



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:56 AM BST

PDB ID : 2NY6  
Title : HIV-1 gp120 Envelope Glycoprotein (M95W, W96C, I109C, T123C, T257S, V275C, S334A, S375W, Q428C, G431C) Complexed with CD4 and Antibody 17b  
Authors : Zhou, T.; Xu, L.; Dey, B.; Hessel, A.J.; Van Ryk, D.; Xiang, S.H.; Yang, X.; Zhang, M.Y.; Zwick, M.B.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Sodroski, J.; Wyatt, R.; Nabel, G.J.; Kwong, P.D.  
Deposited on : 2006-11-20  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

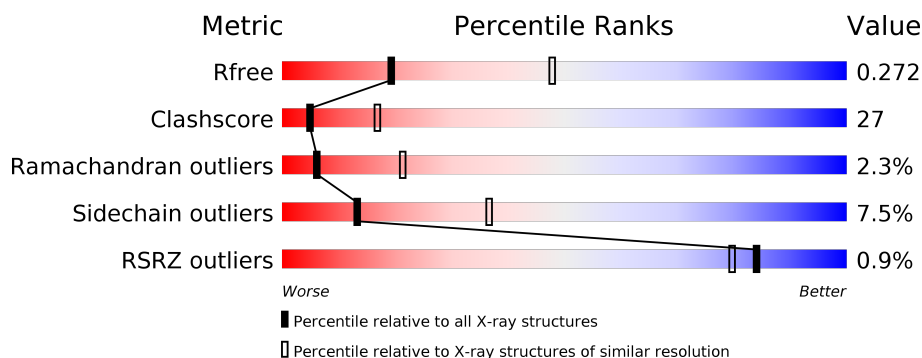
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	317	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>5%</div> <div></div> </div> </div>
2	B	184	<div> <div></div> <div> <div>49%</div> <div>39%</div> <div>10%</div> <div></div> </div> </div>
3	C	214	<div> <div></div> <div> <div>58%</div> <div>39%</div> <div></div> </div> </div>
4	D	229	<div> <div></div> <div> <div>62%</div> <div>31%</div> <div></div> </div> </div>
5	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7332 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 ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2350	1473	410	442	25			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1412	885	247	276	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	MET	-	initiating methionine	UNP P01730

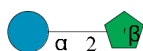
- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	222	Total	C	N	O	S	0	0	0
			1674	1059	280	330	5			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	2	Total	C	O	0	0	0
			23	12	11			

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



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

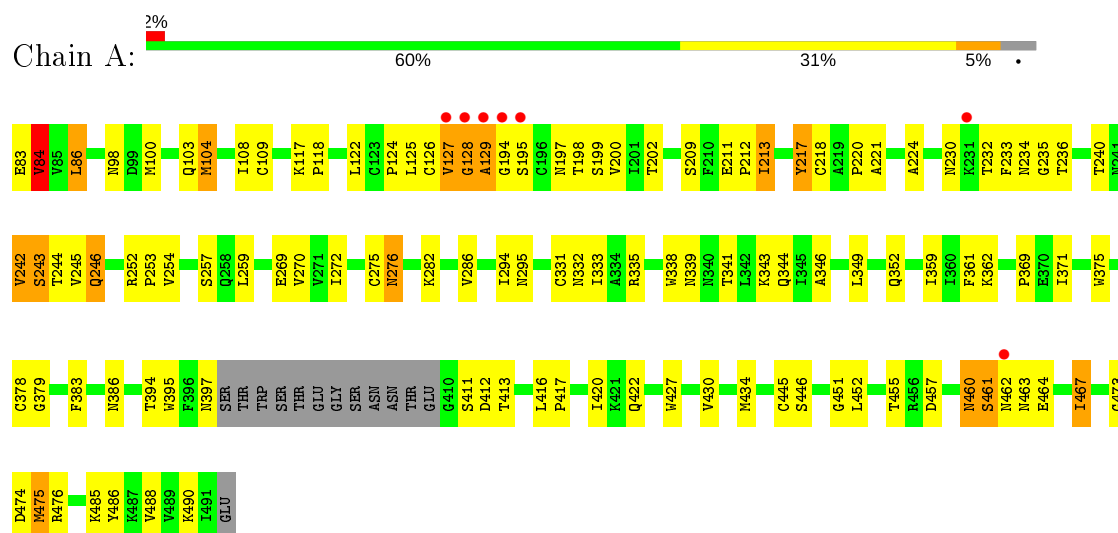
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total 42	O 42	0	0
7	B	17	Total 17	O 17	0	0
7	C	28	Total 28	O 28	0	0
7	D	28	Total 28	O 28	0	0

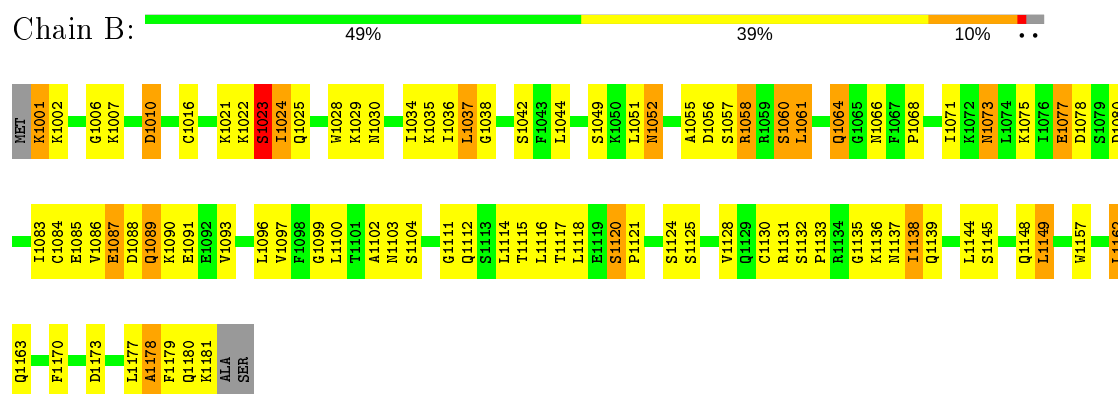
### 3 Residue-property plots

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.

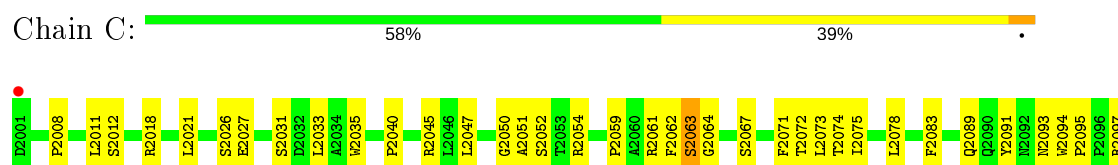
#### • Molecule 1: ENVELOPE GLYCOPROTEIN GP120



#### • Molecule 2: T-cell surface glycoprotein CD4

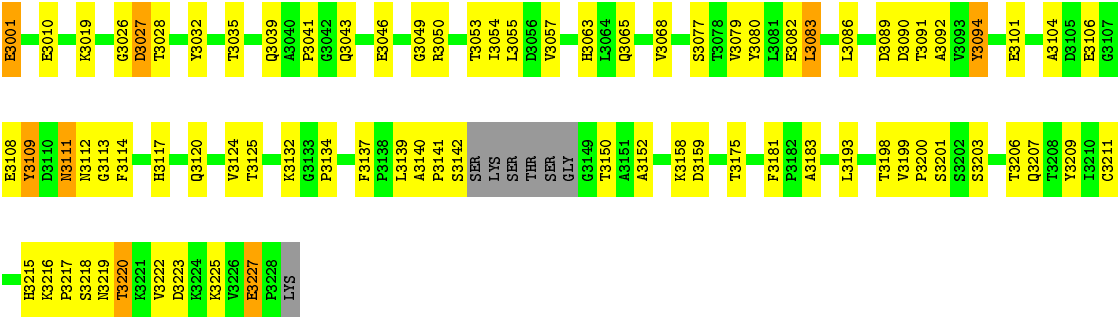


#### • Molecule 3: ANTIBODY 17B, LIGHT CHAIN





• Molecule 4: ANTIBODY 17B, HEAVY CHAIN



• Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.31Å 87.02Å 196.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.37 – 2.80 42.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	78.8 (42.37-2.80) 78.8 (42.36-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.276 0.190 , 0.272	Depositor DCC
$R_{free}$ test set	1188 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GLC, NAG, FRU

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	0.37	0/2398	0.53	0/3252
2	B	0.34	0/1432	0.51	0/1930
3	C	0.38	0/1683	0.53	0/2288
4	D	0.66	4/1713 (0.2%)	0.58	1/2335 (0.0%)
All	All	0.45	4/7226 (0.1%)	0.54	1/9805 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3227	GLU	CD-OE1	13.50	1.40	1.25
4	D	3227	GLU	CG-CD	12.89	1.71	1.51
4	D	3227	GLU	CB-CG	7.88	1.67	1.52
4	D	3227	GLU	CD-OE2	6.83	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3227	GLU	CB-CG-CD	-5.37	99.69	114.20

There are no chirality outliers.

There are no planarity outliers.

### 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	2350	0	2286	119	0
2	B	1412	0	1441	101	0
3	C	1646	0	1590	95	0
4	D	1674	0	1636	87	0
5	E	23	0	21	2	0
6	A	112	0	104	7	0
7	A	42	0	0	16	0
7	B	17	0	0	9	0
7	C	28	0	0	16	0
7	D	28	0	0	17	0
All	All	7332	0	7078	392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (392) 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)
2:B:1121:PRO:CD	7:B:17:HOH:O	1.78	1.25
4:D:3112:ASN:HA	7:D:103:HOH:O	1.43	1.18
1:A:117:LYS:HB2	7:A:978:HOH:O	1.40	1.16
2:B:1121:PRO:HD3	7:B:17:HOH:O	1.34	1.11
3:C:2177:LEU:C	3:C:2177:LEU:HD23	1.74	1.08
3:C:2067:SER:HB3	7:C:36:HOH:O	1.54	1.08
2:B:1075:LYS:HB3	2:B:1077:GLU:OE1	1.57	1.05
4:D:3134:PRO:HD2	7:D:107:HOH:O	1.61	1.00
1:A:422:GLN:NE2	7:A:967:HOH:O	1.95	0.99
1:A:217:TYR:HD1	1:A:218:CYS:N	1.59	0.99
2:B:1121:PRO:CG	7:B:17:HOH:O	1.95	0.98
4:D:3150:THR:HA	7:D:3:HOH:O	1.63	0.97
4:D:3001:GLU:OE1	4:D:3001:GLU:HA	1.61	0.97
4:D:3201:SER:N	7:D:105:HOH:O	1.96	0.96
2:B:1121:PRO:HG3	7:B:17:HOH:O	1.54	0.95
4:D:3027:ASP:OD1	4:D:3032:TYR:OH	1.86	0.93
2:B:1077:GLU:CD	2:B:1077:GLU:H	1.71	0.90
3:C:2067:SER:HA	3:C:2071:PHE:CE2	2.07	0.89
1:A:339:ASN:OD1	6:A:839:NAG:H2	1.73	0.89
4:D:3206:THR:HG23	4:D:3207:GLN:N	1.85	0.88
2:B:1100:LEU:HD23	2:B:1117:THR:O	1.73	0.88
2:B:1058:ARG:HB3	2:B:1058:ARG:HH11	1.38	0.88
1:A:217:TYR:C	1:A:217:TYR:HD1	1.78	0.87
2:B:1180:GLN:HG3	2:B:1181:LYS:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ASN:HB2	7:A:980:HOH:O	1.75	0.86
2:B:1124:SER:HB2	2:B:1163:GLN:NE2	1.90	0.85
4:D:3141:PRO:O	4:D:3142:SER:HB2	1.76	0.84
1:A:455:THR:CG2	2:B:1035:LYS:HZ1	1.92	0.83
4:D:3203:SER:HG	4:D:3209:TYR:HH	1.07	0.83
3:C:2127:LEU:O	7:C:85:HOH:O	1.96	0.83
4:D:3054:ILE:HG23	4:D:3055:LEU:HD13	1.59	0.82
1:A:217:TYR:CD1	1:A:218:CYS:N	2.48	0.82
1:A:104:MET:HA	1:A:104:MET:CE	2.10	0.82
1:A:269:GLU:HB3	6:A:789:NAG:H61	1.61	0.81
1:A:455:THR:CG2	2:B:1035:LYS:NZ	2.44	0.81
2:B:1086:VAL:O	2:B:1088:ASP:N	2.13	0.81
3:C:2094:TRP:HA	3:C:2095:PRO:C	2.02	0.80
3:C:2061:ARG:HG2	7:C:73:HOH:O	1.81	0.80
4:D:3225:LYS:HE2	4:D:3227:GLU:HG3	1.64	0.80
1:A:213:ILE:HD13	1:A:213:ILE:H	1.45	0.80
3:C:2144:ARG:NH2	7:C:84:HOH:O	2.14	0.80
1:A:202:THR:HG22	3:C:2095:PRO:HG3	1.64	0.79
3:C:2061:ARG:N	7:C:73:HOH:O	2.16	0.79
4:D:3206:THR:CG2	4:D:3207:GLN:H	1.95	0.79
2:B:1087:GLU:O	2:B:1088:ASP:HB3	1.81	0.78
4:D:3206:THR:HG23	4:D:3207:GLN:H	1.45	0.78
1:A:217:TYR:CD1	1:A:217:TYR:C	2.54	0.78
1:A:455:THR:HG23	2:B:1035:LYS:HZ1	1.50	0.77
1:A:275:CYS:O	1:A:276:ASN:HB2	1.83	0.77
4:D:3026:GLY:O	4:D:3027:ASP:HB2	1.83	0.77
4:D:3140:ALA:O	7:D:130:HOH:O	2.02	0.76
4:D:3206:THR:CG2	4:D:3207:GLN:N	2.49	0.76
1:A:451:GLY:C	1:A:452:LEU:HD12	2.05	0.76
2:B:1058:ARG:CB	2:B:1058:ARG:HH11	1.99	0.75
3:C:2177:LEU:C	3:C:2177:LEU:CD2	2.50	0.75
3:C:2177:LEU:HD23	3:C:2178:SER:N	2.02	0.75
7:A:967:HOH:O	4:D:3108:GLU:HA	1.87	0.75
1:A:217:TYR:HE1	1:A:218:CYS:O	1.70	0.74
4:D:3200:PRO:HA	7:D:105:HOH:O	1.86	0.74
4:D:3054:ILE:HG23	4:D:3055:LEU:CD1	2.18	0.73
1:A:117:LYS:CB	7:A:978:HOH:O	2.14	0.73
3:C:2183:LEU:C	7:C:41:HOH:O	2.26	0.73
1:A:122:LEU:HD22	1:A:200:VAL:HG22	1.70	0.73
4:D:3193:LEU:C	4:D:3193:LEU:HD12	2.09	0.73
4:D:3050:ARG:NH2	4:D:3101:GLU:OE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:LEU:HA	7:B:108:HOH:O	1.88	0.72
4:D:3216:LYS:N	4:D:3217:PRO:CD	2.53	0.72
2:B:1124:SER:HB2	2:B:1163:GLN:HE21	1.52	0.72
3:C:2054:ARG:NE	7:C:58:HOH:O	1.98	0.72
1:A:83:GLU:O	1:A:84:VAL:HG13	1.88	0.72
3:C:2195:ALA:HA	3:C:2210:SER:HB3	1.71	0.72
2:B:1075:LYS:CB	2:B:1077:GLU:OE1	2.36	0.71
1:A:485:LYS:HD3	7:A:975:HOH:O	1.90	0.71
1:A:117:LYS:HD3	7:A:978:HOH:O	1.90	0.71
3:C:2183:LEU:O	7:C:41:HOH:O	2.08	0.71
2:B:1180:GLN:O	2:B:1181:LYS:HD2	1.90	0.71
3:C:2011:LEU:HB3	3:C:2106:LEU:HD12	1.71	0.71
3:C:2137:LEU:C	3:C:2138:LEU:HD12	2.10	0.71
1:A:217:TYR:CE1	1:A:218:CYS:O	2.43	0.71
3:C:2160:ASN:O	3:C:2181:LEU:HD12	1.89	0.71
1:A:379:GLY:N	7:A:956:HOH:O	1.94	0.71
3:C:2185:LYS:HE2	3:C:2189:GLU:OE2	1.92	0.70
2:B:1099:GLY:O	2:B:1118:LEU:HD12	1.92	0.70
2:B:1061:LEU:HD23	2:B:1061:LEU:N	2.06	0.70
2:B:1088:ASP:O	2:B:1088:ASP:OD1	2.09	0.69
2:B:1073:ASN:HD22	2:B:1073:ASN:C	1.96	0.68
4:D:3134:PRO:HD2	4:D:3220:THR:HG21	1.76	0.68
1:A:122:LEU:CD2	1:A:200:VAL:HG22	2.25	0.67
1:A:83:GLU:OE1	1:A:246:GLN:HG2	1.94	0.67
2:B:1085:GLU:OE2	2:B:1090:LYS:HE3	1.94	0.67
1:A:371:ILE:HD11	1:A:473:GLY:HA3	1.76	0.67
3:C:2188:TYR:O	3:C:2194:TYR:OH	2.12	0.67
4:D:3046:GLU:OE1	4:D:3063:HIS:CE1	2.47	0.67
1:A:98:ASN:OD1	1:A:100:MET:HG3	1.95	0.67
3:C:2054:ARG:NH1	3:C:2062:PHE:O	2.28	0.66
2:B:1066:ASN:O	2:B:1068:PRO:HD3	1.95	0.66
4:D:3001:GLU:OE1	4:D:3001:GLU:CA	2.37	0.66
1:A:104:MET:HE2	1:A:104:MET:HA	1.76	0.66
1:A:379:GLY:CA	7:A:956:HOH:O	2.39	0.66
1:A:242:VAL:CG2	1:A:243:SER:N	2.58	0.66
1:A:209:SER:HB2	1:A:379:GLY:HA2	1.78	0.65
2:B:1178:ALA:O	2:B:1179:PHE:HB3	1.96	0.65
2:B:1061:LEU:HB3	2:B:1066:ASN:HB2	1.78	0.65
1:A:412:ASP:C	1:A:412:ASP:OD1	2.35	0.65
1:A:126:CYS:SG	2:B:1060:SER:HB2	2.37	0.65
3:C:2177:LEU:O	3:C:2177:LEU:HD23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2012:SER:HB3	3:C:2109:LYS:HE2	1.78	0.64
2:B:1058:ARG:CB	2:B:1058:ARG:NH1	2.61	0.64
4:D:3150:THR:O	7:D:39:HOH:O	2.13	0.64
2:B:1089:GLN:HG2	2:B:1090:LYS:N	2.13	0.63
4:D:3120:GLN:N	4:D:3120:GLN:OE1	2.29	0.63
7:A:957:HOH:O	4:D:3108:GLU:HB2	1.97	0.63
1:A:117:LYS:CD	7:A:978:HOH:O	2.44	0.63
1:A:430:VAL:HG12	1:A:430:VAL:O	1.98	0.63
4:D:3222:VAL:HG12	4:D:3223:ASP:N	2.14	0.63
1:A:269:GLU:HB3	6:A:789:NAG:C6	2.29	0.62
2:B:1066:ASN:O	2:B:1068:PRO:CD	2.47	0.62
1:A:341:THR:HA	1:A:344:GLN:HE21	1.64	0.62
3:C:2120:PHE:CD1	4:D:3139:LEU:HB3	2.35	0.62
1:A:125:LEU:HD12	1:A:126:CYS:H	1.64	0.61
4:D:3152:ALA:HB2	4:D:3198:THR:HG22	1.81	0.61
4:D:3090:ASP:O	4:D:3094:TYR:OH	2.15	0.61
2:B:1007:LYS:O	2:B:1010:ASP:HB2	2.01	0.61
4:D:3141:PRO:O	4:D:3142:SER:CB	2.48	0.61
1:A:84:VAL:O	1:A:243:SER:HB3	2.01	0.60
3:C:2184:SER:HA	7:C:41:HOH:O	2.00	0.60
2:B:1073:ASN:O	2:B:1073:ASN:ND2	2.27	0.60
2:B:1086:VAL:HG22	2:B:1087:GLU:N	2.17	0.59
2:B:1115:THR:HB	7:B:66:HOH:O	2.00	0.59
1:A:379:GLY:HA2	7:A:956:HOH:O	2.00	0.59
4:D:3199:VAL:HB	4:D:3200:PRO:HD2	1.85	0.59
1:A:270:VAL:H	6:A:789:NAG:H61	1.68	0.58
2:B:1077:GLU:CD	2:B:1077:GLU:N	2.50	0.58
3:C:2091:TYR:HA	3:C:2098:TYR:CD1	2.38	0.58
1:A:84:VAL:O	1:A:243:SER:CB	2.52	0.58
1:A:269:GLU:HA	6:A:789:NAG:O5	2.04	0.58
6:A:839:NAG:H83	6:A:839:NAG:H3	1.85	0.58
3:C:2073:LEU:HD12	3:C:2074:THR:H	1.69	0.58
3:C:2134:VAL:HG12	3:C:2150:TRP:CH2	2.38	0.57
7:A:967:HOH:O	4:D:3109:TYR:N	2.28	0.57
4:D:3063:HIS:NE2	5:E:2:FRU:H61	2.18	0.57
1:A:104:MET:HE3	1:A:104:MET:HA	1.86	0.57
4:D:3219:ASN:CG	4:D:3219:ASN:O	2.42	0.57
3:C:2059:PRO:HB2	7:C:73:HOH:O	2.04	0.57
3:C:2008:PRO:O	3:C:2104:THR:HG23	2.03	0.57
1:A:127:VAL:O	1:A:128:GLY:C	2.43	0.57
4:D:3199:VAL:HB	4:D:3200:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2153:ASP:OD1	3:C:2193:VAL:HG12	2.04	0.56
3:C:2061:ARG:O	3:C:2075:ILE:HA	2.05	0.56
4:D:3019:LYS:HD3	7:D:96:HOH:O	2.04	0.56
4:D:3200:PRO:CA	7:D:105:HOH:O	2.49	0.56
3:C:2073:LEU:HD12	3:C:2074:THR:N	2.20	0.56
4:D:3108:GLU:OE2	7:D:120:HOH:O	2.17	0.56
1:A:386:ASN:HB3	1:A:417:PRO:HG2	1.88	0.56
2:B:1064:GLN:N	2:B:1064:GLN:OE1	2.39	0.56
3:C:2183:LEU:N	3:C:2183:LEU:HD23	2.21	0.56
3:C:2059:PRO:C	7:C:73:HOH:O	2.44	0.55
1:A:109:CYS:SG	1:A:427:TRP:CZ3	2.99	0.55
1:A:452:LEU:N	1:A:452:LEU:HD12	2.20	0.55
2:B:1180:GLN:HG3	2:B:1181:LYS:N	2.18	0.55
4:D:3215:HIS:HB3	4:D:3220:THR:HG22	1.88	0.55
3:C:2114:ALA:HB2	3:C:2202:GLY:O	2.06	0.55
4:D:3055:LEU:HB3	4:D:3057:VAL:HG23	1.89	0.55
1:A:352:GLN:O	1:A:352:GLN:HG3	2.07	0.55
3:C:2031:SER:O	3:C:2050:GLY:HA2	2.06	0.55
4:D:3094:TYR:CD2	4:D:3094:TYR:N	2.74	0.55
2:B:1023:SER:OG	2:B:1023:SER:O	2.25	0.55
1:A:257:SER:O	1:A:259:LEU:N	2.38	0.54
1:A:461:SER:C	1:A:463:ASN:H	2.08	0.54
1:A:474:ASP:O	1:A:476:ARG:N	2.40	0.54
2:B:1037:LEU:HG	2:B:1044:LEU:HD11	1.90	0.54
3:C:2177:LEU:HA	4:D:3181:PHE:HE2	1.72	0.54
2:B:1037:LEU:HD23	2:B:1037:LEU:C	2.28	0.54
3:C:2093:ASN:O	7:C:86:HOH:O	2.18	0.54
1:A:272:ILE:HG22	1:A:286:VAL:HG22	1.90	0.54
1:A:332:ASN:O	1:A:333:ILE:HG13	2.07	0.54
2:B:1057:SER:OG	2:B:1058:ARG:N	2.41	0.54
3:C:2033:LEU:HD22	3:C:2089:GLN:O	2.08	0.54
1:A:455:THR:HG21	2:B:1035:LYS:NZ	2.23	0.54
3:C:2059:PRO:HD2	3:C:2062:PHE:CD2	2.43	0.54
1:A:128:GLY:O	1:A:129:ALA:HB3	2.08	0.54
1:A:294:ILE:HG23	1:A:294:ILE:O	2.08	0.53
3:C:2130:GLY:O	3:C:2185:LYS:HB2	2.07	0.53
3:C:2107:GLU:O	3:C:2107:GLU:HG3	2.08	0.53
4:D:3028:THR:HG22	7:D:77:HOH:O	2.08	0.53
4:D:3035:THR:HG23	4:D:3049:GLY:O	2.07	0.53
4:D:3216:LYS:N	4:D:3217:PRO:HD3	2.24	0.53
4:D:3027:ASP:OD1	4:D:3032:TYR:CZ	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1016:CYS:HA	2:B:1091:GLU:OE2	2.08	0.53
4:D:3113:GLY:HA2	7:D:12:HOH:O	2.08	0.53
4:D:3225:LYS:HE2	4:D:3227:GLU:CG	2.36	0.53
4:D:3010:GLU:HB2	4:D:3124:VAL:HG22	1.91	0.53
2:B:1083:ILE:HD12	2:B:1083:ILE:N	2.24	0.52
2:B:1131:ARG:HA	2:B:1136:LYS:O	2.10	0.52
1:A:104:MET:O	1:A:108:ILE:HG12	2.09	0.52
1:A:461:SER:O	1:A:463:ASN:N	2.43	0.52
2:B:1180:GLN:HA	2:B:1180:GLN:OE1	2.08	0.52
1:A:84:VAL:CG2	1:A:244:THR:HB	2.39	0.52
4:D:3183:ALA:HA	4:D:3193:LEU:HB3	1.92	0.52
2:B:1028:TRP:CH2	2:B:1084:CYS:HB2	2.45	0.52
2:B:1061:LEU:O	2:B:1064:GLN:HB2	2.09	0.52
4:D:3028:THR:CG2	7:D:77:HOH:O	2.58	0.52
1:A:341:THR:HA	1:A:344:GLN:NE2	2.25	0.51
2:B:1086:VAL:C	2:B:1088:ASP:N	2.62	0.51
2:B:1103:ASN:HA	7:B:29:HOH:O	2.08	0.51
2:B:1112:GLN:O	2:B:1149:LEU:HD22	2.11	0.51
3:C:2183:LEU:N	3:C:2183:LEU:CD2	2.73	0.51
2:B:1073:ASN:ND2	2:B:1073:ASN:C	2.64	0.51
1:A:125:LEU:HD12	1:A:126:CYS:N	2.26	0.51
1:A:461:SER:C	1:A:463:ASN:N	2.64	0.51
1:A:86:LEU:N	1:A:86:LEU:CD1	2.74	0.51
3:C:2045:ARG:NH1	7:C:67:HOH:O	2.17	0.51
2:B:1089:GLN:CG	2:B:1090:LYS:N	2.74	0.51
4:D:3200:PRO:C	7:D:105:HOH:O	2.41	0.51
4:D:3193:LEU:C	4:D:3193:LEU:CD1	2.78	0.50
1:A:362:LYS:HD2	1:A:467:ILE:HG21	1.92	0.50
3:C:2122:PRO:HD3	3:C:2134:VAL:HG22	1.92	0.50
4:D:3091:THR:HG23	4:D:3125:THR:HA	1.93	0.50
2:B:1086:VAL:C	2:B:1088:ASP:H	2.15	0.50
1:A:455:THR:HG22	7:A:972:HOH:O	2.12	0.50
3:C:2026:SER:O	3:C:2027:GLU:HB3	2.11	0.50
3:C:2050:GLY:O	3:C:2051:ALA:HB3	2.11	0.50
1:A:242:VAL:HG23	1:A:243:SER:N	2.25	0.50
4:D:3222:VAL:CG1	4:D:3223:ASP:N	2.74	0.50
2:B:1100:LEU:CD2	2:B:1117:THR:O	2.54	0.49
3:C:2183:LEU:H	3:C:2183:LEU:HD23	1.75	0.49
1:A:84:VAL:HG23	1:A:244:THR:HB	1.93	0.49
1:A:394:THR:HG21	1:A:397:ASN:HD22	1.76	0.49
1:A:109:CYS:SG	1:A:427:TRP:CH2	3.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1075:LYS:N	2:B:1078:ASP:OD2	2.32	0.49
4:D:3027:ASP:OD1	4:D:3032:TYR:CE1	2.65	0.49
2:B:1036:ILE:HD13	2:B:1049:SER:HB3	1.95	0.49
3:C:2021:LEU:N	3:C:2021:LEU:HD12	2.28	0.48
1:A:209:SER:HB2	1:A:379:GLY:CA	2.41	0.48
3:C:2054:ARG:NH1	3:C:2054:ARG:HG3	2.28	0.48
4:D:3101:GLU:OE1	4:D:3111:ASN:N	2.45	0.48
2:B:1088:ASP:C	2:B:1088:ASP:OD1	2.51	0.48
3:C:2134:VAL:HG12	3:C:2150:TRP:HH2	1.79	0.48
3:C:2152:VAL:O	3:C:2155:ALA:HB3	2.14	0.48
2:B:1120:SER:HB3	2:B:1121:PRO:HD2	1.95	0.48
4:D:3079:VAL:HG12	4:D:3080:TYR:N	2.29	0.48
3:C:2035:TRP:O	3:C:2047:LEU:HB2	2.13	0.48
3:C:2136:CYS:HB2	3:C:2150:TRP:CH2	2.49	0.48
3:C:2137:LEU:HD12	3:C:2138:LEU:H	1.79	0.47
3:C:2067:SER:HA	3:C:2071:PHE:CZ	2.48	0.47
1:A:272:ILE:HD12	1:A:349:LEU:HD23	1.95	0.47
2:B:1030:ASN:HB2	2:B:1080:ASP:OD2	2.15	0.47
1:A:338:TRP:O	1:A:341:THR:N	2.47	0.47
3:C:2184:SER:CA	7:C:41:HOH:O	2.60	0.47
1:A:233:PHE:CE2	1:A:235:GLY:HA2	2.49	0.47
1:A:420:ILE:HD12	1:A:420:ILE:N	2.29	0.47
2:B:1007:LYS:HG3	2:B:1170:PHE:CE1	2.50	0.47
2:B:1055:ALA:O	2:B:1056:ASP:HB2	2.14	0.47
1:A:103:GLN:OE1	1:A:103:GLN:HA	2.14	0.47
2:B:1024:ILE:HD12	2:B:1024:ILE:H	1.80	0.47
2:B:1100:LEU:HD23	2:B:1100:LEU:HA	1.62	0.47
3:C:2011:LEU:HD23	3:C:2106:LEU:CD1	2.45	0.47
4:D:3152:ALA:CB	4:D:3198:THR:HG22	2.44	0.47
2:B:1058:ARG:HB2	2:B:1058:ARG:NH1	2.30	0.46
3:C:2054:ARG:HH11	3:C:2054:ARG:HG3	1.79	0.46
3:C:2120:PHE:CE1	4:D:3139:LEU:O	2.68	0.46
1:A:86:LEU:CD1	1:A:86:LEU:H	2.28	0.46
2:B:1103:ASN:OD1	2:B:1104:SER:N	2.48	0.46
2:B:1178:ALA:O	2:B:1179:PHE:CB	2.62	0.46
4:D:3158:LYS:O	4:D:3159:ASP:HB2	2.15	0.46
2:B:1051:LEU:HD21	2:B:1071:ILE:HD13	1.97	0.46
4:D:3063:HIS:CD2	5:E:2:FRU:H61	2.51	0.46
4:D:3207:GLN:HA	4:D:3207:GLN:OE1	2.14	0.46
1:A:211:GLU:HA	1:A:212:PRO:HD2	1.80	0.46
1:A:242:VAL:HG23	1:A:243:SER:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1077:GLU:N	2:B:1077:GLU:OE2	2.47	0.46
4:D:3201:SER:CB	7:D:102:HOH:O	2.63	0.46
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.50	0.46
2:B:1029:LYS:HA	2:B:1034:ILE:O	2.16	0.46
1:A:375:TRP:HA	1:A:383:PHE:O	2.15	0.46
2:B:1066:ASN:C	2:B:1068:PRO:HD3	2.36	0.46
3:C:2138:LEU:HD12	3:C:2138:LEU:N	2.30	0.46
1:A:124:PRO:HA	1:A:198:THR:HA	1.98	0.46
1:A:230:ASN:HB3	1:A:232:THR:O	2.16	0.46
2:B:1111:GLY:HA2	2:B:1148:GLN:HB3	1.98	0.46
1:A:460:ASN:O	1:A:461:SER:HB2	2.15	0.45
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.98	0.45
1:A:86:LEU:HD13	1:A:86:LEU:H	1.81	0.45
2:B:1162:LEU:HD23	2:B:1163:GLN:N	2.31	0.45
3:C:2195:ALA:CA	3:C:2210:SER:HB3	2.43	0.45
1:A:275:CYS:O	1:A:276:ASN:CB	2.58	0.45
1:A:282:LYS:HE2	2:B:1025:GLN:OE1	2.17	0.45
2:B:1051:LEU:CD2	2:B:1071:ILE:HD13	2.47	0.45
4:D:3053:THR:HB	7:D:2:HOH:O	2.16	0.45
1:A:242:VAL:HG22	1:A:243:SER:N	2.29	0.45
1:A:209:SER:HB3	1:A:379:GLY:O	2.17	0.45
3:C:2161:SER:HB3	3:C:2181:LEU:HD13	1.98	0.45
4:D:3201:SER:C	4:D:3203:SER:H	2.20	0.45
2:B:1145:SER:N	7:B:57:HOH:O	2.46	0.45
4:D:3039:GLN:O	4:D:3092:ALA:HB1	2.16	0.45
3:C:2018:ARG:HB2	3:C:2018:ARG:HE	1.55	0.45
3:C:2184:SER:N	7:C:41:HOH:O	2.50	0.45
3:C:2148:VAL:HG13	3:C:2198:VAL:HG22	1.99	0.45
1:A:209:SER:HB2	1:A:379:GLY:C	2.38	0.44
1:A:244:THR:CG2	1:A:245:VAL:N	2.79	0.44
2:B:1086:VAL:CG2	2:B:1087:GLU:N	2.79	0.44
2:B:1115:THR:O	2:B:1115:THR:HG22	2.16	0.44
2:B:1006:GLY:O	2:B:1097:VAL:HA	2.18	0.44
3:C:2063:SER:O	3:C:2073:LEU:HD12	2.18	0.44
3:C:2152:VAL:HB	3:C:2157:GLN:NE2	2.33	0.44
2:B:1128:VAL:O	2:B:1139:GLN:HB2	2.17	0.44
3:C:2142:TYR:CG	3:C:2143:PRO:HA	2.52	0.44
4:D:3112:ASN:HB3	4:D:3114:PHE:CE1	2.52	0.44
1:A:338:TRP:O	1:A:339:ASN:C	2.56	0.44
2:B:1086:VAL:O	2:B:1087:GLU:C	2.53	0.44
1:A:234:ASN:OD1	1:A:236:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD11	7:A:955:HOH:O	2.16	0.44
2:B:1130:CYS:O	2:B:1137:ASN:HA	2.18	0.44
1:A:490:LYS:HD2	1:A:490:LYS:H	1.83	0.44
1:A:386:ASN:CB	1:A:417:PRO:HG2	2.47	0.43
1:A:457:ASP:HB2	1:A:467:ILE:HB	1.99	0.43
1:A:474:ASP:OD1	1:A:476:ARG:NH1	2.51	0.43
2:B:1001:LYS:HD2	2:B:1001:LYS:HA	1.67	0.43
3:C:2137:LEU:HD12	3:C:2138:LEU:N	2.33	0.43
1:A:422:GLN:O	1:A:434:MET:HA	2.17	0.43
3:C:2011:LEU:HB3	3:C:2106:LEU:CD1	2.46	0.43
2:B:1083:ILE:HD12	2:B:1083:ILE:H	1.81	0.43
3:C:2094:TRP:HA	3:C:2095:PRO:O	2.18	0.43
4:D:3094:TYR:HD2	4:D:3094:TYR:N	2.16	0.43
1:A:295:ASN:HD22	6:A:795:NAG:H83	1.83	0.43
1:A:463:ASN:OD1	1:A:464:GLU:N	2.51	0.43
1:A:361:PHE:HE1	1:A:395:TRP:CD1	2.37	0.43
4:D:3001:GLU:OE1	4:D:3117:HIS:HE1	2.00	0.43
2:B:1128:VAL:HB	2:B:1144:LEU:HD11	2.01	0.43
3:C:2112:VAL:HG22	3:C:2143:PRO:HD3	2.00	0.43
1:A:463:ASN:C	1:A:463:ASN:OD1	2.56	0.43
2:B:1162:LEU:HD23	2:B:1162:LEU:C	2.38	0.43
4:D:3083:LEU:HD13	4:D:3086:LEU:HD23	2.00	0.43
2:B:1114:LEU:HB2	2:B:1149:LEU:HD21	2.01	0.43
4:D:3215:HIS:CD2	4:D:3217:PRO:HD2	2.53	0.43
3:C:2148:VAL:HG12	3:C:2148:VAL:O	2.18	0.42
2:B:1162:LEU:CD2	2:B:1162:LEU:C	2.87	0.42
4:D:3054:ILE:O	4:D:3054:ILE:HG12	2.19	0.42
4:D:3083:LEU:HB3	4:D:3086:LEU:HD21	2.00	0.42
2:B:1066:ASN:O	2:B:1068:PRO:HD2	2.18	0.42
4:D:3068:VAL:HA	4:D:3082:GLU:O	2.18	0.42
1:A:117:LYS:HA	1:A:118:PRO:HD3	1.82	0.42
4:D:3104:ALA:O	4:D:3106:GLU:N	2.53	0.42
4:D:3104:ALA:C	4:D:3106:GLU:N	2.73	0.42
1:A:213:ILE:CD1	1:A:213:ILE:H	2.22	0.42
3:C:2169:ASP:HB3	3:C:2172:ASP:OD1	2.20	0.42
1:A:224:ALA:O	1:A:488:VAL:HA	2.18	0.42
3:C:2156:LEU:HD13	3:C:2157:GLN:O	2.20	0.42
3:C:2187:ASP:O	3:C:2190:LYS:HB3	2.20	0.42
4:D:3193:LEU:O	4:D:3193:LEU:HD12	2.19	0.42
4:D:3218:SER:OG	4:D:3220:THR:HB	2.20	0.42
3:C:2095:PRO:HD2	3:C:2097:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3041:PRO:C	4:D:3043:GLN:H	2.22	0.41
3:C:2126:GLN:HG3	4:D:3137:PHE:CE2	2.54	0.41
4:D:3216:LYS:N	4:D:3217:PRO:HD2	2.35	0.41
1:A:220:PRO:O	1:A:221:ALA:C	2.57	0.41
2:B:1114:LEU:HD12	2:B:1114:LEU:HA	1.77	0.41
3:C:2156:LEU:HA	3:C:2156:LEU:HD22	1.89	0.41
4:D:3134:PRO:CD	7:D:107:HOH:O	2.40	0.41
1:A:346:ALA:HA	1:A:359:ILE:HG21	2.03	0.41
2:B:1135:GLY:O	2:B:1136:LYS:C	2.58	0.41
3:C:2161:SER:HB3	3:C:2181:LEU:CD1	2.50	0.41
1:A:335:ARG:NE	1:A:411:SER:O	2.41	0.41
2:B:1132:SER:HB2	2:B:1133:PRO:HD2	2.02	0.41
3:C:2062:PHE:N	7:C:73:HOH:O	2.48	0.41
3:C:2133:SER:HA	3:C:2181:LEU:O	2.20	0.41
1:A:254:VAL:HG13	1:A:254:VAL:O	2.21	0.41
2:B:1051:LEU:O	2:B:1052:ASN:C	2.57	0.41
3:C:2052:SER:HB3	3:C:2064:GLY:O	2.21	0.41
1:A:295:ASN:O	1:A:331:CYS:HA	2.20	0.41
3:C:2139:ASN:CG	3:C:2140:ASN:OD1	2.59	0.41
2:B:1102:ALA:HA	2:B:1116:LEU:HD23	2.01	0.41
3:C:2078:LEU:HA	3:C:2078:LEU:HD23	1.87	0.41
3:C:2138:LEU:CD1	3:C:2138:LEU:N	2.83	0.41
3:C:2145:GLU:CD	3:C:2145:GLU:H	2.23	0.41
1:A:198:THR:O	7:A:973:HOH:O	2.22	0.41
1:A:252:ARG:HD2	1:A:252:ARG:H	1.86	0.41
3:C:2054:ARG:HD3	3:C:2059:PRO:O	2.21	0.41
3:C:2078:LEU:HD13	3:C:2083:PHE:CE2	2.56	0.41
1:A:209:SER:CB	1:A:379:GLY:C	2.89	0.40
1:A:485:LYS:HE3	1:A:486:TYR:CE1	2.55	0.40
2:B:1138:ILE:HD11	2:B:1157:TRP:HZ3	1.85	0.40
2:B:1001:LYS:C	2:B:1001:LYS:HE2	2.40	0.40
2:B:1132:SER:HB2	2:B:1133:PRO:CD	2.51	0.40
2:B:1178:ALA:N	7:B:108:HOH:O	2.30	0.40
3:C:2115:PRO:HB3	3:C:2141:PHE:HB3	2.02	0.40
4:D:3104:ALA:C	4:D:3106:GLU:H	2.24	0.40
3:C:2067:SER:HA	3:C:2071:PHE:HE2	1.74	0.40
3:C:2094:TRP:CA	3:C:2095:PRO:C	2.81	0.40
1:A:126:CYS:HB3	1:A:127:VAL:H	1.55	0.40
3:C:2172:ASP:OD1	3:C:2172:ASP:C	2.60	0.40
2:B:1038:GLY:O	2:B:1044:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	300/317 (95%)	265 (88%)	23 (8%)	12 (4%)	3	9
2	B	179/184 (97%)	159 (89%)	15 (8%)	5 (3%)	5	17
3	C	212/214 (99%)	190 (90%)	20 (9%)	2 (1%)	17	46
4	D	218/229 (95%)	198 (91%)	18 (8%)	2 (1%)	17	46
All	All	909/944 (96%)	812 (89%)	76 (8%)	21 (2%)	6	21

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	461	SER
1	A	475	MET
2	B	1023	SER
2	B	1052	ASN
2	B	1087	GLU
4	D	3027	ASP
1	A	127	VAL
1	A	128	GLY
1	A	194	GLY
1	A	195	SER
1	A	462	ASN
2	B	1022	LYS
3	C	2188	TYR
1	A	84	VAL
1	A	129	ALA
1	A	197	ASN
4	D	3065	GLN
1	A	246	GLN
2	B	1178	ALA
3	C	2040	PRO

### 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	269/281 (96%)	251 (93%)	18 (7%)	16	43
2	B	164/166 (99%)	141 (86%)	23 (14%)	3	11
3	C	184/184 (100%)	176 (96%)	8 (4%)	29	62
4	D	187/193 (97%)	176 (94%)	11 (6%)	19	49
All	All	804/824 (98%)	744 (92%)	60 (8%)	13	37

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	86	LEU
1	A	104	MET
1	A	199	SER
1	A	213	ILE
1	A	217	TYR
1	A	240	THR
1	A	242	VAL
1	A	243	SER
1	A	343	LYS
1	A	369	PRO
1	A	413	THR
1	A	416	LEU
1	A	445	CYS
1	A	446	SER
1	A	460	ASN
1	A	467	ILE
1	A	475	MET
2	B	1001	LYS
2	B	1002	LYS
2	B	1010	ASP
2	B	1021	LYS
2	B	1023	SER
2	B	1024	ILE

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Mol	Chain	Res	Type
2	B	1037	LEU
2	B	1042	SER
2	B	1058	ARG
2	B	1060	SER
2	B	1061	LEU
2	B	1064	GLN
2	B	1073	ASN
2	B	1077	GLU
2	B	1089	GLN
2	B	1093	VAL
2	B	1096	LEU
2	B	1120	SER
2	B	1125	SER
2	B	1138	ILE
2	B	1149	LEU
2	B	1162	LEU
2	B	1173	ASP
3	C	2063	SER
3	C	2072	THR
3	C	2116	SER
3	C	2127	LEU
3	C	2144	ARG
3	C	2171	LYS
3	C	2177	LEU
3	C	2183	LEU
4	D	3001	GLU
4	D	3077	SER
4	D	3083	LEU
4	D	3089	ASP
4	D	3094	TYR
4	D	3109	TYR
4	D	3111	ASN
4	D	3132	LYS
4	D	3175	THR
4	D	3211	CYS
4	D	3220	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	344	GLN

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Mol	Chain	Res	Type
2	B	1089	GLN
4	D	3111	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 ⓘ

2 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	$\# Z  > 2$
5	GLC	E	1	5	11,11,12	0.57	0	15,15,17	0.93	0
5	FRU	E	2	5	11,12,12	0.70	0	10,18,18	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	E	1	5	-	0/2/19/22	0/1/1/1
5	FRU	E	2	5	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

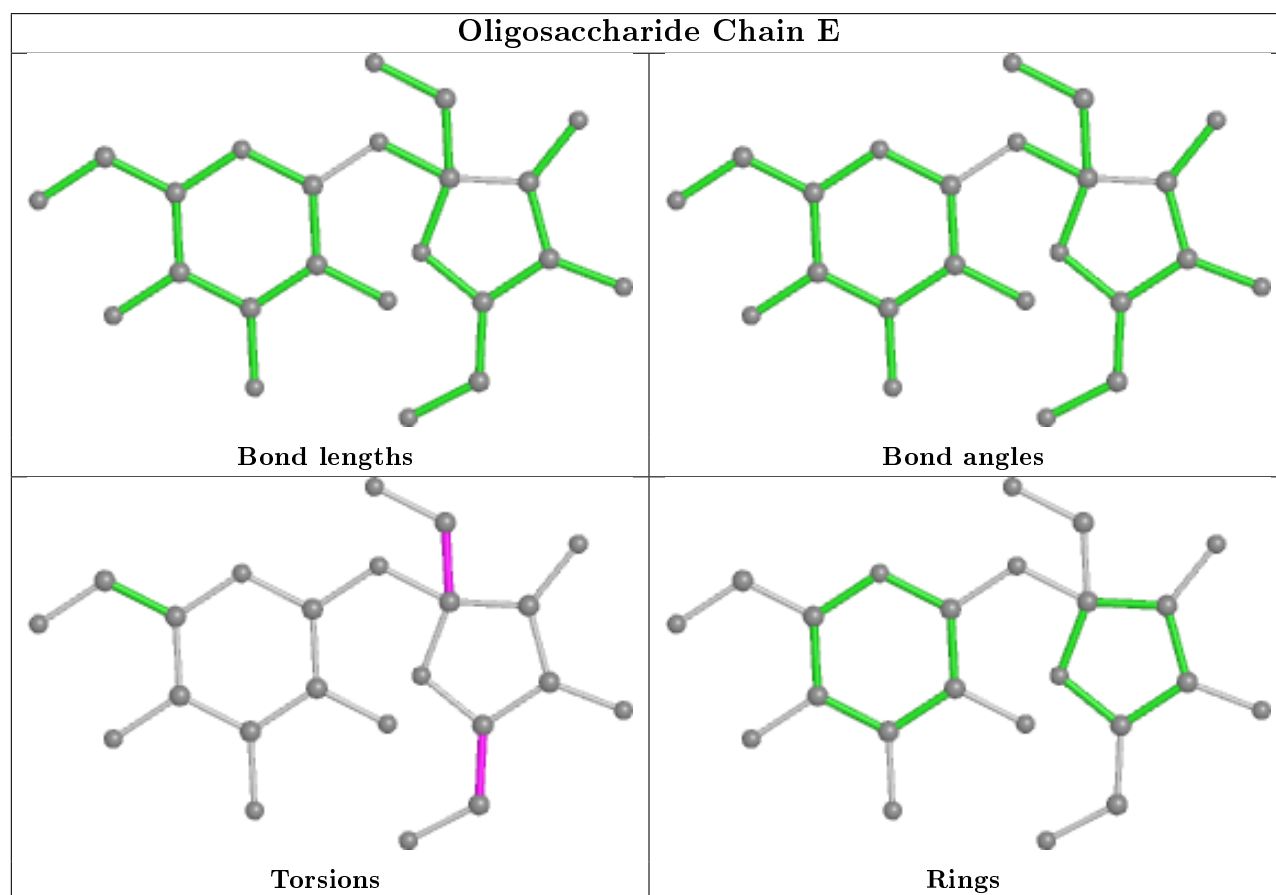
Mol	Chain	Res	Type	Atoms
5	E	2	FRU	O1-C1-C2-C3
5	E	2	FRU	O1-C1-C2-O2
5	E	2	FRU	O1-C1-C2-O5
5	E	2	FRU	O5-C5-C6-O6
5	E	2	FRU	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	FRU	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 ⓘ

8 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
6	NAG	A	795	1	14,14,15	0.54	0	17,19,21	0.94	1 (5%)
6	NAG	A	948	1	14,14,15	0.56	0	17,19,21	0.89	0
6	NAG	A	789	1	14,14,15	0.55	0	17,19,21	1.26	2 (11%)
6	NAG	A	734	1	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
6	NAG	A	776	1	14,14,15	0.47	0	17,19,21	1.10	2 (11%)
6	NAG	A	762	1	14,14,15	0.68	0	17,19,21	1.27	2 (11%)
6	NAG	A	839	1	14,14,15	0.51	0	17,19,21	1.21	2 (11%)
6	NAG	A	886	1	14,14,15	0.72	0	17,19,21	1.44	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	795	1	-	2/6/23/26	0/1/1/1
6	NAG	A	948	1	-	2/6/23/26	0/1/1/1
6	NAG	A	789	1	-	4/6/23/26	0/1/1/1
6	NAG	A	734	1	-	4/6/23/26	0/1/1/1
6	NAG	A	776	1	-	2/6/23/26	0/1/1/1
6	NAG	A	762	1	-	0/6/23/26	0/1/1/1
6	NAG	A	839	1	-	4/6/23/26	0/1/1/1
6	NAG	A	886	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	886	NAG	C4-C3-C2	-3.99	105.17	111.02
6	A	789	NAG	C2-N2-C7	-3.93	117.31	122.90
6	A	776	NAG	O5-C5-C6	2.91	111.76	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	839	NAG	C1-O5-C5	2.89	116.11	112.19
6	A	886	NAG	C3-C4-C5	-2.85	105.15	110.24
6	A	839	NAG	O5-C1-C2	2.79	115.70	111.29
6	A	762	NAG	C2-N2-C7	-2.76	118.97	122.90
6	A	762	NAG	O5-C1-C2	-2.52	107.31	111.29
6	A	789	NAG	O5-C1-C2	-2.36	107.56	111.29
6	A	795	NAG	O5-C5-C6	2.29	110.79	107.20
6	A	734	NAG	O5-C5-C6	2.20	110.65	107.20
6	A	776	NAG	C2-N2-C7	-2.03	120.01	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	795	NAG	C8-C7-N2-C2
6	A	789	NAG	C8-C7-N2-C2
6	A	789	NAG	O7-C7-N2-C2
6	A	734	NAG	C8-C7-N2-C2
6	A	734	NAG	O7-C7-N2-C2
6	A	839	NAG	C3-C2-N2-C7
6	A	839	NAG	C8-C7-N2-C2
6	A	839	NAG	O7-C7-N2-C2
6	A	886	NAG	C3-C2-N2-C7
6	A	886	NAG	C8-C7-N2-C2
6	A	886	NAG	O7-C7-N2-C2
6	A	734	NAG	O5-C5-C6-O6
6	A	948	NAG	O5-C5-C6-O6
6	A	789	NAG	O5-C5-C6-O6
6	A	795	NAG	O7-C7-N2-C2
6	A	734	NAG	C4-C5-C6-O6
6	A	789	NAG	C4-C5-C6-O6
6	A	776	NAG	C8-C7-N2-C2
6	A	948	NAG	C4-C5-C6-O6
6	A	776	NAG	O7-C7-N2-C2
6	A	839	NAG	O5-C5-C6-O6
6	A	886	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	795	NAG	1	0
6	A	789	NAG	4	0
6	A	839	NAG	2	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	304/317 (95%)	-0.32	7 (2%) 60 51	28, 53, 104, 162	0
2	B	181/184 (98%)	-0.34	0 100 100	35, 61, 96, 112	0
3	C	214/214 (100%)	-0.60	1 (0%) 91 88	25, 48, 91, 116	0
4	D	222/229 (96%)	-0.60	0 100 100	28, 45, 90, 120	0
All	All	921/944 (97%)	-0.46	8 (0%) 84 80	25, 51, 98, 162	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	8.1
1	A	195	SER	4.5
1	A	194	GLY	3.1
1	A	127	VAL	2.6
1	A	128	GLY	2.2
1	A	231	LYS	2.2
3	C	2001	ASP	2.1
1	A	462	ASN	2.1

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

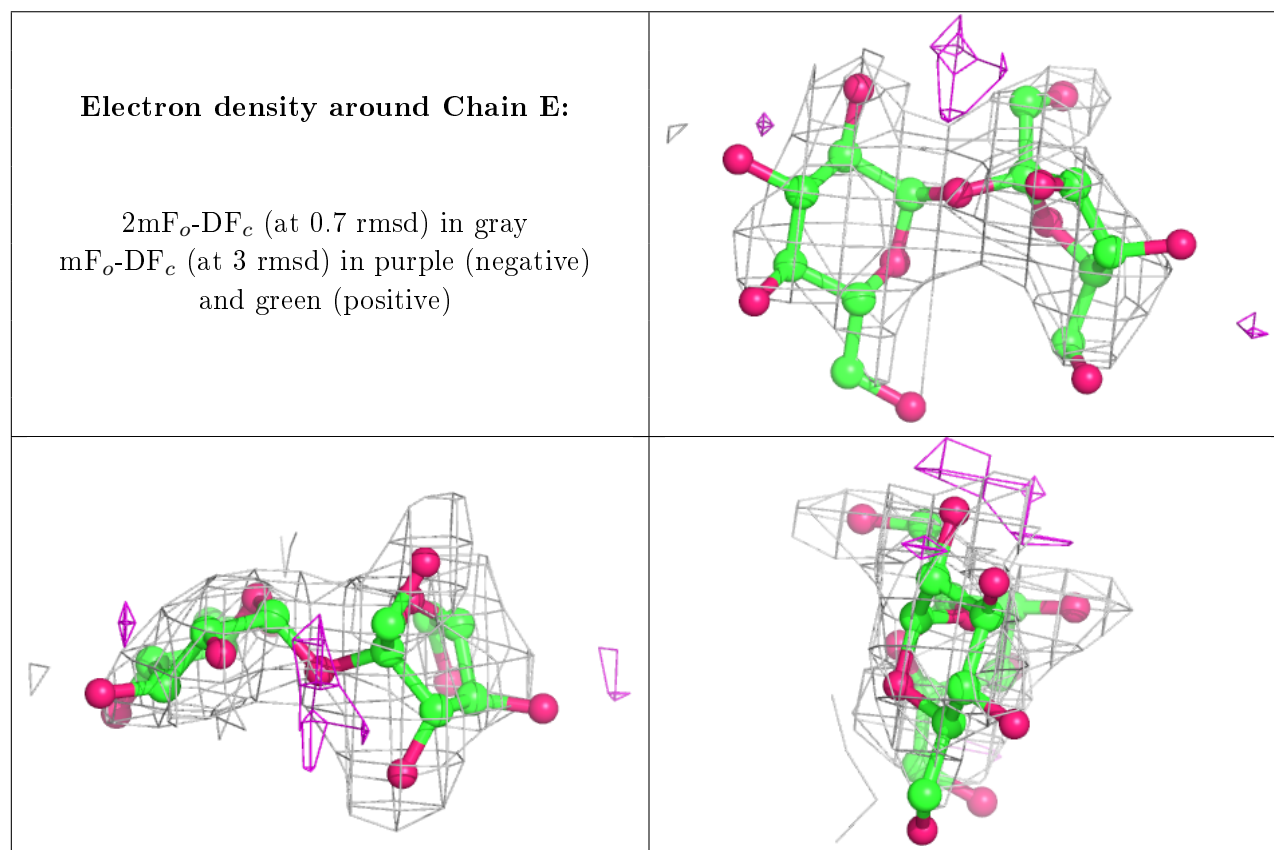
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	FRU	E	2	12/12	0.84	0.32	94,96,97,98	0
5	GLC	E	1	11/12	0.90	0.31	99,100,101,101	0

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



## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	734	14/15	0.87	0.21	85,88,89,89	0
6	NAG	A	839	14/15	0.88	0.32	82,84,86,86	0
6	NAG	A	948	14/15	0.92	0.15	62,64,65,66	0
6	NAG	A	886	14/15	0.92	0.14	58,59,61,61	0
6	NAG	A	776	14/15	0.93	0.17	69,71,74,75	0
6	NAG	A	789	14/15	0.96	0.14	46,49,55,57	0
6	NAG	A	795	14/15	0.97	0.14	39,43,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	762	14/15	0.98	0.11	32,36,41,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.