22	1:B:665:ASP:OD1	2.06	0.56
1:B:961:ARG:N	6:B:1102:HOH:O	1.96	0.55
1:A:568:GLN:HG2	1:A:940:LYS:HD2	1.88	0.55
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.88	0.55
1:A:660:VAL:HG12	1:A:695:ALA:HA	1.89	0.55
1:B:57:THR:HG22	1:B:58:ASN:HA	1.89	0.55
1:A:778:MET:HE3	1:A:807:TYR:CB	2.36	0.55
1:B:152:VAL:HG21	1:B:156:LEU:CD1	2.36	0.55
1:B:640:TRP:O	1:B:644:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:VAL:HG12	1:A:561:LEU:CD2	2.36	0.55
1:B:436:ILE:HD11	1:B:457:LYS:HG2	1.89	0.55
1:B:586:TRP:HB2	1:B:588:ILE:HD11	1.89	0.55
1:A:640:TRP:O	1:A:644:ILE:HD12	2.06	0.55
1:B:431:ASN:OD1	5:B:1007:NAG:O5	2.21	0.54
1:A:294:ASN:N	5:A:1011:NAG:H82	2.16	0.54
1:A:594:THR:CG2	1:A:614:LEU:HD11	2.36	0.54
1:B:960:THR:N	6:B:1102:HOH:O	2.41	0.54
1:A:407:THR:HG1	1:A:408:TYR:HD2	1.53	0.54
1:B:185:ARG:HD3	6:B:1128:HOH:O	2.07	0.54
1:B:332:ALA:HB3	1:B:333:PRO:HD3	1.88	0.54
1:B:801:THR:C	6:B:1101:HOH:O	2.44	0.54
1:B:370:HIS:NE2	6:B:1108:HOH:O	2.34	0.54
1:B:194:LEU:HD12	1:B:196:VAL:HG22	1.90	0.54
1:A:55:VAL:HG23	1:A:56:ALA:O	2.07	0.54
1:B:70:PRO:CD	1:B:109:ILE:CG2	2.85	0.53
1:A:236:MET:HE1	1:A:320:LEU:HD22	1.91	0.53
1:B:611:THR:CA	1:B:612:LEU:CB	2.85	0.53
5:A:1011:NAG:H2	6:A:1103:HOH:O	2.08	0.53
1:B:70:PRO:HD3	1:B:109:ILE:HG21	1.91	0.53
1:B:140:LEU:HD22	6:B:1106:HOH:O	2.08	0.53
1:B:388:ASP:HB3	1:B:391:LEU:HD13	1.91	0.53
1:B:594:THR:CG2	1:B:618:THR:HG21	2.39	0.53
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.89	0.53
1:B:70:PRO:CD	1:B:109:ILE:HG21	2.39	0.53
1:B:566:PHE:HB2	1:B:632:ILE:HD11	1.91	0.53
1:A:690:GLU:CG	1:A:696:LEU:HG	2.38	0.53
1:B:561:LEU:HB2	1:B:611:THR:CG2	2.39	0.53
1:B:961:ARG:HB2	6:B:1148:HOH:O	2.07	0.53
1:B:388:ASP:HB3	1:B:391:LEU:CD1	2.39	0.52
1:A:820:GLU:O	1:A:824:ILE:HG13	2.09	0.52
1:A:150:LEU:HD11	1:A:166:MET:HE2	1.92	0.52
1:B:140:LEU:CD2	6:B:1106:HOH:O	2.58	0.52
1:B:676:THR:HA	6:B:1124:HOH:O	2.10	0.52
1:A:328:ILE:CD1	1:A:343:THR:HG22	2.39	0.52
1:B:552:VAL:HG12	1:B:561:LEU:CD2	2.40	0.52
1:B:328:ILE:CD1	1:B:343:THR:HG22	2.39	0.52
1:A:328:ILE:HD11	1:A:343:THR:HG22	1.92	0.52
1:A:436:ILE:HD11	1:A:542:THR:CB	2.40	0.52
1:A:647:LEU:HD22	1:A:686:TYR:CE2	2.45	0.52
1:A:183:THR:HG22	1:A:193:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:HG3	1:A:890:GLY:O	2.09	0.51
1:B:150:LEU:HD11	1:B:166:MET:HE2	1.92	0.51
1:B:152:VAL:HG21	1:B:156:LEU:HD12	1.92	0.51
1:B:224:ILE:HG13	1:B:224:ILE:O	2.10	0.51
1:A:118:THR:O	1:A:119:ASN:HB2	2.11	0.51
1:B:328:ILE:HD11	1:B:343:THR:HG22	1.92	0.51
1:A:666:VAL:HG11	1:A:680:ALA:HA	1.93	0.51
1:B:548:PRO:CB	1:B:588:ILE:CD1	2.88	0.51
1:B:586:TRP:HB3	1:B:588:ILE:CG1	2.40	0.51
1:B:183:THR:HG22	1:B:193:ILE:HD13	1.92	0.51
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.93	0.51
1:B:393:GLU:OE1	6:B:1108:HOH:O	2.19	0.50
1:B:561:LEU:CB	1:B:611:THR:CG2	2.89	0.50
1:A:55:VAL:CG2	1:A:62:PHE:HB2	2.38	0.50
5:A:1011:NAG:H61	6:A:1162:HOH:O	2.11	0.50
1:A:327:ALA:HB2	1:A:349:LEU:HD23	1.93	0.50
1:A:738:SER:O	1:A:751:ARG:CD	2.60	0.50
1:A:739:TRP:CZ2	1:A:766:CYS:SG	3.05	0.50
1:B:160:LEU:HA	6:B:1114:HOH:O	2.11	0.50
1:A:152:VAL:HG21	1:A:156:LEU:CD1	2.41	0.50
1:A:457:LYS:HG2	1:A:461:ILE:HD13	1.94	0.49
1:A:466:LYS:HZ2	5:A:1006:NAG:H81	1.76	0.49
1:A:739:TRP:HZ2	1:A:766:CYS:SG	2.34	0.49
1:B:430:LEU:HD23	1:B:936:GLU:HB2	1.93	0.49
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.94	0.49
1:A:453:VAL:C	1:A:455:TYR:H	2.20	0.49
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.94	0.49
1:B:541:TRP:HZ2	1:B:588:ILE:HG12	1.69	0.49
1:A:55:VAL:CG2	1:A:56:ALA:N	2.74	0.49
1:B:224:ILE:CD1	1:B:232:ALA:HB3	1.95	0.49
1:B:666:VAL:HG11	1:B:680:ALA:HA	1.94	0.49
1:B:738:SER:O	1:B:751:ARG:CD	2.61	0.49
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.94	0.49
1:A:604:ILE:O	1:A:605:LEU:CB	2.60	0.49
1:A:257:VAL:HG12	1:A:258:LYS:N	2.28	0.48
1:B:132:LYS:HD2	1:B:135:LYS:HD3	1.95	0.48
1:A:443:PRO:HA	1:A:446:ILE:HD11	1.93	0.48
1:A:912:GLN:HE21	1:A:916:LEU:HD13	1.78	0.48
1:B:457:LYS:NZ	6:B:1117:HOH:O	2.46	0.48
1:B:484:LYS:O	1:B:488:ARG:NH1	2.47	0.48
1:B:561:LEU:HB2	1:B:611:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:ILE:O	1:B:605:LEU:CB	2.61	0.48
1:B:464:MET:CE	1:B:630:TYR:H	2.27	0.47
1:B:561:LEU:CG	1:B:611:THR:CG2	2.81	0.47
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.96	0.47
1:A:690:GLU:O	1:A:696:LEU:HD21	2.14	0.47
1:A:727:LEU:HD21	1:A:763:HIS:HB2	1.97	0.47
1:A:570:VAL:CG1	1:A:571:PHE:H	2.13	0.47
1:A:647:LEU:HD23	1:A:651:HIS:HB2	1.96	0.47
1:B:70:PRO:HD2	1:B:109:ILE:CG2	2.44	0.47
1:B:109:ILE:HD13	1:B:148:ILE:O	2.14	0.47
1:A:54:PRO:O	1:A:55:VAL:HG12	2.15	0.47
1:A:93:ALA:HB3	1:A:168:PHE:CE1	2.50	0.47
1:A:889:LEU:C	1:A:889:LEU:HD12	2.40	0.47
1:B:236:MET:HG2	1:B:256:THR:HG22	1.97	0.47
1:B:430:LEU:HD23	1:B:936:GLU:CB	2.44	0.47
1:A:464:MET:CE	1:A:630:TYR:H	2.28	0.47
1:B:561:LEU:HD12	1:B:611:THR:CB	2.41	0.47
1:B:640:TRP:CD1	1:B:675:LEU:HD21	2.50	0.47
1:B:126:GLU:HB2	1:B:160:LEU:HD23	1.97	0.47
1:B:561:LEU:N	1:B:611:THR:CG2	2.78	0.46
1:A:690:GLU:C	1:A:696:LEU:HD11	2.39	0.46
1:B:70:PRO:HD2	1:B:109:ILE:HG22	1.98	0.46
1:B:450:PHE:O	1:B:895:ARG:NH2	2.46	0.46
1:B:889:LEU:HD12	1:B:889:LEU:C	2.41	0.46
1:B:549:LEU:CD1	1:B:632:ILE:HD12	2.44	0.46
1:A:841:ILE:HD12	1:A:871:LEU:HD21	1.97	0.46
1:A:640:TRP:CD1	1:A:675:LEU:HD11	2.51	0.46
1:A:604:ILE:HD12	1:A:604:ILE:N	2.31	0.46
1:A:723:LYS:O	1:A:727:LEU:HD12	2.16	0.46
1:B:93:ALA:HB3	1:B:168:PHE:CE1	2.51	0.46
1:B:591:THR:O	1:B:624:ASN:N	2.49	0.46
1:B:549:LEU:HD21	6:B:1150:HOH:O	2.15	0.46
1:A:731:LYS:N	1:A:732:PRO:HD2	2.30	0.46
1:A:421:CYS:CB	1:A:460:CYS:HG	2.25	0.45
1:A:605:LEU:HD23	1:A:605:LEU:C	2.41	0.45
1:A:496:TRP:CZ2	1:A:542:THR:HG21	2.50	0.45
1:B:604:ILE:N	1:B:604:ILE:HD12	2.31	0.45
1:B:727:LEU:HD21	1:B:763:HIS:HB2	1.97	0.45
1:A:56:ALA:CB	1:A:57:THR:HA	2.42	0.45
1:A:236:MET:HE1	1:A:320:LEU:CD2	2.46	0.45
1:A:917:PHE:O	1:A:921:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:HD11	1:B:538:MET:SD	2.56	0.45
1:A:236:MET:HG2	1:A:256:THR:HG22	1.97	0.45
1:A:744:SER:OG	1:A:745:VAL:N	2.50	0.45
1:B:57:THR:CB	1:B:58:ASN:HA	2.47	0.45
1:A:257:VAL:HG11	1:A:487:TYR:CD1	2.51	0.45
1:A:846:GLU:OE1	6:A:1102:HOH:O	2.21	0.45
1:A:293:ARG:NH2	4:E:3:MAN:O2	2.50	0.45
1:A:496:TRP:HZ2	1:A:542:THR:HG21	1.82	0.45
1:B:461:ILE:O	1:B:465:LEU:CD1	2.65	0.45
1:B:723:LYS:O	1:B:727:LEU:HD12	2.17	0.45
1:A:152:VAL:HG21	1:A:156:LEU:HD12	1.98	0.45
1:B:118:THR:O	1:B:119:ASN:HB2	2.17	0.45
1:B:731:LYS:N	1:B:732:PRO:HD2	2.30	0.45
1:A:591:THR:O	1:A:624:ASN:N	2.50	0.45
1:B:845:MET:O	1:B:886:LYS:HE3	2.17	0.44
1:A:884:LEU:HD12	1:A:887:PHE:O	2.18	0.44
1:B:744:SER:OG	1:B:745:VAL:N	2.50	0.44
1:B:647:LEU:CD2	1:B:683:MET:CG	2.96	0.44
1:B:960:THR:CB	6:B:1105:HOH:O	2.64	0.44
1:A:407:THR:OG1	1:A:408:TYR:CD2	2.66	0.44
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.53	0.44
1:A:183:THR:CG2	1:A:193:ILE:HD13	2.47	0.44
1:A:922:GLU:HA	1:A:926:SER:HB2	2.00	0.44
1:B:453:VAL:C	1:B:455:TYR:H	2.26	0.43
1:A:710:MET:O	1:A:713:ARG:O	2.37	0.43
1:A:132:LYS:HB2	1:A:133:PRO:CD	2.48	0.43
1:B:594:THR:HG21	1:B:618:THR:HG21	2.00	0.43
1:A:444:THR:O	1:A:447:GLN:HG2	2.18	0.43
1:B:398:TYR:CE1	1:B:402:ILE:HG13	2.54	0.43
1:B:865:ARG:HH11	1:B:865:ARG:HG2	1.83	0.43
1:A:111:HIS:HE1	6:A:1111:HOH:O	2.02	0.43
1:A:540:THR:OG1	1:A:544:GLN:NE2	2.51	0.43
1:A:691:THR:HA	1:A:696:LEU:HD11	1.99	0.43
1:B:403:ALA:O	1:B:407:THR:HG22	2.19	0.43
1:A:355:THR:HG21	1:A:817:SER:CB	2.48	0.43
1:B:710:MET:O	1:B:713:ARG:O	2.36	0.43
1:A:562:GLN:HG3	1:A:609:THR:HG22	2.00	0.43
1:B:183:THR:CG2	1:B:193:ILE:HD13	2.49	0.43
1:B:496:TRP:HZ2	1:B:542:THR:HG21	1.82	0.43
1:B:62:PHE:CZ	1:B:109:ILE:HD11	2.53	0.42
1:B:654:LEU:HA	6:B:1127:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:MET:HE1	1:B:804:GLY:HA2	1.99	0.42
1:B:865:ARG:HG2	1:B:865:ARG:NH1	2.34	0.42
1:B:908:LYS:HE3	1:B:942:ILE:HG21	2.01	0.42
1:B:417:PHE:O	1:B:420:VAL:HG22	2.18	0.42
1:B:594:THR:HG23	1:B:618:THR:HG21	2.01	0.42
1:B:634:HIS:CE1	1:B:675:LEU:HD11	2.55	0.42
1:A:569:GLY:C	1:A:570:VAL:CG2	2.92	0.42
1:B:674:ARG:C	1:B:675:LEU:HD12	2.44	0.42
1:A:132:LYS:O	1:A:133:PRO:C	2.63	0.42
1:A:547:ILE:HD12	1:A:630:TYR:CE2	2.54	0.42
1:A:563:GLN:HE22	1:A:605:LEU:HD21	1.84	0.42
1:B:599:VAL:CG2	1:B:601:HIS:NE2	2.83	0.42
1:B:755:LEU:HB3	1:B:793:ILE:HD13	2.00	0.42
1:A:57:THR:OG1	1:A:58:ASN:N	2.47	0.42
1:B:221:SER:HA	6:B:1129:HOH:O	2.19	0.42
1:B:547:ILE:HD12	1:B:630:TYR:CE2	2.54	0.42
1:B:586:TRP:CB	1:B:588:ILE:HD11	2.49	0.42
1:B:923:ALA:O	1:B:924:GLN:HG2	2.20	0.42
1:B:958:VAL:O	6:B:1102:HOH:O	2.22	0.42
1:A:738:SER:O	1:A:751:ARG:HD2	2.20	0.42
1:B:320:LEU:HD13	1:B:320:LEU:N	2.34	0.42
1:A:88:SER:HG	1:A:90:ASP:CG	2.28	0.41
1:A:945:LEU:HD22	1:A:949:LEU:HD22	2.02	0.41
1:B:318:TYR:OH	1:B:320:LEU:HD22	2.20	0.41
1:A:436:ILE:HD12	1:A:436:ILE:C	2.45	0.41
1:B:592:TYR:CZ	1:B:601:HIS:HB2	2.56	0.41
1:A:74:ILE:N	1:A:74:ILE:HD12	2.35	0.41
1:A:109:ILE:HD11	1:A:149:ALA:HB2	2.03	0.41
1:B:550:LEU:HB3	6:B:1110:HOH:O	2.19	0.41
1:B:616:GLU:HG3	1:B:617:LYS:O	2.21	0.41
1:A:316:ILE:HD11	1:A:483:LYS:HG3	2.03	0.41
1:A:569:GLY:C	1:A:570:VAL:HG23	2.45	0.41
1:B:543:LEU:O	1:B:543:LEU:HD23	2.21	0.41
1:A:248:LEU:HD22	2:C:1:NAG:H83	2.02	0.41
1:A:443:PRO:O	1:A:447:GLN:NE2	2.54	0.41
1:B:154:GLU:O	1:B:154:GLU:HG3	2.20	0.41
1:A:755:LEU:HB3	1:A:793:ILE:HD13	2.02	0.41
1:B:57:THR:CG2	1:B:58:ASN:HA	2.50	0.41
1:B:106:GLN:O	1:B:152:VAL:HG22	2.20	0.41
1:A:106:GLN:O	1:A:152:VAL:HG22	2.20	0.41
1:B:145:HIS:CD2	6:B:1111:HOH:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:MET:HE2	1:A:630:TYR:H	1.86	0.41
1:A:890:GLY:HA3	1:A:928:LEU:HD21	2.02	0.41
1:B:200:GLU:HA	1:B:201:PRO:HA	1.91	0.41
1:A:77:HIS:HD2	3:D:1:NAG:H82	1.85	0.40
5:A:1011:NAG:O7	6:A:1103:HOH:O	2.22	0.40
1:B:738:SER:O	1:B:751:ARG:HD2	2.21	0.40
1:A:540:THR:HG1	1:A:586:TRP:CD1	2.40	0.40
1:B:877:ARG:HA	1:B:917:PHE:CE1	2.57	0.40
1:A:693:SER:OG	1:A:750:LEU:HD22	2.21	0.40
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.57	0.40
1:B:464:MET:HE2	1:B:630:TYR:H	1.86	0.40
1:A:690:GLU:CG	1:A:696:LEU:CD2	3.00	0.40
1:B:476:LYS:NZ	6:B:1107:HOH:O	2.18	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:A:531:ASN:ND2	1:B:585:LEU:CD1[1_554]	1.90	0.30

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	864/967 (89%)	793 (92%)	57 (7%)	14 (2%)	7	32
1	B	854/967 (88%)	787 (92%)	55 (6%)	12 (1%)	9	34
All	All	1718/1934 (89%)	1580 (92%)	112 (6%)	26 (2%)	8	33

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	605	LEU
1	B	119	ASN
1	B	605	LEU
1	A	583	ARG
1	A	604	ILE
1	A	923	ALA
1	B	133	PRO
1	B	604	ILE
1	B	612	LEU
1	B	925	GLY
1	B	926	SER
1	A	451	ASP
1	B	451	ASP
1	A	57	THR
1	A	355	THR
1	A	920	SER
1	A	925	GLY
1	A	529	GLY
1	B	355	THR
1	B	610	ASP
1	B	744	SER
1	B	920	SER
1	A	133	PRO
1	A	570	VAL
1	A	55	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	782/870 (90%)	719 (92%)	63 (8%)	11	36
1	B	774/870 (89%)	710 (92%)	64 (8%)	10	35
All	All	1556/1740 (89%)	1429 (92%)	127 (8%)	10	36

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	60	GLU
1	A	71	SER
1	A	92	VAL
1	A	94	SER
1	A	99	VAL
1	A	109	ILE
1	A	110	LEU
1	A	132	LYS
1	A	157	THR
1	A	196	VAL
1	A	350	LEU
1	A	355	THR
1	A	383	MET
1	A	389	ILE
1	A	419	ASN
1	A	423	GLU
1	A	424	VAL
1	A	425	ILE
1	A	433	SER
1	A	436	ILE
1	A	446	ILE
1	A	447	GLN
1	A	452	GLU
1	A	453	VAL
1	A	461	ILE
1	A	469	LEU
1	A	478	ILE
1	A	479	ILE
1	A	500	SER
1	A	501	ASN
1	A	533	GLU
1	A	543	LEU
1	A	547	ILE
1	A	552	VAL
1	A	557	CYS
1	A	568	GLN
1	A	571	PHE
1	A	583	ARG
1	A	585	LEU
1	A	588	ILE
1	A	593	SER
1	A	595	SER

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Mol	Chain	Res	Type
1	A	611	THR
1	A	653	LEU
1	A	658	ASP
1	A	676	THR
1	A	698	GLU
1	A	722	LEU
1	A	727	LEU
1	A	744	SER
1	A	762	ASN
1	A	784	LEU
1	A	792	LYS
1	A	802	THR
1	A	811	GLN
1	A	814	LEU
1	A	889	LEU
1	A	915	LYS
1	A	916	LEU
1	A	920	SER
1	A	924	GLN
1	A	928	LEU
1	B	57	THR
1	B	60	GLU
1	B	61	ARG
1	B	92	VAL
1	B	94	SER
1	B	99	VAL
1	B	109	ILE
1	B	110	LEU
1	B	135	LYS
1	B	139	VAL
1	B	154	GLU
1	B	233	LEU
1	B	245	GLU
1	B	257	VAL
1	B	320	LEU
1	B	350	LEU
1	B	367	VAL
1	B	383	MET
1	B	389	ILE
1	B	419	ASN
1	B	423	GLU
1	B	424	VAL

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Mol	Chain	Res	Type
1	B	425	ILE
1	B	426	THR
1	B	433	SER
1	B	446	ILE
1	B	469	LEU
1	B	476	LYS
1	B	478	ILE
1	B	479	ILE
1	B	498	SER
1	B	533	GLU
1	B	534	VAL
1	B	535	LYS
1	B	540	THR
1	B	547	ILE
1	B	552	VAL
1	B	554	GLN
1	B	557	CYS
1	B	560	ARG
1	B	583	ARG
1	B	585	LEU
1	B	595	SER
1	B	606	LYS
1	B	610	ASP
1	B	614	LEU
1	B	617	LYS
1	B	625	VAL
1	B	632	ILE
1	B	642	GLN
1	B	652	THR
1	B	658	ASP
1	B	700	LEU
1	B	722	LEU
1	B	727	LEU
1	B	744	SER
1	B	762	ASN
1	B	784	LEU
1	B	889	LEU
1	B	920	SER
1	B	924	GLN
1	B	927	HIS
1	B	928	LEU
1	B	960	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	159	HIS
1	A	230	HIS
1	A	252	HIS
1	A	301	GLN
1	A	338	ASN
1	A	370	HIS
1	A	456	ASN
1	A	463	ASN
1	A	544	GLN
1	A	587	HIS
1	A	601	HIS
1	A	800	GLN
1	A	811	GLN
1	A	834	GLN
1	A	912	GLN
1	A	959	ASN
1	B	111	HIS
1	B	119	ASN
1	B	159	HIS
1	B	230	HIS
1	B	301	GLN
1	B	370	HIS
1	B	445	GLN
1	B	447	GLN
1	B	456	ASN
1	B	463	ASN
1	B	480	GLN
1	B	501	ASN
1	B	785	ASN
1	B	800	GLN
1	B	833	HIS
1	B	959	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.61	0	17,19,21	1.73	2 (11%)
2	NAG	C	2	2	14,14,15	0.71	1 (7%)	17,19,21	1.70	5 (29%)
2	MAN	C	3	2	11,11,12	0.51	0	15,15,17	1.57	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.59	0	17,19,21	1.11	1 (5%)
3	NAG	D	2	3	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
4	NAG	E	1	1,4	14,14,15	0.73	0	17,19,21	2.15	3 (17%)
4	NAG	E	2	4	14,14,15	0.54	0	17,19,21	1.96	5 (29%)
4	MAN	E	3	4	11,11,12	0.65	0	15,15,17	1.51	4 (26%)
4	MAN	E	4	4	11,11,12	0.52	0	15,15,17	2.20	3 (20%)
3	NAG	F	1	1,3	14,14,15	0.59	0	17,19,21	1.06	1 (5%)
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	1.39	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	MAN	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	2.03	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C1-O5-C5	7.11	121.71	112.19
4	E	1	NAG	C1-O5-C5	7.04	121.63	112.19
2	C	1	NAG	C1-O5-C5	5.12	119.05	112.19
2	C	3	MAN	C1-O5-C5	4.18	117.79	112.19
4	E	2	NAG	C1-O5-C5	4.14	117.73	112.19
2	C	2	NAG	C1-O5-C5	3.83	117.32	112.19
4	E	2	NAG	C2-N2-C7	-3.81	117.80	122.90
3	F	2	NAG	C1-O5-C5	3.62	117.03	112.19
3	F	1	NAG	C1-O5-C5	3.30	116.60	112.19
2	C	2	NAG	O5-C1-C2	-3.24	106.28	111.29
4	E	3	MAN	C1-C2-C3	3.22	114.33	109.64
3	D	2	NAG	C1-O5-C5	3.15	116.40	112.19
4	E	3	MAN	O4-C4-C3	2.99	117.42	110.38
4	E	2	NAG	C4-C3-C2	-2.98	106.65	111.02
4	E	2	NAG	O4-C4-C3	2.79	116.96	110.38
4	E	4	MAN	C1-C2-C3	2.78	113.69	109.64
2	C	2	NAG	C2-N2-C7	-2.69	119.29	122.90
2	C	3	MAN	C1-C2-C3	2.62	113.46	109.64
3	F	2	NAG	O5-C1-C2	2.61	115.33	111.29
3	D	1	NAG	C4-C3-C2	2.53	114.72	111.02
4	E	4	MAN	C2-C3-C4	-2.49	106.49	110.86
2	C	1	NAG	C3-C4-C5	-2.45	105.79	110.23
4	E	2	NAG	C1-C2-N2	2.45	114.29	110.43
4	E	1	NAG	O5-C1-C2	-2.43	107.54	111.29
3	F	2	NAG	C2-N2-C7	-2.42	119.65	122.90
4	E	1	NAG	C3-C4-C5	-2.41	105.85	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C5-C4	2.37	116.59	110.83
2	C	3	MAN	C6-C5-C4	-2.27	107.43	113.02
4	E	3	MAN	O3-C3-C2	-2.11	105.75	110.05
2	C	2	NAG	C6-C5-C4	-2.10	107.85	113.02
4	E	3	MAN	O4-C4-C5	-2.06	104.25	109.32
3	D	2	NAG	C2-N2-C7	-2.05	120.15	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

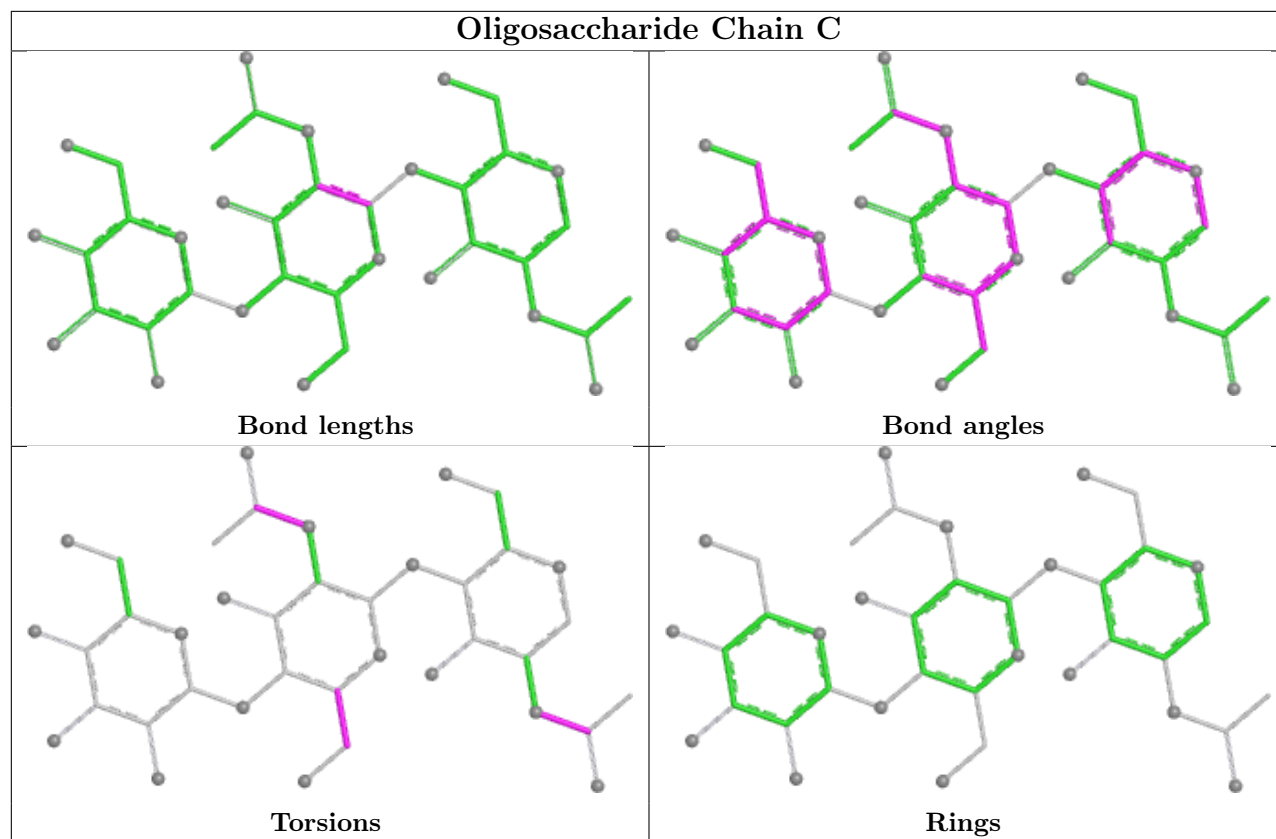
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
4	E	4	MAN	C4-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C1-C2-N2-C7

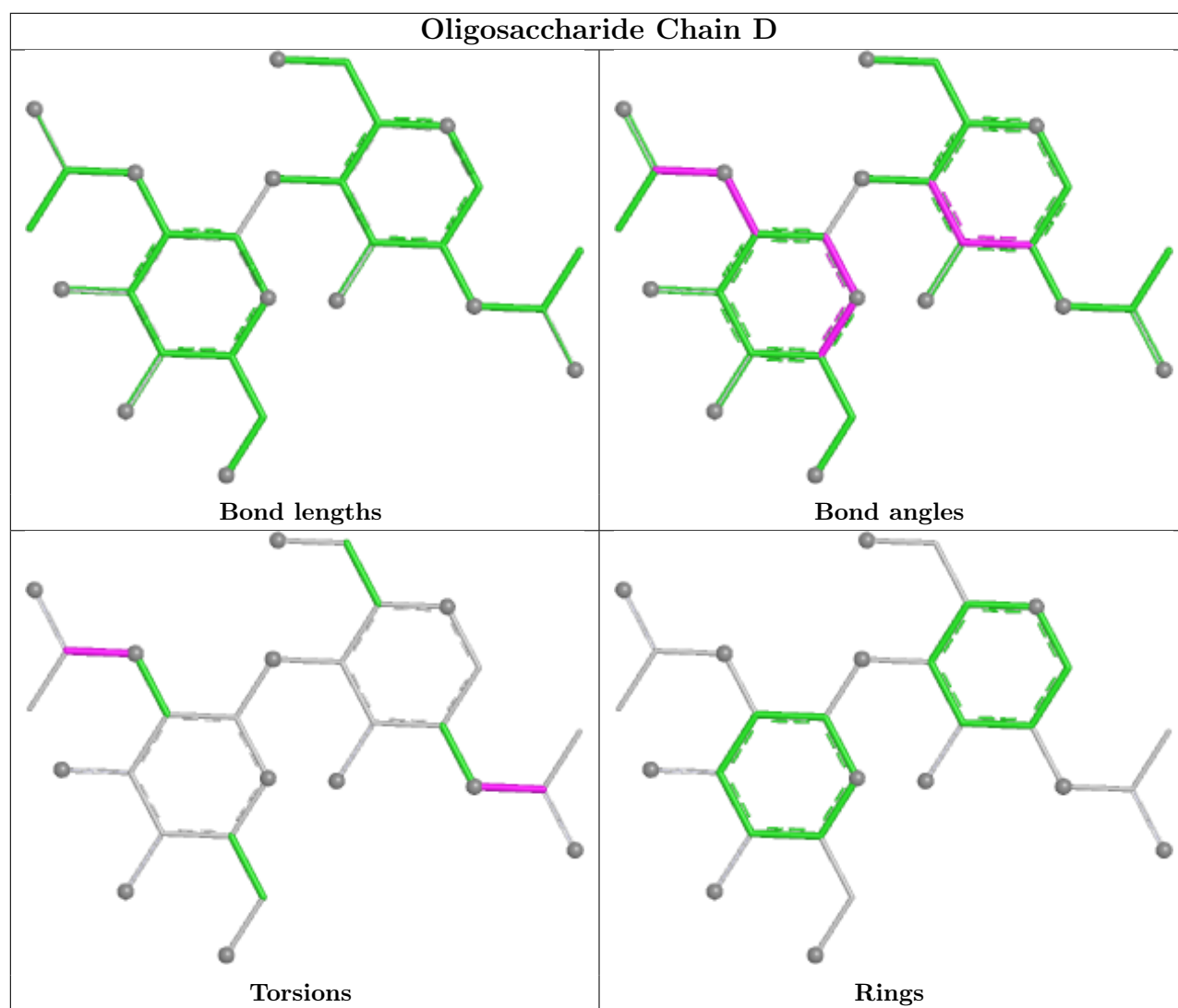
There are no ring outliers.

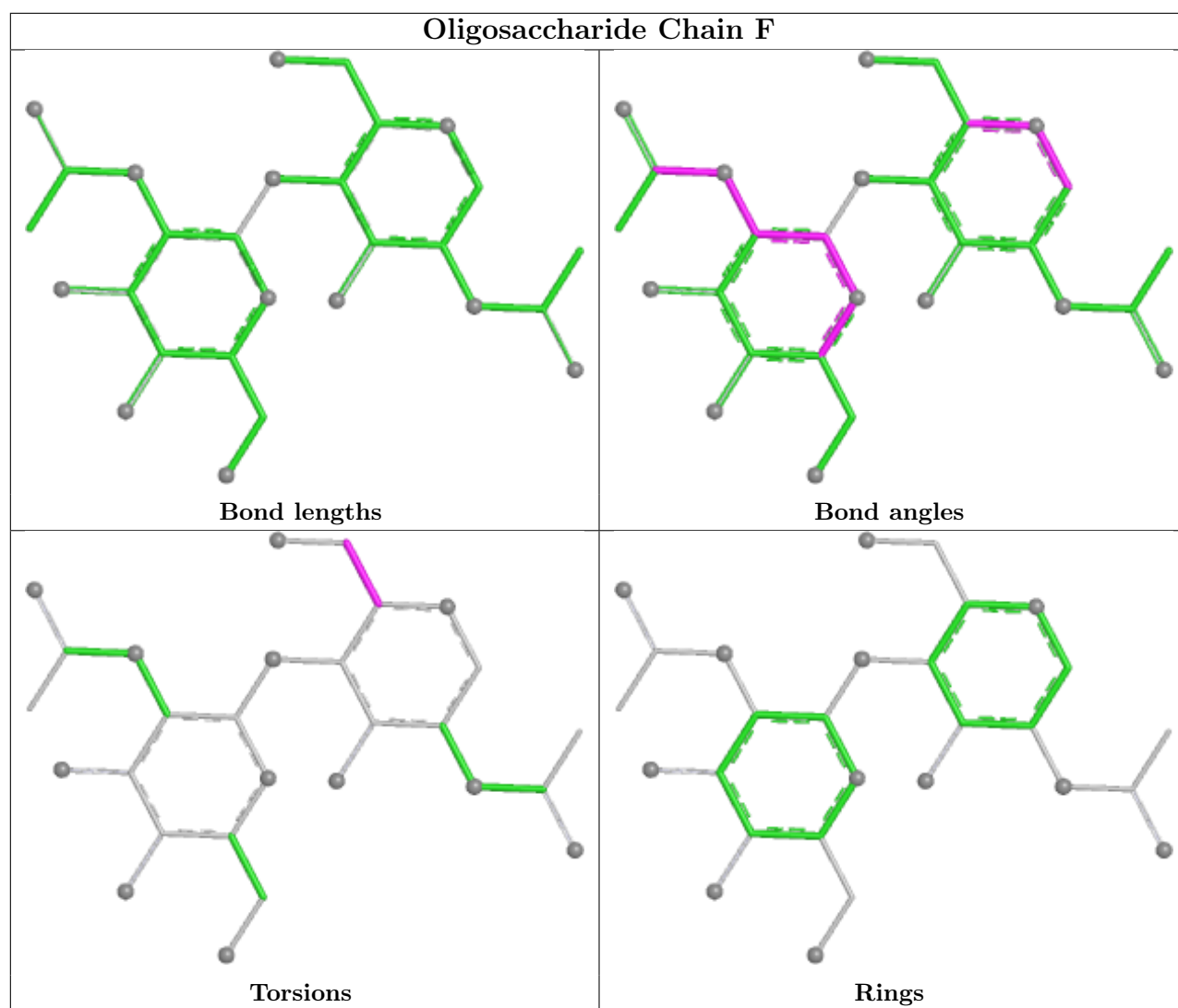
4 monomers are involved in 4 short contacts:

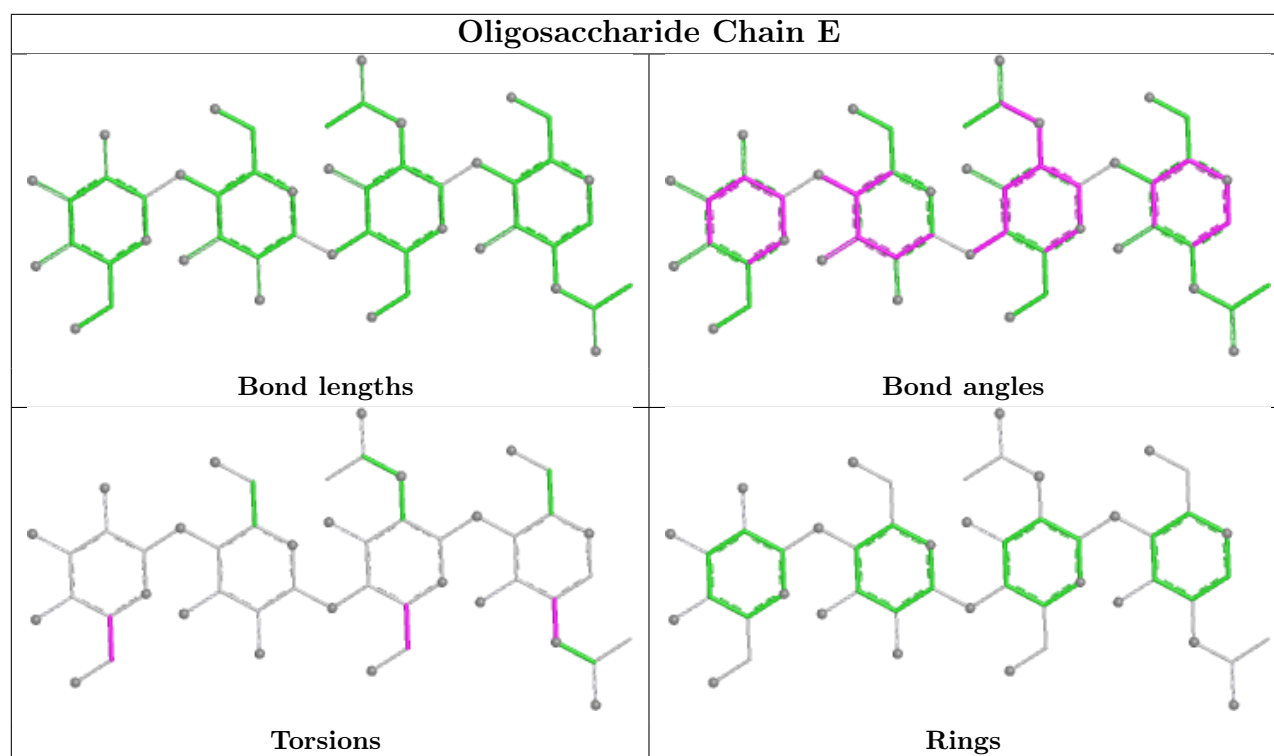
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	MAN	1	0
3	D	1	NAG	1	0
2	C	1	NAG	1	0
4	E	3	MAN	2	0

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









5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1010	1	14,14,15	0.85	1 (7%)	17,19,21	2.27	2 (11%)
5	NAG	A	1012	1	14,14,15	0.90	1 (7%)	17,19,21	0.53	0
5	NAG	A	1006	1	14,14,15	0.43	0	17,19,21	1.70	4 (23%)
5	NAG	A	1011	1	14,14,15	0.74	0	17,19,21	0.76	0
5	NAG	A	1009	1	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
5	NAG	B	1007	1	14,14,15	0.82	0	17,19,21	1.07	1 (5%)
5	NAG	A	1007	1	14,14,15	0.58	0	17,19,21	0.61	0
5	NAG	B	1008	1	14,14,15	0.59	0	17,19,21	1.09	1 (5%)
5	NAG	A	1008	1	14,14,15	0.56	0	17,19,21	1.96	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
5	NAG	A	1010	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1012	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1011	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1007	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1008	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1010	NAG	C1-C2	2.54	1.55	1.52
5	A	1012	NAG	C1-C2	2.02	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1010	NAG	C1-O5-C5	7.79	122.63	112.19
5	A	1008	NAG	C1-O5-C5	5.71	119.84	112.19
5	A	1006	NAG	C1-O5-C5	4.85	118.69	112.19
5	A	1010	NAG	O5-C1-C2	3.20	116.24	111.29
5	A	1008	NAG	O5-C1-C2	3.19	116.22	111.29
5	A	1008	NAG	C4-C3-C2	-3.07	106.52	111.02
5	A	1008	NAG	C2-N2-C7	-2.52	119.53	122.90
5	B	1008	NAG	C1-O5-C5	2.34	115.32	112.19
5	A	1009	NAG	C1-O5-C5	2.33	115.31	112.19
5	A	1006	NAG	O5-C5-C4	2.16	116.09	110.83
5	A	1006	NAG	C4-C3-C2	-2.06	108.00	111.02
5	A	1006	NAG	C2-N2-C7	-2.02	120.20	122.90
5	B	1007	NAG	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1008	NAG	C8-C7-N2-C2
5	A	1008	NAG	O7-C7-N2-C2
5	A	1010	NAG	C8-C7-N2-C2
5	A	1010	NAG	O7-C7-N2-C2
5	A	1012	NAG	O5-C5-C6-O6
5	A	1011	NAG	O5-C5-C6-O6
5	A	1011	NAG	C4-C5-C6-O6
5	A	1012	NAG	C4-C5-C6-O6
5	A	1007	NAG	C8-C7-N2-C2
5	A	1009	NAG	C8-C7-N2-C2
5	B	1007	NAG	C4-C5-C6-O6
5	A	1007	NAG	O7-C7-N2-C2
5	A	1009	NAG	O7-C7-N2-C2
5	A	1010	NAG	C4-C5-C6-O6
5	B	1007	NAG	O5-C5-C6-O6
5	A	1010	NAG	C3-C2-N2-C7
5	A	1008	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1012	NAG	1	0
5	A	1006	NAG	2	0
5	A	1011	NAG	6	0
5	B	1007	NAG	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	871/967 (90%)	-0.15	9 (1%)	79 59	33, 69, 108, 146	1 (0%)
1	B	862/967 (89%)	0.01	14 (1%)	70 47	20, 78, 116, 135	0
All	All	1733/1934 (89%)	-0.07	23 (1%)	75 53	20, 73, 113, 146	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	611	THR	8.7
1	B	610	ASP	5.5
1	A	54	PRO	3.8
1	B	612	LEU	3.7
1	B	502	SER	3.1
1	A	447	GLN	2.9
1	B	925	GLY	2.8
1	B	588	ILE	2.5
1	B	440	ALA	2.4
1	A	454	SER	2.3
1	B	538	MET	2.2
1	A	436	ILE	2.2
1	A	882[A]	HIS	2.2
1	A	696	LEU	2.2
1	B	133	PRO	2.2
1	B	882	HIS	2.1
1	A	532	ALA	2.1
1	B	609	THR	2.1
1	A	888	ASP	2.0
1	B	615	PRO	2.0
1	A	452	GLU	2.0
1	B	55	VAL	2.0
1	B	884	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

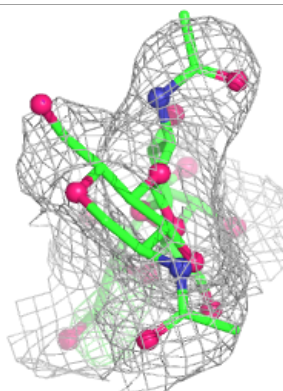
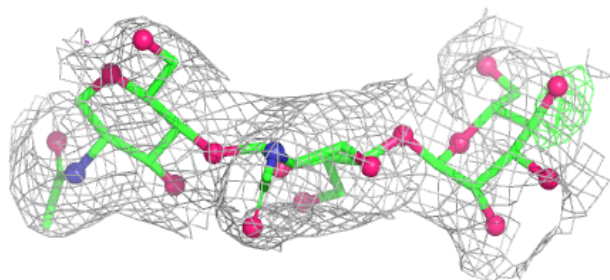
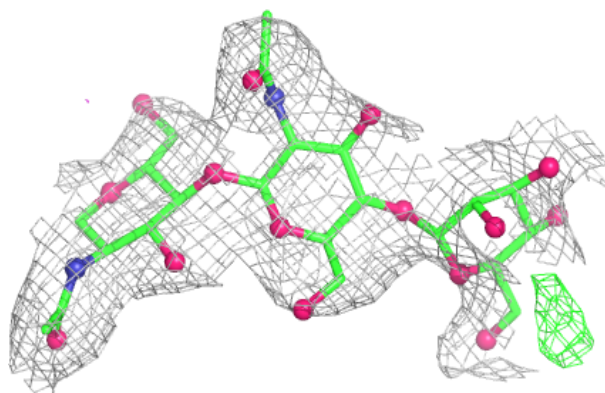
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	E	3	11/12	0.43	0.13	100,151,166,167	0
4	MAN	E	4	11/12	0.48	0.13	106,144,168,193	0
2	MAN	C	3	11/12	0.53	0.12	81,145,174,188	0
3	NAG	F	2	14/15	0.83	0.12	89,120,146,147	0
3	NAG	D	2	14/15	0.86	0.10	46,103,145,150	0
3	NAG	F	1	14/15	0.87	0.09	55,102,112,134	0
2	NAG	C	2	14/15	0.87	0.10	69,100,122,136	0
4	NAG	E	1	14/15	0.88	0.11	26,88,112,113	0
4	NAG	E	2	14/15	0.92	0.10	99,122,163,191	0
2	NAG	C	1	14/15	0.92	0.10	40,70,99,123	0
3	NAG	D	1	14/15	0.92	0.10	46,67,83,93	0

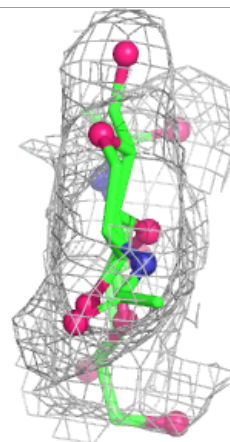
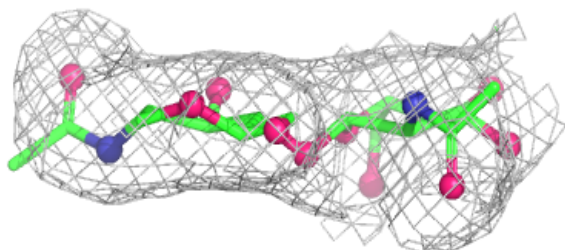
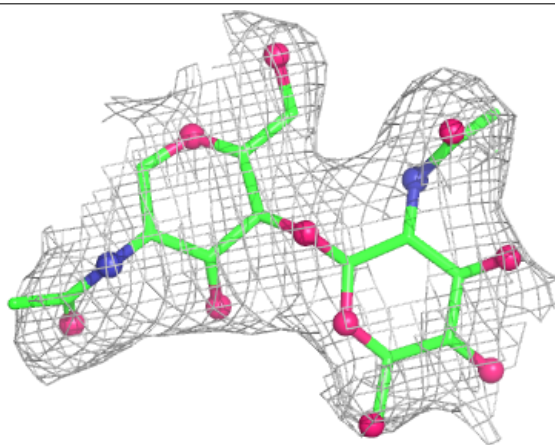
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

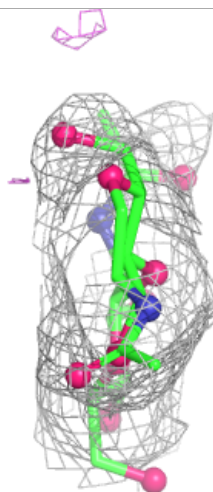
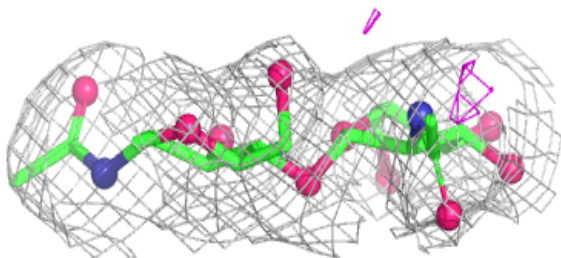
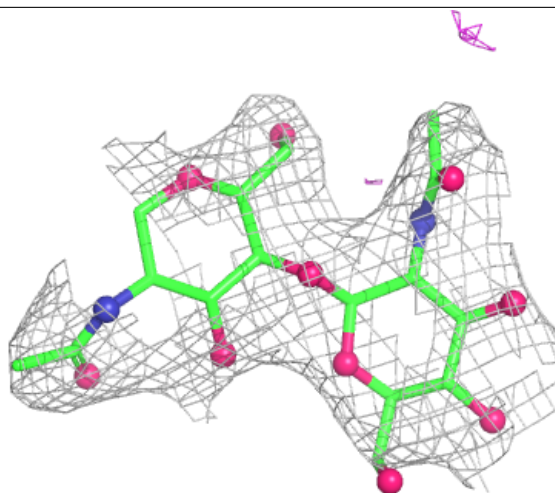
**Electron density around Chain D:**

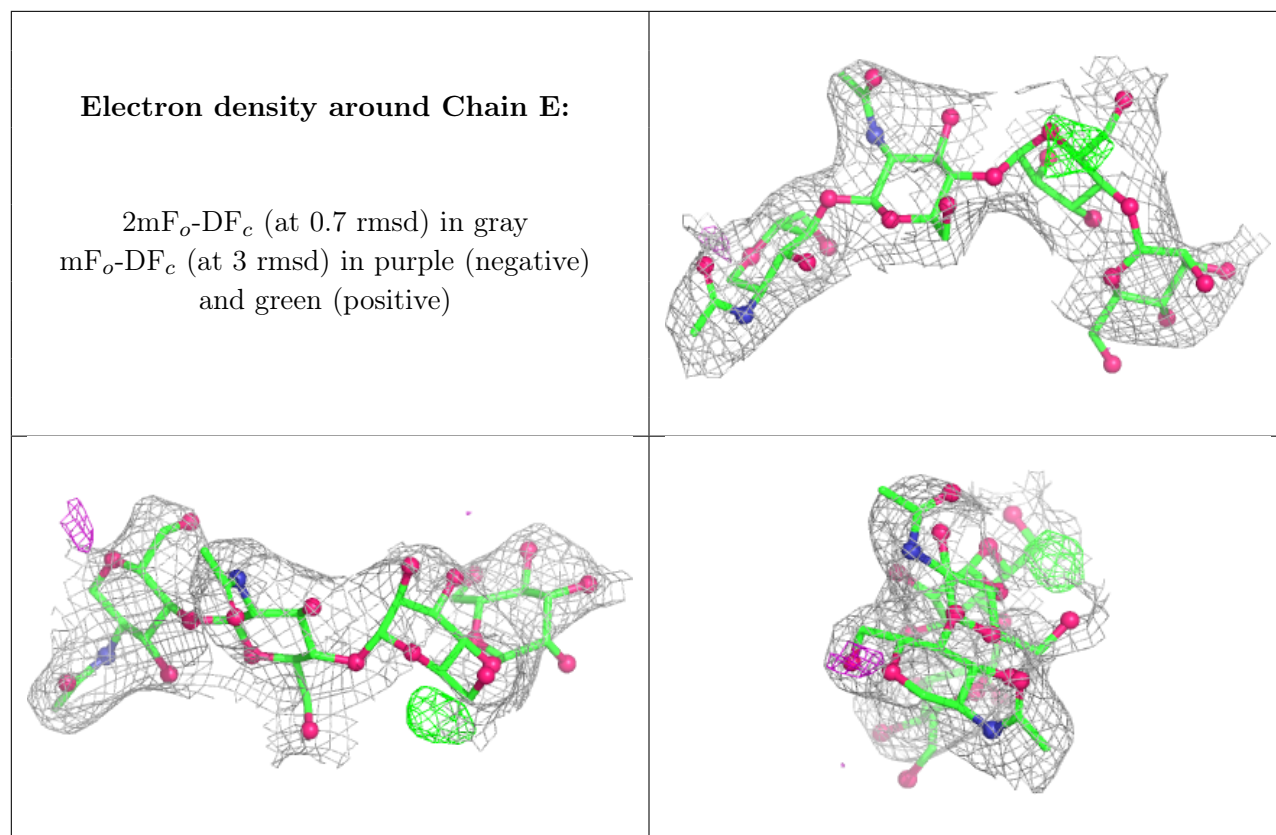
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

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
5	NAG	A	1009	14/15	0.42	0.16	92,170,183,186	0
5	NAG	B	1007	14/15	0.51	0.12	125,162,193,205	0
5	NAG	B	1008	14/15	0.56	0.12	72,135,184,187	0
5	NAG	A	1010	14/15	0.57	0.14	103,153,172,186	0
5	NAG	A	1008	14/15	0.68	0.16	109,152,178,178	0
5	NAG	A	1011	14/15	0.68	0.14	114,133,166,168	0
5	NAG	A	1012	14/15	0.70	0.10	109,156,196,208	0
5	NAG	A	1007	14/15	0.84	0.12	80,133,164,185	0
5	NAG	A	1006	14/15	0.88	0.11	84,132,146,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.