



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 04:21 PM EST

PDB ID : 4FNU  
Title : Crystal structure of GH36 alpha-galactosidase AgaA A355E D478A from *Geobacillus stearothermophilus* in complex with stachyose  
Authors : Merceron, R.; Foucault, M.; Haser, R.; Mattes, R.; Watzlawick, H.; Gouet, P.  
Deposited on : 2012-06-20  
Resolution : 3.60 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.

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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

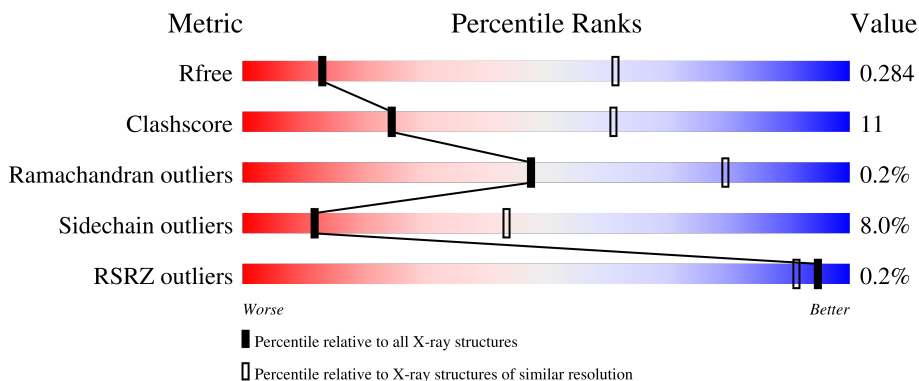
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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.



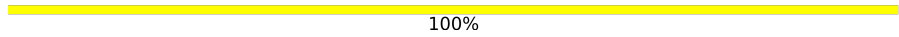

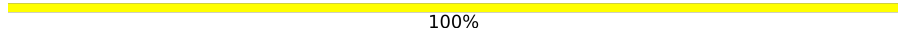
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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  $\geq 3$ , 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	729	 66% 28% . .
1	B	729	 69% 26% . .
1	C	729	 69% 27% . .
1	D	729	 71% 26% . .
2	E	4	 50% 50%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	4	 100%
2	G	4	 50% 50%
2	H	4	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	E	4	-	-	-	X
2	GLC	G	3	-	-	-	X
2	FRU	G	4	-	-	-	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23332 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.

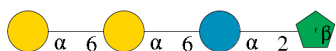
- Molecule 1 is a protein called Alpha-galactosidase AgaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	718	5788	3675	1020	1070	23	0	0	0
1	B	718	5788	3675	1020	1070	23	0	0	0
1	C	718	5788	3675	1020	1070	23	0	0	0
1	D	718	5788	3675	1020	1070	23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
A	478	ALA	ASP	engineered mutation	UNP Q9ALJ4
B	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
B	478	ALA	ASP	engineered mutation	UNP Q9ALJ4
C	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
C	478	ALA	ASP	engineered mutation	UNP Q9ALJ4
D	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
D	478	ALA	ASP	engineered mutation	UNP Q9ALJ4

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	4	45	24	21	0	0	0

*Continued on next page...*

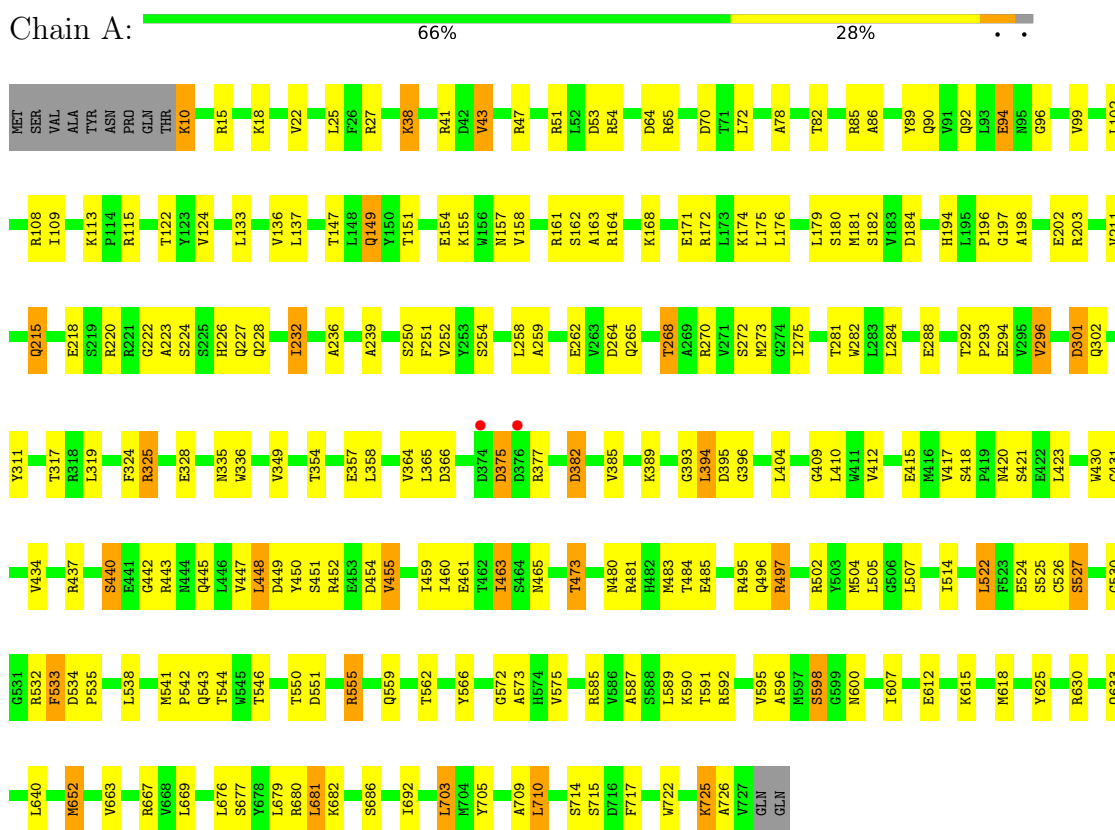
*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	4	Total	C	O	0	0	0
			45	24	21			
2	G	4	Total	C	O	0	0	0
			45	24	21			
2	H	4	Total	C	O	0	0	0
			45	24	21			

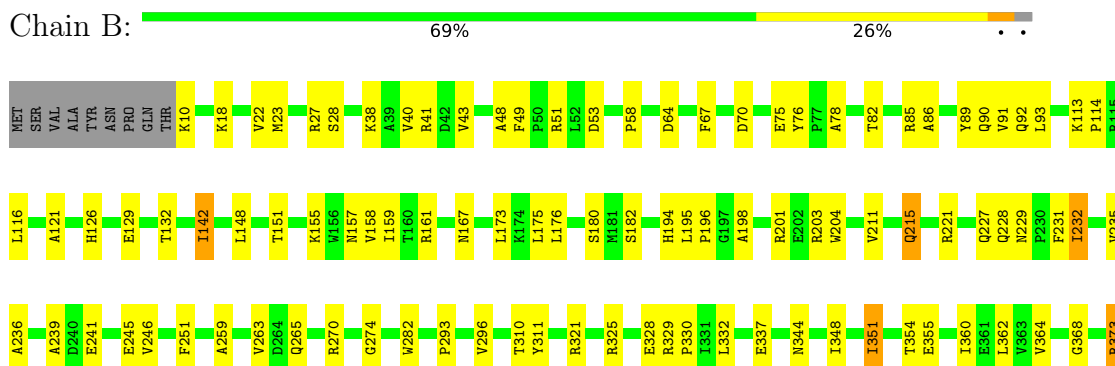
### 3 Residue-property plots [i](#)

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

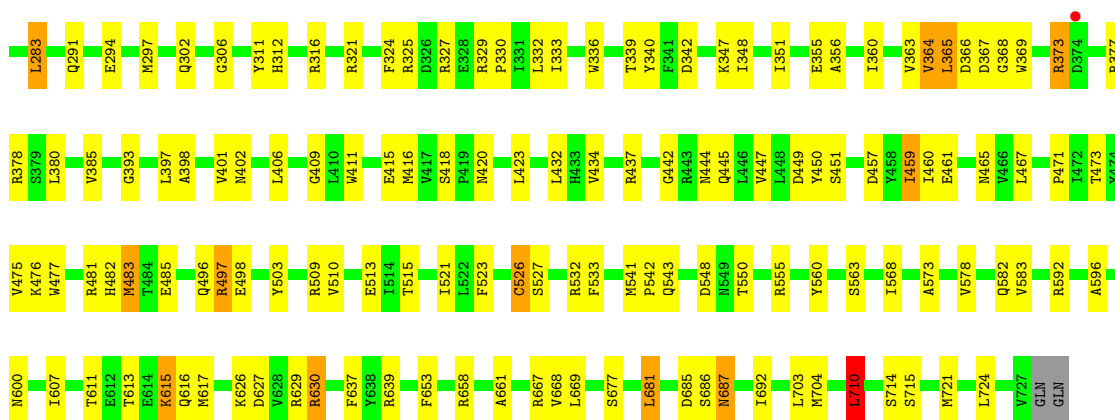
- Molecule 1: Alpha-galactosidase AgaA



- Molecule 1: Alpha-galactosidase AgaA



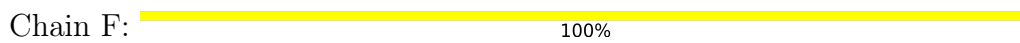




- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.07Å 154.07Å 238.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 3.60 19.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.92-3.60) 99.7 (19.92-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 3.62Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.238 , 0.282 0.238 , 0.284	Depositor DCC
$R_{free}$ test set	1906 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.0	Xtrriage
Anisotropy	0.223	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 19.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, GLA, GLC

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	0.22	0/5935	0.42	0/8046
1	B	0.22	0/5935	0.40	0/8046
1	C	0.22	0/5935	0.41	0/8046
1	D	0.22	0/5935	0.42	1/8046 (0.0%)
All	All	0.22	0/23740	0.41	1/32184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	710	LEU	CA-CB-CG	5.87	128.81	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5788	0	5621	147	0
1	B	5788	0	5621	130	0
1	C	5788	0	5621	139	0
1	D	5788	0	5621	124	0
2	E	45	0	39	4	0
2	F	45	0	39	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	45	0	39	2	0
2	H	45	0	39	0	0
All	All	23332	0	22640	501	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 11.

All (501) 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:681:LEU:HD11	1:B:703:LEU:HB3	1.61	0.81
1:B:684:LEU:H	1:B:704:MET:HE3	1.45	0.81
1:B:113:LYS:HD2	1:B:151:THR:HG21	1.66	0.78
1:A:113:LYS:HD2	1:A:151:THR:HG21	1.66	0.77
1:C:348:ILE:HD11	1:C:397:LEU:HD11	1.65	0.76
1:D:667:ARG:NH2	1:D:715:SER:O	2.20	0.75
1:A:317:THR:O	1:A:325:ARG:NH1	2.20	0.75
1:D:568:ILE:HD11	1:D:637:PHE:HB2	1.69	0.75
1:C:51:ARG:HH21	1:C:67:PHE:HA	1.51	0.73
1:A:281:THR:HG22	1:A:497:ARG:HB2	1.69	0.73
1:D:548:ASP:O	1:D:582:GLN:NE2	2.21	0.73
1:C:92:GLN:HB3	1:C:174:LYS:HB3	1.70	0.73
1:C:317:THR:O	1:C:325:ARG:NH1	2.22	0.72
1:A:686:SER:O	1:B:41:ARG:NH1	2.23	0.72
1:D:327:ARG:O	1:D:329:ARG:NH1	2.23	0.71
1:A:113:LYS:NZ	1:A:122:THR:O	2.22	0.71
1:B:75:GLU:OE1	1:B:161:ARG:NH1	2.24	0.71
1:C:681:LEU:HD12	1:C:703:LEU:HD13	1.73	0.71
1:C:351:ILE:HD11	1:C:607:ILE:HB	1.72	0.70
1:B:328:GLU:HB3	1:B:629:ARG:HD2	1.72	0.70
1:C:41:ARG:NH2	1:D:686:SER:O	2.24	0.70
1:D:27:ARG:NH2	1:D:61:ASP:OD2	2.25	0.70
1:B:232:ILE:HG12	1:B:259:ALA:HB1	1.73	0.69
1:B:368:GLY:HA2	1:B:373:ARG:HB3	1.73	0.69
1:D:368:GLY:HA2	1:D:373:ARG:HB3	1.74	0.69
1:C:316:ARG:HG3	1:C:317:THR:HG23	1.73	0.69
1:B:86:ALA:O	1:B:270:ARG:NH1	2.26	0.69
1:B:431:CYS:HA	1:B:448:LEU:HA	1.75	0.68
1:A:533:PHE:HE1	1:A:546:THR:HG22	1.58	0.68
1:D:380:LEU:HB2	1:D:418:SER:HB2	1.75	0.68
1:C:691:GLU:HA	1:C:697:VAL:HA	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ASP:OD1	1:C:509:ARG:NH2	2.27	0.66
1:A:211:VAL:H	1:A:215:GLN:HE21	1.44	0.66
1:A:555:ARG:HH11	1:A:555:ARG:HG3	1.61	0.65
1:D:365:LEU:HD11	1:D:369:TRP:HB3	1.78	0.65
1:D:578:VAL:HG13	1:D:592:ARG:HH11	1.62	0.65
1:C:333:ILE:HG22	1:C:360:ILE:HG21	1.78	0.64
1:B:27:ARG:NH2	1:B:64:ASP:OD2	2.31	0.64
1:B:211:VAL:H	1:B:215:GLN:HE21	1.44	0.64
1:D:401:VAL:HG12	1:D:406:LEU:HB2	1.78	0.64
1:A:70:ASP:O	1:A:85:ARG:NH1	2.30	0.64
1:D:142:ILE:HG13	1:D:173:LEU:HD11	1.79	0.64
1:C:281:THR:HG22	1:C:497:ARG:HB2	1.80	0.64
1:C:625:TYR:OH	1:C:633:GLN:NE2	2.30	0.63
1:D:398:ALA:O	1:D:402:ASN:ND2	2.30	0.63
1:A:497:ARG:NH1	1:D:98:THR:OG1	2.31	0.63
1:A:440:SER:HB3	1:D:60:PRO:HA	1.79	0.63
1:A:41:ARG:NH2	1:B:689:ASP:OD1	2.32	0.62
1:B:440:SER:HB3	1:C:60:PRO:HA	1.80	0.62
1:C:652:MET:HE1	1:C:682:LYS:H	1.64	0.62
1:C:680:ARG:HH21	1:C:705:TYR:HA	1.64	0.62
1:C:442:GLY:H	1:C:481:ARG:HE	1.47	0.62
1:A:364:VAL:HG22	1:A:409:GLY:HA3	1.82	0.61
1:C:283:LEU:HD22	1:C:494:GLU:HG3	1.82	0.61
1:C:250:SER:HB3	1:C:296:VAL:HG13	1.82	0.61
1:D:218:GLU:OE2	1:D:220:ARG:NH2	2.33	0.61
1:C:390:LEU:HD11	1:C:397:LEU:HB2	1.81	0.61
1:A:301:ASP:N	1:A:301:ASP:OD1	2.33	0.61
1:A:546:THR:OG1	1:A:555:ARG:NH2	2.33	0.61
1:A:172:ARG:HH22	1:A:174:LYS:HE2	1.65	0.61
1:A:65:ARG:NH2	1:D:444:ASN:OD1	2.32	0.60
1:C:583:VAL:HG23	1:C:585:ARG:H	1.65	0.60
1:A:431:CYS:HA	1:A:448:LEU:HA	1.83	0.60
1:D:457:ASP:OD1	1:D:509:ARG:NH2	2.32	0.60
1:A:252:VAL:HG12	1:A:535:PRO:HB2	1.83	0.60
1:C:429:ASP:OD1	1:C:429:ASP:N	2.34	0.60
1:C:474:TYR:OH	1:C:524:GLU:OE2	2.20	0.59
1:C:590:LYS:O	1:C:594:HIS:ND1	2.35	0.59
1:D:174:LYS:HB3	1:D:283:LEU:HD12	1.82	0.59
1:C:102:LEU:HD21	1:C:137:LEU:HD13	1.84	0.59
1:B:411:TRP:HD1	1:B:476:LYS:HE2	1.67	0.59
1:B:594:HIS:ND1	1:B:721:MET:SD	2.73	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ARG:HG2	1:D:420:ASN:HB3	1.84	0.59
1:D:461:GLU:O	1:D:465:ASN:ND2	2.34	0.59
1:D:59:ASN:OD1	1:D:65:ARG:NH1	2.35	0.59
1:C:114:PRO:HD3	1:C:132:THR:HG21	1.85	0.59
1:C:193:ILE:HD11	1:C:205:ILE:HB	1.85	0.59
1:C:355:GLU:HA	1:C:358:LEU:HD12	1.85	0.59
1:B:445:GLN:O	1:B:481:ARG:NH1	2.36	0.58
1:B:610:LEU:HD23	1:B:614:GLU:HB3	1.85	0.58
1:B:235:VAL:HG12	1:B:246:VAL:HG13	1.85	0.58
1:C:699:GLY:H	1:D:44:ARG:HG3	1.68	0.58
1:A:461:GLU:O	1:A:465:ASN:ND2	2.36	0.58
1:C:185:PHE:HB2	1:C:269:ALA:HB3	1.84	0.58
1:D:467:LEU:HD21	1:D:475:VAL:HG21	1.86	0.58
1:C:238:ASN:ND2	1:D:240:ASP:OD2	2.37	0.58
1:A:681:LEU:HD13	1:A:703:LEU:HB3	1.86	0.57
1:D:117:ASN:HB3	1:D:291:GLN:HG3	1.87	0.57
1:C:316:ARG:NH1	1:C:633:GLN:O	2.38	0.57
1:D:434:VAL:HG22	1:D:485:GLU:HB3	1.86	0.57
1:A:452:ARG:HB2	1:A:455:VAL:HG23	1.86	0.57
1:A:595:VAL:O	1:A:598:SER:OG	2.22	0.57
1:A:335:ASN:ND2	1:A:366:ASP:OD2	2.38	0.57
1:A:54:ARG:NH1	1:B:673:ASN:OD1	2.35	0.56
1:D:125:GLU:OE2	1:D:325:ARG:NH2	2.39	0.56
1:B:201:ARG:HA	1:B:558:ILE:HD11	1.86	0.56
1:C:252:VAL:HG12	1:C:535:PRO:HB2	1.87	0.56
1:C:205:ILE:H	1:C:644:PHE:HE2	1.51	0.56
1:C:364:VAL:HG12	1:C:409:GLY:HA3	1.87	0.56
1:A:86:ALA:O	1:A:270:ARG:NH1	2.39	0.56
1:B:377:ARG:NH1	1:B:444:ASN:OD1	2.39	0.56
1:B:175:LEU:HB2	1:B:282:TRP:HB3	1.86	0.56
1:A:434:VAL:HG23	1:A:437:ARG:HB2	1.89	0.55
1:A:497:ARG:HE	1:A:497:ARG:HA	1.71	0.55
1:B:241:GLU:OE2	1:B:639:ARG:NH1	2.39	0.55
1:B:583:VAL:O	1:D:714:SER:OG	2.24	0.55
1:C:75:GLU:OE1	1:C:161:ARG:NH1	2.39	0.55
1:D:339:THR:OG1	1:D:342:ASP:O	2.24	0.55
1:A:27:ARG:NH2	1:A:64:ASP:OD2	2.39	0.55
1:D:447:VAL:HG13	1:D:481:ARG:HD3	1.87	0.55
1:A:85:ARG:HE	1:A:270:ARG:NH2	2.04	0.55
1:C:252:VAL:HG22	1:C:294:GLU:O	2.07	0.55
1:C:380:LEU:HB2	1:C:418:SER:HB2	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD22	1:A:137:LEU:HB3	1.88	0.54
1:B:195:LEU:HB2	1:B:229:ASN:HB3	1.90	0.54
1:A:587:ALA:O	1:A:592:ARG:NH2	2.39	0.54
1:C:195:LEU:HB2	1:C:229:ASN:HB3	1.89	0.54
1:B:203:ARG:NE	1:B:562:THR:OG1	2.34	0.54
1:A:663:VAL:HG21	1:A:681:LEU:HD21	1.90	0.54
1:D:411:TRP:HD1	1:D:476:LYS:HE2	1.73	0.54
1:A:10:LYS:HB3	1:A:25:LEU:HB2	1.90	0.54
1:A:612:GLU:HA	1:A:615:LYS:HE3	1.90	0.54
1:A:680:ARG:NH2	1:B:245:GLU:OE2	2.39	0.54
1:A:250:SER:HB3	1:A:296:VAL:HG13	1.89	0.53
1:C:158:VAL:HG13	1:C:296:VAL:HG23	1.91	0.53
1:A:158:VAL:HG13	1:A:296:VAL:HG23	1.90	0.53
1:D:373:ARG:NH1	1:D:378:ARG:O	2.42	0.53
1:C:149:GLN:HE22	1:C:164:ARG:HB2	1.74	0.53
1:C:434:VAL:HG23	1:C:437:ARG:HB2	1.91	0.53
1:A:198:ALA:HB2	1:D:265:GLN:HB2	1.91	0.53
1:C:175:LEU:HB2	1:C:282:TRP:HB3	1.90	0.53
1:A:705:TYR:CD1	1:B:38:LYS:HE3	2.43	0.53
1:B:450:TYR:HE2	1:B:507:LEU:HD13	1.73	0.53
1:A:714:SER:OG	1:C:583:VAL:O	2.27	0.52
1:C:313:GLU:HA	1:C:316:ARG:HG2	1.91	0.52
1:C:687:ASN:HA	1:D:41:ARG:HH22	1.74	0.52
1:B:452:ARG:HE	1:B:490:ALA:HB2	1.74	0.52
1:C:467:LEU:HG	1:C:472:ILE:HG21	1.91	0.52
1:C:507:LEU:HD21	1:C:532:ARG:HH12	1.74	0.52
1:B:198:ALA:HB2	1:C:265:GLN:HB2	1.91	0.52
1:A:227:GLN:HG3	1:D:265:GLN:HB3	1.92	0.52
1:A:555:ARG:HD2	1:A:559:GLN:HG3	1.90	0.52
1:B:265:GLN:HB2	1:C:198:ALA:HB2	1.91	0.52
1:C:22:VAL:HG21	1:C:43:VAL:HG21	1.92	0.52
1:C:475:VAL:HG23	1:C:521:ILE:HD11	1.90	0.52
1:A:203:ARG:HE	1:A:562:THR:HB	1.74	0.52
1:A:232:ILE:HG12	1:A:259:ALA:HB1	1.91	0.52
1:A:591:THR:HG21	1:A:717:PHE:O	2.10	0.52
1:B:373:ARG:NH1	1:B:378:ARG:O	2.43	0.52
1:B:578:VAL:HG11	1:B:587:ALA:H	1.75	0.52
1:D:329:ARG:O	1:D:629:ARG:NH2	2.43	0.51
1:D:385:VAL:HG21	1:D:393:GLY:HA2	1.93	0.51
1:D:481:ARG:NH1	1:D:482:HIS:O	2.43	0.51
1:C:392:ASN:HB3	1:C:396:GLY:HA3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HB3	1:D:150:TYR:HB2	1.92	0.51
1:D:211:VAL:HG13	1:D:215:GLN:NE2	2.25	0.51
1:A:162:SER:HB3	1:A:294:GLU:HA	1.92	0.51
1:C:337:GLU:HB2	1:C:604:GLU:HG2	1.92	0.51
1:C:218:GLU:OE2	1:C:220:ARG:NH2	2.44	0.51
1:B:555:ARG:HD2	1:B:559:GLN:HG3	1.93	0.51
1:C:275:ILE:HD11	1:C:293:PRO:HD2	1.92	0.51
1:D:333:ILE:HG22	1:D:360:ILE:HG21	1.93	0.51
1:D:543:GLN:OE1	1:D:600:ASN:ND2	2.44	0.51
1:A:530:GLY:N	1:A:546:THR:O	2.44	0.51
1:A:211:VAL:HG22	1:A:215:GLN:HG3	1.92	0.51
1:A:725:LYS:NZ	1:A:726:ALA:O	2.31	0.51
1:C:546:THR:OG1	1:C:555:ARG:NH1	2.40	0.51
1:B:434:VAL:HG23	1:B:437:ARG:HB2	1.93	0.51
1:C:324:PHE:HA	1:C:327:ARG:HG3	1.92	0.51
1:B:626:LYS:HB3	1:B:629:ARG:HH21	1.75	0.51
1:B:504:MET:HE3	1:B:507:LEU:HD23	1.92	0.50
1:A:215:GLN:OE1	1:A:215:GLN:N	2.42	0.50
1:C:573:ALA:HB1	1:C:596:ALA:HA	1.93	0.50
1:B:116:LEU:HD12	1:B:121:ALA:HB2	1.93	0.50
1:B:441:GLU:HA	1:B:481:ARG:HH12	1.77	0.50
1:C:202:GLU:HG3	1:C:226:HIS:HB3	1.94	0.50
1:C:411:TRP:HD1	1:C:476:LYS:HE3	1.74	0.50
1:D:75:GLU:OE1	1:D:161:ARG:NH1	2.44	0.50
1:A:447:VAL:HG23	1:A:481:ARG:HD3	1.94	0.50
1:C:483:MET:HB2	1:C:486:ILE:HD11	1.93	0.50
1:B:552:ALA:HB2	1:B:592:ARG:HA	1.93	0.50
1:A:22:VAL:HG21	1:A:43:VAL:HG21	1.94	0.49
1:A:252:VAL:HG22	1:A:294:GLU:O	2.12	0.49
1:A:41:ARG:NH1	1:B:686:SER:O	2.43	0.49
1:B:496:GLN:NE2	1:B:497:ARG:HG2	2.27	0.49
1:D:363:VAL:HG23	1:D:406:LEU:HD22	1.94	0.49
1:D:661:ALA:HB3	1:D:724:LEU:HB2	1.93	0.49
1:B:70:ASP:OD2	1:C:221:ARG:NH2	2.40	0.49
1:C:240:ASP:OD1	1:D:238:ASN:ND2	2.38	0.49
1:D:195:LEU:HB2	1:D:229:ASN:HB3	1.95	0.49
1:A:161:ARG:HE	1:A:181:MET:HB2	1.77	0.49
1:A:442:GLY:O	1:A:445:GLN:HG2	2.11	0.49
1:B:92:GLN:HB2	1:B:176:LEU:HD11	1.94	0.49
1:C:192:TRP:HZ3	1:C:232:ILE:HD11	1.77	0.49
1:D:202:GLU:HG3	1:D:226:HIS:HB3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:VAL:HG21	1:C:587:ALA:H	1.77	0.49
1:C:691:GLU:HG3	1:C:725:LYS:HG3	1.95	0.49
1:D:113:LYS:HD3	1:D:151:THR:HG21	1.95	0.49
1:B:380:LEU:HB2	1:B:418:SER:HB2	1.95	0.49
1:B:576:SER:O	1:B:592:ARG:NH1	2.45	0.49
1:B:460:ILE:HA	1:B:514:ILE:HD11	1.94	0.48
1:C:622:VAL:HG12	1:C:626:LYS:HE3	1.95	0.48
1:D:611:THR:O	1:D:615:LYS:HG2	2.13	0.48
1:B:51:ARG:HD2	1:B:51:ARG:HA	1.56	0.48
1:B:411:TRP:CD1	1:B:476:LYS:HE2	2.48	0.48
1:D:92:GLN:HB3	1:D:174:LYS:HG3	1.95	0.48
1:D:555:ARG:HH22	1:D:573:ALA:HA	1.78	0.48
1:C:496:GLN:NE2	1:C:497:ARG:HG2	2.28	0.48
1:B:428:PRO:O	1:B:439:ARG:NH1	2.46	0.48
1:D:509:ARG:NH1	1:D:513:GLU:OE2	2.46	0.48
1:D:582:GLN:N	1:D:582:GLN:OE1	2.46	0.48
1:A:161:ARG:HH21	1:A:182:SER:H	1.61	0.48
1:B:551:ASP:OD2	1:B:585:ARG:NH1	2.44	0.48
1:A:38:LYS:HB3	1:B:705:TYR:CG	2.49	0.48
1:A:184:ASP:OD1	1:A:270:ARG:NE	2.30	0.48
1:A:440:SER:OG	1:A:485:GLU:OE2	2.31	0.48
1:A:709:ALA:HB3	1:B:48:ALA:HB3	1.96	0.48
1:B:606:ASP:OD2	1:B:609:LYS:NZ	2.30	0.48
1:C:697:VAL:HG22	1:D:44:ARG:HH21	1.78	0.48
1:A:669:LEU:HD21	1:C:669:LEU:HD21	1.96	0.48
1:D:460:ILE:HD11	1:D:510:VAL:HA	1.95	0.48
1:D:560:TYR:CZ	1:D:639:ARG:HD2	2.49	0.48
1:C:113:LYS:HD2	1:C:151:THR:HG21	1.96	0.47
1:C:568:ILE:HD11	1:C:599:GLY:HA2	1.96	0.47
1:A:459:ILE:O	1:A:463:ILE:HG12	2.14	0.47
1:C:51:ARG:HD2	1:C:51:ARG:HA	1.56	0.47
1:C:111:LYS:NZ	1:C:131:GLU:HB3	2.29	0.47
1:A:99:VAL:HG21	1:D:485:GLU:HA	1.95	0.47
1:A:147:THR:HB	1:A:164:ARG:HB3	1.97	0.47
1:A:382:ASP:OD1	1:A:382:ASP:N	2.46	0.47
1:B:22:VAL:HG21	1:B:43:VAL:HG21	1.96	0.47
1:B:496:GLN:HE22	1:B:497:ARG:HG2	1.78	0.47
1:C:442:GLY:N	1:C:481:ARG:HE	2.12	0.47
1:A:175:LEU:HB2	1:A:282:TRP:HB3	1.96	0.47
1:A:705:TYR:HB3	1:B:38:LYS:HB3	1.96	0.47
1:B:85:ARG:HE	1:B:270:ARG:NH2	2.12	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:SER:OG	1:B:544:THR:HG23	2.15	0.47
1:B:680:ARG:HH21	1:B:705:TYR:HA	1.79	0.47
1:C:394:LEU:HB3	1:C:470:ALA:HB2	1.96	0.47
1:D:235:VAL:HG13	1:D:239:ALA:HB3	1.96	0.47
1:A:53:ASP:OD1	1:A:65:ARG:HD2	2.15	0.47
1:D:356:ALA:HB2	1:D:406:LEU:HD11	1.96	0.47
1:A:265:GLN:HB2	1:D:198:ALA:HB2	1.96	0.47
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.80	0.47
1:C:73:LEU:HD22	1:C:184:ASP:HB3	1.96	0.47
1:C:388:ARG:HA	1:C:388:ARG:HD3	1.70	0.47
1:C:215:GLN:HG2	1:C:261:ILE:HG23	1.97	0.46
1:C:533:PHE:HE1	1:C:546:THR:HG22	1.80	0.46
1:D:366:ASP:OD1	1:D:367:ASP:N	2.43	0.46
1:D:677:SER:HB2	1:D:710:LEU:HD11	1.97	0.46
1:B:329:ARG:HA	1:B:330:PRO:HD3	1.82	0.46
1:D:161:ARG:HD3	1:D:297:MET:HE1	1.97	0.46
1:B:265:GLN:HB3	1:C:227:GLN:HG3	1.96	0.46
1:C:628:VAL:O	1:C:632:VAL:HG13	2.15	0.46
1:D:397:LEU:O	1:D:401:VAL:HG23	2.16	0.46
2:G:2:GLA:O2	2:G:4:FRU:H4	2.15	0.46
1:A:149:GLN:HE21	1:A:149:GLN:HB2	1.53	0.46
1:A:236:ALA:HB3	1:A:239:ALA:HB2	1.98	0.46
1:B:23:MET:HE3	1:B:75:GLU:HG3	1.97	0.46
1:D:14:LEU:HD11	1:D:150:TYR:HB3	1.97	0.46
1:D:58:PRO:HB2	1:D:82:THR:HG22	1.97	0.46
1:D:221:ARG:HD3	1:D:482:HIS:CE1	2.50	0.46
1:A:415:GLU:HA	1:A:450:TYR:HE2	1.80	0.46
1:A:535:PRO:HD3	1:A:566:TYR:HE1	1.81	0.46
1:A:555:ARG:HG3	1:A:555:ARG:NH1	2.27	0.46
1:A:227:GLN:OE1	1:A:227:GLN:N	2.48	0.46
1:A:375:ASP:OD1	1:A:375:ASP:N	2.47	0.46
1:B:227:GLN:OE1	1:B:227:GLN:N	2.47	0.46
1:B:93:LEU:HD13	1:B:142:ILE:HD11	1.96	0.46
1:C:222:GLY:HA3	1:C:483:MET:SD	2.56	0.46
1:D:227:GLN:OE1	1:D:227:GLN:N	2.47	0.46
1:D:432:LEU:HB2	1:D:447:VAL:HG23	1.97	0.46
1:D:236:ALA:HB3	1:D:239:ALA:HB2	1.98	0.46
1:D:283:LEU:N	1:D:498:GLU:OE2	2.43	0.46
1:D:442:GLY:O	1:D:445:GLN:HG2	2.15	0.46
1:A:394:LEU:HD12	1:A:395:ASP:N	2.32	0.46
1:B:385:VAL:HG12	1:B:394:LEU:HD13	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:GLU:OE2	1:D:477:TRP:NE1	2.48	0.46
1:A:417:VAL:HG23	1:A:448:LEU:HD22	1.97	0.45
1:C:91:VAL:HG11	1:C:173:LEU:HD23	1.97	0.45
1:C:147:THR:HB	1:C:164:ARG:HB3	1.98	0.45
1:C:472:ILE:HG23	1:C:521:ILE:HD12	1.97	0.45
1:C:640:LEU:HD12	1:C:640:LEU:HA	1.81	0.45
1:D:102:LEU:HD22	1:D:137:LEU:HB3	1.99	0.45
1:A:640:LEU:HD13	1:A:679:LEU:HD11	1.97	0.45
1:B:337:GLU:HB2	1:B:604:GLU:HG2	1.98	0.45
1:B:460:ILE:HG13	1:B:461:GLU:N	2.31	0.45
1:A:324:PHE:CD2	1:A:522:LEU:HD12	2.51	0.45
1:B:38:LYS:HE2	1:B:38:LYS:HB2	1.84	0.45
1:C:416:MET:HE2	1:C:445:GLN:HE21	1.82	0.45
1:A:336:TRP:CE3	2:E:1:GLA:H62	2.52	0.45
1:B:532:ARG:HE	1:B:532:ARG:HB3	1.54	0.45
1:D:687:ASN:O	1:D:687:ASN:ND2	2.43	0.45
1:A:526:CYS:SG	2:E:1:GLA:H2	2.56	0.45
1:A:262:GLU:HB3	1:A:270:ARG:HB3	1.98	0.45
1:C:105:LYS:HA	1:C:105:LYS:HD2	1.76	0.45
1:C:227:GLN:OE1	1:C:227:GLN:N	2.49	0.45
1:C:351:ILE:HG12	1:C:607:ILE:HD13	1.99	0.45
1:C:598:SER:OG	1:C:651:TRP:NE1	2.50	0.45
1:B:167:ASN:ND2	1:B:173:LEU:HD13	2.31	0.45
1:B:373:ARG:HD2	1:B:373:ARG:HA	1.54	0.45
1:A:559:GLN:HA	1:A:562:THR:HG22	1.98	0.45
1:A:663:VAL:HB	1:A:722:TRP:HB2	1.99	0.45
1:B:180:SER:H	1:B:274:GLY:HA3	1.82	0.45
1:B:221:ARG:HD3	1:B:482:HIS:ND1	2.32	0.45
1:C:421:SER:O	1:C:425:ARG:HG3	2.17	0.45
1:C:467:LEU:HD21	1:C:475:VAL:HG21	1.99	0.45
1:D:162:SER:HB3	1:D:294:GLU:HA	1.98	0.45
1:A:502:ARG:HA	1:A:505:LEU:HB2	1.99	0.44
1:B:58:PRO:HB2	1:B:82:THR:HG22	1.99	0.44
1:B:355:GLU:HB3	1:B:360:ILE:HD12	1.98	0.44
1:B:583:VAL:HG23	1:B:585:ARG:H	1.81	0.44
1:B:442:GLY:H	1:B:481:ARG:NH1	2.15	0.44
1:B:450:TYR:HB2	1:B:503:TYR:CD1	2.52	0.44
1:D:91:VAL:HG13	1:D:175:LEU:HD23	2.00	0.44
1:D:475:VAL:HG23	1:D:521:ILE:HD11	1.97	0.44
1:D:541:MET:HA	1:D:542:PRO:HD3	1.82	0.44
1:C:261:ILE:HD11	1:C:269:ALA:HB1	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:SER:OG	1:A:715:SER:N	2.51	0.44
1:B:554:SER:O	1:B:558:ILE:HG12	2.17	0.44
1:D:351:ILE:O	1:D:355:GLU:HG3	2.16	0.44
1:A:572:GLY:HA2	1:A:600:ASN:OD1	2.18	0.44
1:C:205:ILE:HG23	1:C:561:GLY:HA2	1.99	0.44
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.82	0.44
1:A:541:MET:HA	1:A:542:PRO:HD3	1.85	0.44
1:A:677:SER:HB2	1:A:710:LEU:HD22	2.00	0.44
1:B:194:HIS:CD2	1:B:196:PRO:HD3	2.53	0.44
1:C:652:MET:HG2	1:C:663:VAL:HA	1.98	0.44
1:D:73:LEU:HD12	1:D:73:LEU:H	1.82	0.44
1:D:398:ALA:HB3	1:D:471:PRO:HD2	1.99	0.44
1:A:92:GLN:HB2	1:A:176:LEU:HD11	1.99	0.44
1:A:354:THR:O	1:A:358:LEU:HD13	2.17	0.44
1:A:551:ASP:O	1:A:555:ARG:HB2	2.18	0.44
1:C:225:SER:N	1:C:531:GLY:O	2.50	0.44
1:D:450:TYR:HB2	1:D:503:TYR:CD1	2.53	0.44
1:D:568:ILE:HD13	1:D:653:PHE:HE1	1.83	0.44
1:C:352:ALA:HA	1:C:355:GLU:HG2	1.99	0.44
1:C:387:ARG:NH2	1:C:391:PRO:O	2.51	0.44
1:D:434:VAL:HG23	1:D:437:ARG:HB2	1.99	0.44
1:A:551:ASP:OD1	1:A:585:ARG:HB3	2.18	0.44
1:B:158:VAL:HG13	1:B:296:VAL:HG13	2.00	0.43
1:A:223:ALA:HA	1:A:254:SER:O	2.18	0.43
1:B:51:ARG:HH21	1:B:67:PHE:HA	1.82	0.43
1:B:465:ASN:OD1	1:B:465:ASN:N	2.50	0.43
1:B:692:ILE:HG13	1:B:724:LEU:HG	2.00	0.43
1:C:156:TRP:NE1	1:C:313:GLU:OE2	2.50	0.43
1:A:168:LYS:HE3	1:A:168:LYS:HB3	1.79	0.43
1:D:104:TYR:OH	1:D:107:HIS:ND1	2.28	0.43
1:A:385:VAL:HG11	1:A:393:GLY:HA2	1.99	0.43
1:C:236:ALA:HB3	1:C:239:ALA:HB2	1.99	0.43
1:C:275:ILE:HD12	1:C:275:ILE:H	1.84	0.43
1:C:316:ARG:HH12	1:C:569:SER:HB3	1.83	0.43
1:D:523:PHE:HB3	1:D:541:MET:HG2	2.01	0.43
1:A:254:SER:HA	1:A:534:ASP:OD2	2.18	0.43
1:A:430:TRP:CE3	1:A:455:VAL:HG13	2.54	0.43
1:C:450:TYR:HB2	1:C:503:TYR:CD1	2.54	0.43
1:A:667:ARG:HH11	1:A:667:ARG:HG2	1.83	0.43
1:B:18:LYS:HG2	1:B:157:ASN:HD21	1.83	0.43
1:C:202:GLU:OE1	1:C:202:GLU:N	2.46	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:HB2	1:C:532:ARG:HA	2.00	0.43
1:C:504:MET:HG3	1:C:508:TYR:CE2	2.54	0.43
1:D:222:GLY:HA3	1:D:483:MET:SD	2.58	0.43
1:D:312:HIS:NE2	1:D:563:SER:O	2.41	0.43
1:B:686:SER:HB2	1:B:701:ASP:HB3	2.01	0.43
1:C:162:SER:HB3	1:C:294:GLU:HA	2.00	0.43
1:C:308:SER:OG	1:C:639:ARG:NH2	2.37	0.43
1:A:18:LYS:HE3	1:A:38:LYS:HD2	2.01	0.43
1:B:421:SER:O	1:B:425:ARG:HG3	2.19	0.43
1:C:607:ILE:HA	1:C:610:LEU:HD21	1.99	0.43
1:D:373:ARG:NH1	1:D:378:ARG:H	2.16	0.43
1:A:454:ASP:OD2	1:A:454:ASP:N	2.52	0.43
1:C:285:GLN:N	1:C:288:GLU:OE2	2.46	0.43
1:A:218:GLU:OE2	1:A:220:ARG:NH2	2.52	0.43
1:A:652:MET:SD	1:A:681:LEU:HD23	2.59	0.43
1:B:332:LEU:HB3	1:B:362:LEU:HD23	2.01	0.43
1:C:333:ILE:HD11	1:C:607:ILE:HD11	2.01	0.43
1:C:578:VAL:HG11	1:C:586:VAL:HG13	2.01	0.43
1:B:401:VAL:HG13	1:B:406:LEU:HB2	2.01	0.42
1:D:613:THR:O	1:D:616:GLN:HG2	2.18	0.42
1:A:473:THR:O	1:A:473:THR:OG1	2.36	0.42
1:C:49:PHE:CZ	1:C:51:ARG:HD3	2.54	0.42
1:D:211:VAL:HG13	1:D:215:GLN:HE21	1.84	0.42
1:A:449:ASP:OD2	1:A:451:SER:OG	2.25	0.42
1:D:25:LEU:HD11	1:D:29:GLY:HA2	2.01	0.42
1:D:626:LYS:HA	1:D:629:ARG:HD2	2.00	0.42
1:A:78:ALA:HB2	1:A:89:TYR:CE2	2.55	0.42
1:A:163:ALA:H	1:A:292:THR:HG22	1.83	0.42
1:B:555:ARG:HH12	1:B:573:ALA:HA	1.83	0.42
1:C:530:GLY:N	1:C:546:THR:O	2.53	0.42
1:D:459:ILE:HD13	1:D:459:ILE:HA	1.86	0.42
1:A:194:HIS:CD2	1:A:196:PRO:HD3	2.54	0.42
1:A:525:SER:HB2	1:A:544:THR:HG23	2.01	0.42
1:C:511:MET:HE3	1:C:511:MET:HB2	1.87	0.42
1:A:179:LEU:HD13	1:A:272:SER:HB2	2.01	0.42
1:A:573:ALA:HB1	1:A:596:ALA:HA	2.01	0.42
1:D:364:VAL:HG13	1:D:409:GLY:HA3	2.01	0.42
1:A:251:PHE:CE1	1:A:293:PRO:HB2	2.55	0.42
1:A:527:SER:OG	1:A:532:ARG:HD2	2.20	0.42
1:B:236:ALA:HB3	1:B:239:ALA:HB2	2.02	0.42
1:C:515:THR:HG22	1:C:523:PHE:CD2	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:LYS:HB3	1:C:644:PHE:HE1	1.85	0.42
1:D:302:GLN:HB3	1:D:306:GLY:HA3	2.02	0.42
1:A:96:GLY:O	1:D:497:ARG:HD2	2.19	0.42
1:A:319:LEU:HD23	1:A:538:LEU:HD23	2.01	0.42
1:B:417:VAL:HG13	1:B:423:LEU:HD21	2.01	0.42
1:B:461:GLU:OE2	1:B:517:ARG:NH2	2.52	0.42
1:C:692:ILE:HG12	1:C:724:LEU:HG	2.01	0.42
1:D:347:LYS:HD3	1:D:347:LYS:HA	1.76	0.42
1:A:480:ASN:ND2	2:E:2:GLA:O4	2.53	0.42
1:A:524:GLU:OE1	1:A:543:GLN:NE2	2.49	0.42
1:B:49:PHE:CZ	1:B:51:ARG:HD3	2.54	0.42
1:B:251:PHE:CE1	1:B:293:PRO:HB2	2.55	0.42
1:C:252:VAL:O	1:C:252:VAL:HG23	2.20	0.42
1:A:180:SER:HA	1:A:292:THR:HG21	2.02	0.42
1:A:196:PRO:HB3	1:A:228:GLN:HE22	1.83	0.42
1:A:264:ASP:OD1	1:A:268:THR:HG23	2.19	0.42
1:B:151:THR:O	1:B:159:ILE:HA	2.20	0.42
1:B:481:ARG:HG2	1:B:482:HIS:N	2.35	0.42
1:B:524:GLU:OE1	1:B:543:GLN:NE2	2.52	0.42
1:C:161:ARG:NH2	1:C:182:SER:H	2.18	0.42
1:C:711:PRO:HG2	1:C:720:MET:HE1	2.02	0.42
1:D:78:ALA:HB2	1:D:89:TYR:CE2	2.54	0.42
1:D:329:ARG:HA	1:D:330:PRO:HD3	1.86	0.42
1:A:222:GLY:HA3	1:A:483:MET:SD	2.60	0.41
1:A:284:LEU:HD23	1:A:288:GLU:HG3	2.01	0.41
1:B:76:TYR:HB2	1:B:148:LEU:HD21	2.01	0.41
1:B:229:ASN:O	1:B:231:PHE:N	2.52	0.41
1:C:254:SER:OG	1:C:534:ASP:OD2	2.25	0.41
1:C:625:TYR:CE2	1:C:629:ARG:HB2	2.55	0.41
1:A:109:ILE:HG12	1:A:133:LEU:HD13	2.01	0.41
1:B:449:ASP:O	1:B:455:VAL:HG21	2.19	0.41
1:D:373:ARG:HD2	1:D:373:ARG:HA	1.61	0.41
1:A:18:LYS:HG2	1:A:157:ASN:HD21	1.84	0.41
1:A:625:TYR:OH	1:A:633:GLN:NE2	2.41	0.41
1:B:113:LYS:HA	1:B:114:PRO:HD3	1.94	0.41
1:B:196:PRO:HD2	1:B:204:TRP:O	2.20	0.41
1:D:316:ARG:O	1:D:325:ARG:HG3	2.20	0.41
1:A:504:MET:HE3	1:A:507:LEU:HD23	2.03	0.41
1:D:18:LYS:HD2	1:D:18:LYS:HA	1.82	0.41
1:D:336:TRP:O	1:D:340:TYR:HD1	2.04	0.41
1:D:692:ILE:HG13	1:D:724:LEU:HG	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:CYS:O	1:B:460:ILE:HG12	2.21	0.41
1:B:701:ASP:OD1	1:B:701:ASP:N	2.53	0.41
1:A:275:ILE:HD11	1:A:293:PRO:HD2	2.02	0.41
1:A:395:ASP:OD1	1:A:396:GLY:N	2.53	0.41
1:A:484:THR:HG23	1:D:82:THR:H	1.86	0.41
1:A:495:ARG:O	1:A:497:ARG:N	2.54	0.41
1:B:515:THR:HG22	1:B:523:PHE:CD2	2.56	0.41
1:B:681:LEU:HD13	1:B:684:LEU:HD12	2.02	0.41
1:A:197:GLY:O	1:A:227:GLN:HA	2.20	0.41
1:A:480:ASN:HB3	2:E:2:GLA:O4	2.21	0.41
1:C:678:TYR:CE2	1:D:186:PRO:HB2	2.55	0.41
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.89	0.41
1:B:551:ASP:O	1:B:555:ARG:HB2	2.20	0.41
1:B:669:LEU:HD21	1:D:669:LEU:HD21	2.01	0.41
1:C:329:ARG:HA	1:C:330:PRO:HD3	1.80	0.41
1:C:467:LEU:HD11	1:C:475:VAL:HG21	2.03	0.41
1:A:94:GLU:OE2	1:A:171:GLU:HG2	2.21	0.41
1:A:258:LEU:O	1:A:273:MET:HA	2.21	0.41
1:B:78:ALA:HB2	1:B:89:TYR:CE2	2.56	0.41
1:B:82:THR:H	1:C:484:THR:HG23	1.86	0.41
1:B:196:PRO:HB3	1:B:228:GLN:HE22	1.86	0.41
1:B:678:TYR:HA	1:B:709:ALA:HA	2.03	0.41
1:C:285:GLN:O	1:C:288:GLU:HG2	2.21	0.41
1:C:336:TRP:HB3	1:C:604:GLU:OE2	2.21	0.41
1:C:495:ARG:O	1:C:497:ARG:N	2.54	0.41
1:C:572:GLY:HA2	1:C:600:ASN:HB3	2.03	0.41
1:C:708:VAL:HA	1:D:46:ALA:O	2.21	0.41
1:D:324:PHE:HA	1:D:327:ARG:HB2	2.03	0.41
1:D:526:CYS:SG	1:D:527:SER:N	2.94	0.41
1:D:573:ALA:HB1	1:D:596:ALA:HA	2.03	0.41
1:A:328:GLU:OE1	1:A:630:ARG:HG2	2.21	0.41
1:B:227:GLN:HG3	1:C:265:GLN:HB3	2.02	0.41
1:C:607:ILE:O	1:C:610:LEU:HG	2.21	0.41
1:D:630:ARG:HD3	1:D:630:ARG:HA	1.63	0.41
1:A:70:ASP:HB2	1:A:82:THR:O	2.20	0.40
1:A:202:GLU:OE2	1:A:226:HIS:HD2	2.03	0.40
1:C:221:ARG:HD3	1:C:482:HIS:ND1	2.36	0.40
1:D:449:ASP:OD1	1:D:451:SER:OG	2.23	0.40
1:A:443:ARG:H	1:D:65:ARG:NH1	2.20	0.40
1:B:27:ARG:HB3	1:B:28:SER:H	1.59	0.40
1:B:53:ASP:OD2	2:G:4:FRU:O4	2.25	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:THR:HG21	1:B:717:PHE:O	2.21	0.40
1:B:647:ASN:OD1	1:B:668:VAL:HG13	2.20	0.40
1:A:460:ILE:HG13	1:A:461:GLU:N	2.35	0.40
1:B:161:ARG:NH2	1:B:182:SER:H	2.19	0.40
1:B:612:GLU:OE2	1:B:615:LYS:NZ	2.54	0.40
1:B:626:LYS:HB3	1:B:629:ARG:NH2	2.36	0.40
1:D:57:SER:HA	1:D:58:PRO:HD3	1.94	0.40
1:D:172:ARG:HH11	1:D:172:ARG:HG2	1.86	0.40
1:D:515:THR:HG22	1:D:523:PHE:CD2	2.57	0.40
1:D:681:LEU:CD1	1:D:703:LEU:HB2	2.50	0.40
1:A:38:LYS:HG2	1:B:705:TYR:CE2	2.57	0.40
1:A:418:SER:O	1:A:421:SER:OG	2.33	0.40
1:A:600:ASN:HA	1:A:625:TYR:OH	2.21	0.40
1:B:713:ARG:HB2	1:B:718:ILE:HD13	2.03	0.40
1:C:547:SER:O	1:C:555:ARG:NH2	2.54	0.40
1:A:47:ARG:HH21	1:B:678:TYR:HE1	1.69	0.40
1:B:344:ASN:HA	1:B:389:LYS:HB2	2.03	0.40
1:B:351:ILE:O	1:B:355:GLU:HG3	2.21	0.40
1:D:658:ARG:HB3	1:D:685:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	716/729 (98%)	683 (95%)	32 (4%)	1 (0%)	51 83
1	B	716/729 (98%)	685 (96%)	30 (4%)	1 (0%)	51 83
1	C	716/729 (98%)	683 (95%)	32 (4%)	1 (0%)	51 83
1	D	716/729 (98%)	682 (95%)	32 (4%)	2 (0%)	41 75
All	All	2864/2916 (98%)	2733 (95%)	126 (4%)	5 (0%)	47 79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	B	496	GLN
1	C	496	GLN
1	D	496	GLN
1	D	526	CYS

### 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	608/618 (98%)	545 (90%)	63 (10%)	7 33
1	B	608/618 (98%)	555 (91%)	53 (9%)	10 41
1	C	608/618 (98%)	567 (93%)	41 (7%)	16 50
1	D	608/618 (98%)	570 (94%)	38 (6%)	18 53
All	All	2432/2472 (98%)	2237 (92%)	195 (8%)	12 43

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	15	ARG
1	A	38	LYS
1	A	43	VAL
1	A	51	ARG
1	A	72	LEU
1	A	90	GLN
1	A	94	GLU
1	A	108	ARG
1	A	115	ARG
1	A	124	VAL
1	A	136	VAL
1	A	149	GLN
1	A	154	GLU
1	A	155	LYS

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	215	GLN
1	A	224	SER
1	A	232	ILE
1	A	268	THR
1	A	296	VAL
1	A	301	ASP
1	A	302	GLN
1	A	311	TYR
1	A	325	ARG
1	A	349	VAL
1	A	357	GLU
1	A	365	LEU
1	A	375	ASP
1	A	377	ARG
1	A	382	ASP
1	A	389	LYS
1	A	394	LEU
1	A	404	LEU
1	A	410	LEU
1	A	412	VAL
1	A	420	ASN
1	A	423	LEU
1	A	440	SER
1	A	448	LEU
1	A	455	VAL
1	A	463	ILE
1	A	473	THR
1	A	497	ARG
1	A	514	ILE
1	A	522	LEU
1	A	527	SER
1	A	533	PHE
1	A	550	THR
1	A	555	ARG
1	A	575	VAL
1	A	589	LEU
1	A	590	LYS
1	A	598	SER
1	A	607	ILE
1	A	618	MET
1	A	652	MET
1	A	676	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	681	LEU
1	A	682	LYS
1	A	692	ILE
1	A	703	LEU
1	A	710	LEU
1	A	725	LYS
1	B	10	LYS
1	B	40	VAL
1	B	90	GLN
1	B	91	VAL
1	B	126	HIS
1	B	129	GLU
1	B	132	THR
1	B	142	ILE
1	B	155	LYS
1	B	215	GLN
1	B	232	ILE
1	B	263	VAL
1	B	310	THR
1	B	311	TYR
1	B	321	ARG
1	B	325	ARG
1	B	348	ILE
1	B	351	ILE
1	B	354	THR
1	B	364	VAL
1	B	373	ARG
1	B	382	ASP
1	B	394	LEU
1	B	410	LEU
1	B	412	VAL
1	B	440	SER
1	B	448	LEU
1	B	465	ASN
1	B	473	THR
1	B	497	ARG
1	B	522	LEU
1	B	532	ARG
1	B	533	PHE
1	B	544	THR
1	B	550	THR
1	B	555	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	562	THR
1	B	569	SER
1	B	589	LEU
1	B	592	ARG
1	B	595	VAL
1	B	610	LEU
1	B	612	GLU
1	B	615	LYS
1	B	618	MET
1	B	627	ASP
1	B	667	ARG
1	B	668	VAL
1	B	678	TYR
1	B	681	LEU
1	B	682	LYS
1	B	710	LEU
1	B	721	MET
1	C	15	ARG
1	C	28	SER
1	C	34	VAL
1	C	51	ARG
1	C	105	LYS
1	C	108	ARG
1	C	109	ILE
1	C	127	GLU
1	C	136	VAL
1	C	232	ILE
1	C	241	GLU
1	C	261	ILE
1	C	283	LEU
1	C	291	GLN
1	C	292	THR
1	C	296	VAL
1	C	310	THR
1	C	311	TYR
1	C	325	ARG
1	C	332	LEU
1	C	351	ILE
1	C	378	ARG
1	C	382	ASP
1	C	394	LEU
1	C	399	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	416	MET
1	C	420	ASN
1	C	421	SER
1	C	429	ASP
1	C	483	MET
1	C	497	ARG
1	C	509	ARG
1	C	533	PHE
1	C	550	THR
1	C	590	LYS
1	C	610	LEU
1	C	612	GLU
1	C	617	MET
1	C	630	ARG
1	C	632	VAL
1	C	686	SER
1	D	40	VAL
1	D	65	ARG
1	D	132	THR
1	D	142	ILE
1	D	214	VAL
1	D	224	SER
1	D	261	ILE
1	D	268	THR
1	D	283	LEU
1	D	311	TYR
1	D	321	ARG
1	D	332	LEU
1	D	348	ILE
1	D	364	VAL
1	D	365	LEU
1	D	373	ARG
1	D	377	ARG
1	D	416	MET
1	D	423	LEU
1	D	459	ILE
1	D	473	THR
1	D	483	MET
1	D	497	ARG
1	D	532	ARG
1	D	533	PHE
1	D	550	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	583	VAL
1	D	607	ILE
1	D	615	LYS
1	D	617	MET
1	D	627	ASP
1	D	630	ARG
1	D	668	VAL
1	D	681	LEU
1	D	687	ASN
1	D	704	MET
1	D	710	LEU
1	D	721	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	291	GLN
1	A	302	GLN
1	C	291	GLN
1	C	445	GLN
1	C	621	GLN
1	D	580	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](#)

16 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	GLA	E	1	2	11,11,12	2.57	2 (18%)	15,15,17	0.94	0
2	GLA	E	2	2	11,11,12	2.51	2 (18%)	15,15,17	1.73	2 (13%)
2	GLC	E	3	2	11,11,12	2.38	2 (18%)	15,15,17	1.34	1 (6%)
2	FRU	E	4	2	11,12,12	1.69	4 (36%)	10,18,18	1.65	2 (20%)
2	GLA	F	1	2	11,11,12	2.63	2 (18%)	15,15,17	1.15	1 (6%)
2	GLA	F	2	2	11,11,12	2.46	3 (27%)	15,15,17	2.43	7 (46%)
2	GLC	F	3	2	11,11,12	2.60	4 (36%)	15,15,17	1.58	4 (26%)
2	FRU	F	4	2	11,12,12	1.70	4 (36%)	10,18,18	1.96	4 (40%)
2	GLA	G	1	2	11,11,12	2.62	2 (18%)	15,15,17	1.30	1 (6%)
2	GLA	G	2	2	11,11,12	2.47	2 (18%)	15,15,17	2.24	5 (33%)
2	GLC	G	3	2	11,11,12	2.33	2 (18%)	15,15,17	2.14	7 (46%)
2	FRU	G	4	2	11,12,12	1.67	2 (18%)	10,18,18	1.89	4 (40%)
2	GLA	H	1	2	11,11,12	2.56	3 (27%)	15,15,17	1.29	1 (6%)
2	GLA	H	2	2	11,11,12	2.38	3 (27%)	15,15,17	2.28	6 (40%)
2	GLC	H	3	2	11,11,12	2.43	3 (27%)	15,15,17	1.77	5 (33%)
2	FRU	H	4	2	11,12,12	1.70	3 (27%)	10,18,18	2.03	4 (40%)

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	GLA	E	1	2	-	1/2/19/22	0/1/1/1
2	GLA	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	FRU	E	4	2	-	3/5/24/24	0/1/1/1
2	GLA	F	1	2	-	1/2/19/22	0/1/1/1
2	GLA	F	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	FRU	F	4	2	-	3/5/24/24	0/1/1/1
2	GLA	G	1	2	-	0/2/19/22	0/1/1/1
2	GLA	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	1/2/19/22	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	G	4	2	-	5/5/24/24	0/1/1/1
2	GLA	H	1	2	-	1/2/19/22	0/1/1/1
2	GLA	H	2	2	-	1/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	FRU	H	4	2	-	5/5/24/24	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLA	C2-C3	-7.38	1.41	1.52
2	F	1	GLA	C2-C3	-7.35	1.41	1.52
2	E	1	GLA	C2-C3	-7.27	1.41	1.52
2	E	2	GLA	C2-C3	-7.14	1.42	1.52
2	H	1	GLA	C2-C3	-7.04	1.42	1.52
2	F	2	GLA	C2-C3	-6.94	1.42	1.52
2	G	2	GLA	C2-C3	-6.88	1.42	1.52
2	F	3	GLC	C2-C3	-6.52	1.42	1.52
2	H	2	GLA	C2-C3	-6.46	1.43	1.52
2	H	3	GLC	C2-C3	-6.39	1.43	1.52
2	E	3	GLC	C2-C3	-6.32	1.43	1.52
2	G	3	GLC	C2-C3	-5.82	1.43	1.52
2	F	3	GLC	O5-C1	4.12	1.50	1.43
2	G	3	GLC	O5-C1	3.79	1.49	1.43
2	H	1	GLA	O5-C1	3.52	1.49	1.43
2	G	1	GLA	O5-C1	3.49	1.49	1.43
2	H	3	GLC	O5-C1	3.40	1.49	1.43
2	F	1	GLA	O5-C1	3.31	1.49	1.43
2	E	1	GLA	O5-C1	3.29	1.49	1.43
2	E	3	GLC	O5-C1	3.26	1.48	1.43
2	G	4	FRU	C4-C5	-2.96	1.45	1.53
2	H	4	FRU	C4-C5	-2.84	1.45	1.53
2	F	4	FRU	C4-C5	-2.80	1.45	1.53
2	E	4	FRU	C4-C5	-2.68	1.46	1.53
2	H	4	FRU	O3-C3	-2.59	1.37	1.42
2	H	2	GLA	O5-C1	2.57	1.47	1.43
2	E	4	FRU	O5-C2	-2.56	1.39	1.43
2	G	4	FRU	O3-C3	-2.43	1.37	1.42
2	G	2	GLA	O5-C1	2.43	1.47	1.43
2	F	4	FRU	O3-C3	-2.43	1.37	1.42
2	E	4	FRU	O3-C3	-2.40	1.38	1.42
2	F	2	GLA	O5-C1	2.39	1.47	1.43
2	E	2	GLA	O5-C1	2.23	1.47	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	GLC	O2-C2	-2.19	1.38	1.43
2	H	2	GLA	C4-C3	-2.17	1.46	1.52
2	F	3	GLC	C4-C3	-2.16	1.46	1.52
2	F	4	FRU	O2-C2	2.14	1.44	1.40
2	F	2	GLA	C4-C3	-2.14	1.46	1.52
2	E	4	FRU	O2-C2	2.12	1.44	1.40
2	F	4	FRU	O5-C2	-2.10	1.40	1.43
2	H	3	GLC	O2-C2	-2.06	1.39	1.43
2	H	4	FRU	O5-C2	-2.03	1.40	1.43
2	H	1	GLA	O5-C5	-2.02	1.39	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	GLC	C1-C2-C3	5.17	116.02	109.67
2	G	2	GLA	O5-C5-C6	4.97	114.99	107.20
2	F	2	GLA	C1-C2-C3	4.87	115.65	109.67
2	H	2	GLA	O5-C5-C6	4.54	114.33	107.20
2	F	2	GLA	O5-C5-C6	4.40	114.11	107.20
2	G	2	GLA	C1-C2-C3	4.31	114.97	109.67
2	H	4	FRU	O1-C1-C2	4.03	120.43	111.86
2	F	4	FRU	O1-C1-C2	3.96	120.28	111.86
2	H	2	GLA	C1-O5-C5	3.91	117.50	112.19
2	E	2	GLA	O5-C5-C6	3.86	113.26	107.20
2	H	2	GLA	C1-C2-C3	3.72	114.24	109.67
2	E	2	GLA	C3-C4-C5	3.71	116.85	110.24
2	G	4	FRU	O1-C1-C2	3.62	119.56	111.86
2	F	3	GLC	C1-C2-C3	3.56	114.04	109.67
2	E	4	FRU	O1-C1-C2	3.45	119.20	111.86
2	F	2	GLA	C2-C3-C4	3.31	116.62	110.89
2	H	3	GLC	C3-C4-C5	3.26	116.06	110.24
2	G	3	GLC	C2-C3-C4	3.22	116.47	110.89
2	F	2	GLA	C3-C4-C5	3.01	115.60	110.24
2	H	1	GLA	C1-C2-C3	2.98	113.33	109.67
2	E	3	GLC	C1-C2-C3	2.89	113.22	109.67
2	H	3	GLC	O5-C1-C2	-2.87	106.34	110.77
2	G	1	GLA	C1-C2-C3	2.80	113.11	109.67
2	G	4	FRU	O5-C5-C6	2.72	116.43	108.85
2	H	4	FRU	C6-C5-C4	-2.70	108.58	115.09
2	G	3	GLC	O5-C5-C6	2.68	111.41	107.20
2	G	2	GLA	C2-C3-C4	2.67	115.52	110.89
2	H	2	GLA	O3-C3-C4	-2.67	104.17	110.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	GLA	C3-C4-C5	2.60	114.87	110.24
2	F	2	GLA	O2-C2-C3	-2.58	104.97	110.14
2	F	3	GLC	O5-C5-C6	2.58	111.25	107.20
2	G	3	GLC	C3-C4-C5	2.51	114.72	110.24
2	H	4	FRU	O5-C5-C6	2.49	115.77	108.85
2	H	3	GLC	O4-C4-C3	-2.48	104.61	110.35
2	H	3	GLC	O5-C5-C6	2.44	111.03	107.20
2	F	4	FRU	O5-C5-C6	2.43	115.63	108.85
2	G	4	FRU	O6-C6-C5	2.41	119.56	111.29
2	G	4	FRU	C6-C5-C4	-2.40	109.31	115.09
2	E	4	FRU	O5-C5-C6	2.37	115.45	108.85
2	F	3	GLC	O2-C2-C3	-2.35	105.44	110.14
2	F	4	FRU	C6-C5-C4	-2.23	109.71	115.09
2	F	2	GLA	O3-C3-C4	-2.22	105.22	110.35
2	G	3	GLC	O2-C2-C3	-2.21	105.71	110.14
2	H	4	FRU	O6-C6-C5	2.20	118.83	111.29
2	F	3	GLC	O4-C4-C3	-2.18	105.31	110.35
2	G	3	GLC	O6-C6-C5	2.15	118.67	111.29
2	F	4	FRU	O6-C6-C5	2.13	118.58	111.29
2	H	2	GLA	C2-C3-C4	2.12	114.57	110.89
2	G	2	GLA	O6-C6-C5	2.10	118.50	111.29
2	F	2	GLA	C1-O5-C5	2.07	115.00	112.19
2	H	3	GLC	C2-C3-C4	2.07	114.48	110.89
2	G	3	GLC	O4-C4-C3	-2.07	105.56	110.35
2	H	2	GLA	O6-C6-C5	2.02	118.21	111.29
2	F	1	GLA	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	FRU	O1-C1-C2-C3
2	E	4	FRU	O1-C1-C2-O2
2	E	4	FRU	O1-C1-C2-O5
2	G	4	FRU	O1-C1-C2-C3
2	G	4	FRU	O1-C1-C2-O2
2	G	4	FRU	O1-C1-C2-O5
2	G	4	FRU	O5-C5-C6-O6
2	G	4	FRU	C4-C5-C6-O6
2	H	4	FRU	O5-C5-C6-O6
2	H	4	FRU	C4-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

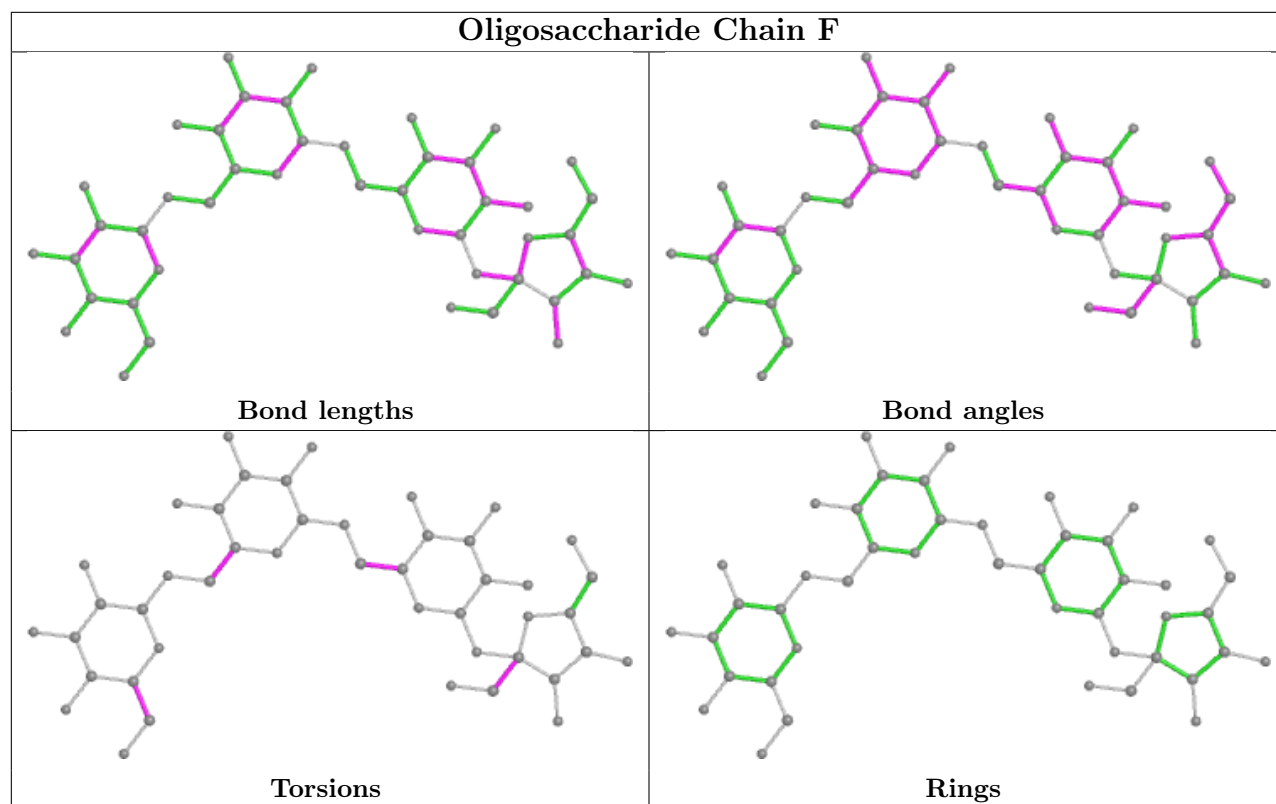
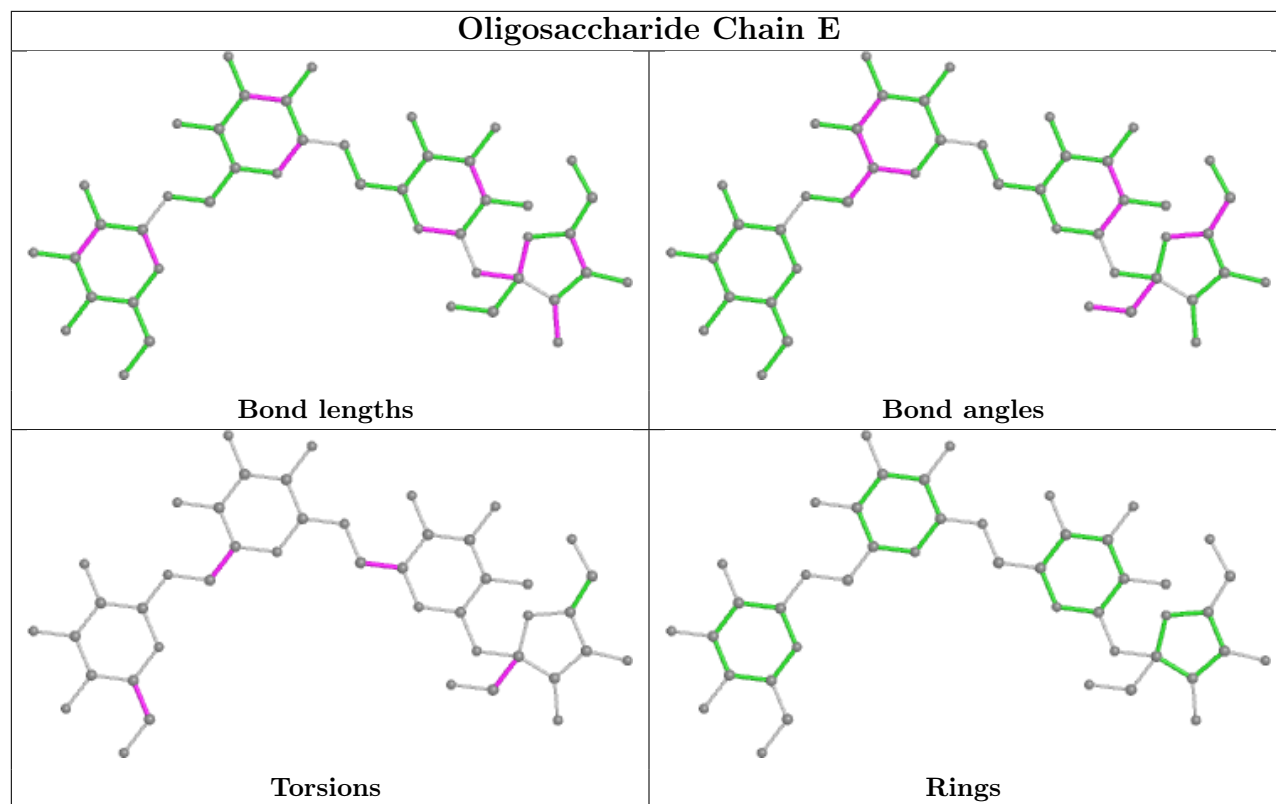
Mol	Chain	Res	Type	Atoms
2	F	2	GLA	C4-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	E	2	GLA	C4-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6
2	F	2	GLA	O5-C5-C6-O6
2	E	2	GLA	O5-C5-C6-O6
2	F	4	FRU	O1-C1-C2-O5
2	E	1	GLA	O5-C5-C6-O6
2	G	3	GLC	O5-C5-C6-O6
2	H	2	GLA	C4-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	F	4	FRU	O1-C1-C2-C3
2	H	4	FRU	O1-C1-C2-O5
2	F	4	FRU	O1-C1-C2-O2
2	H	4	FRU	O1-C1-C2-O2
2	F	1	GLA	O5-C5-C6-O6
2	H	4	FRU	O1-C1-C2-C3
2	H	1	GLA	O5-C5-C6-O6

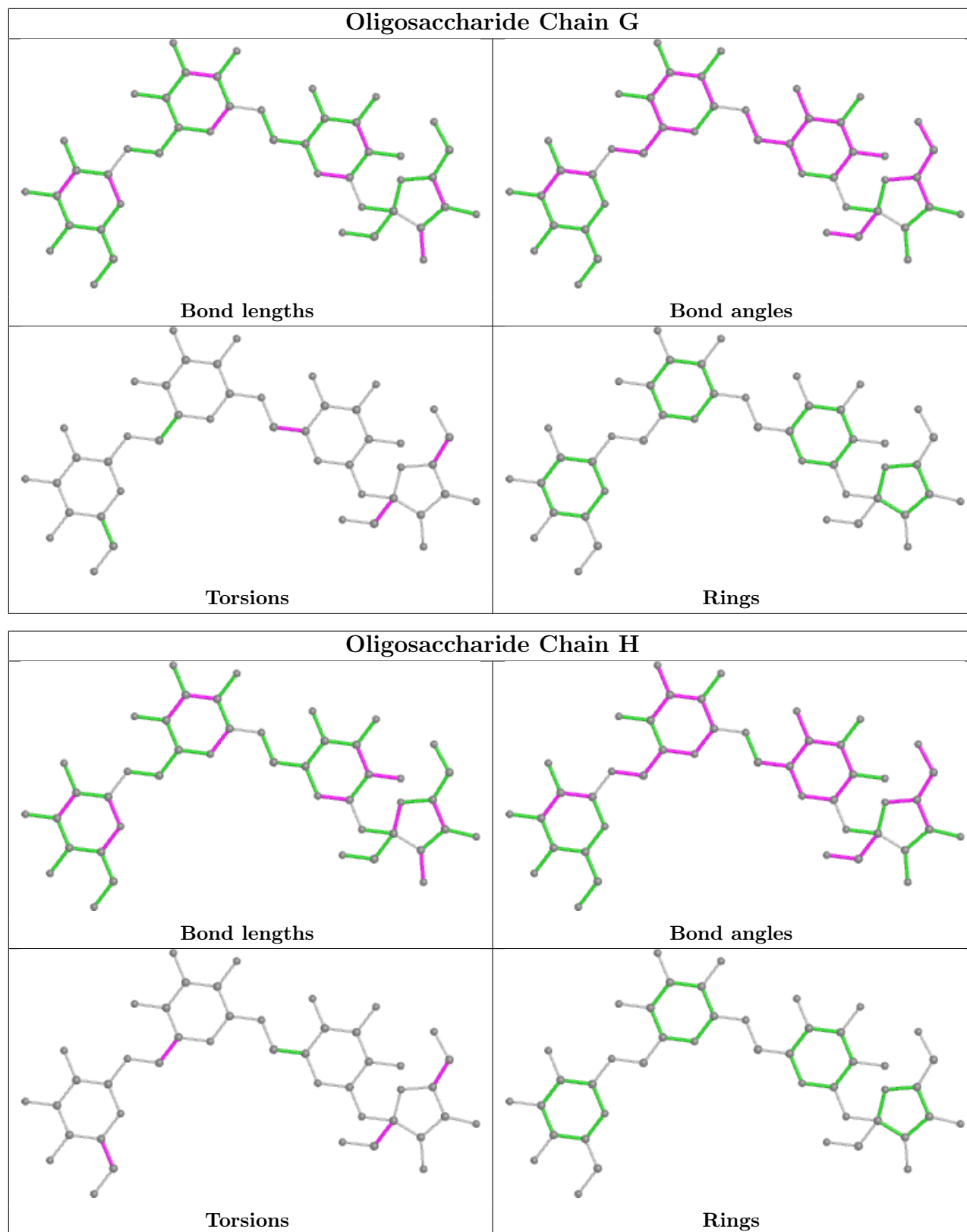
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	GLA	1	0
2	E	1	GLA	2	0
2	E	2	GLA	2	0
2	G	4	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 [i](#)

There are no ligands in this entry.

## 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	718/729 (98%)	-0.36	2 (0%) 94 88	61, 101, 145, 173	0
1	B	718/729 (98%)	-0.51	0 100 100	56, 90, 127, 144	0
1	C	718/729 (98%)	-0.31	3 (0%) 92 86	71, 113, 139, 163	0
1	D	718/729 (98%)	-0.45	1 (0%) 95 93	62, 93, 126, 151	0
All	All	2872/2916 (98%)	-0.41	6 (0%) 95 91	56, 100, 136, 173	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	SER	2.7
1	C	323	ALA	2.6
1	A	376	ASP	2.5
1	A	374	ASP	2.1
1	C	405	GLY	2.1
1	D	374	ASP	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.

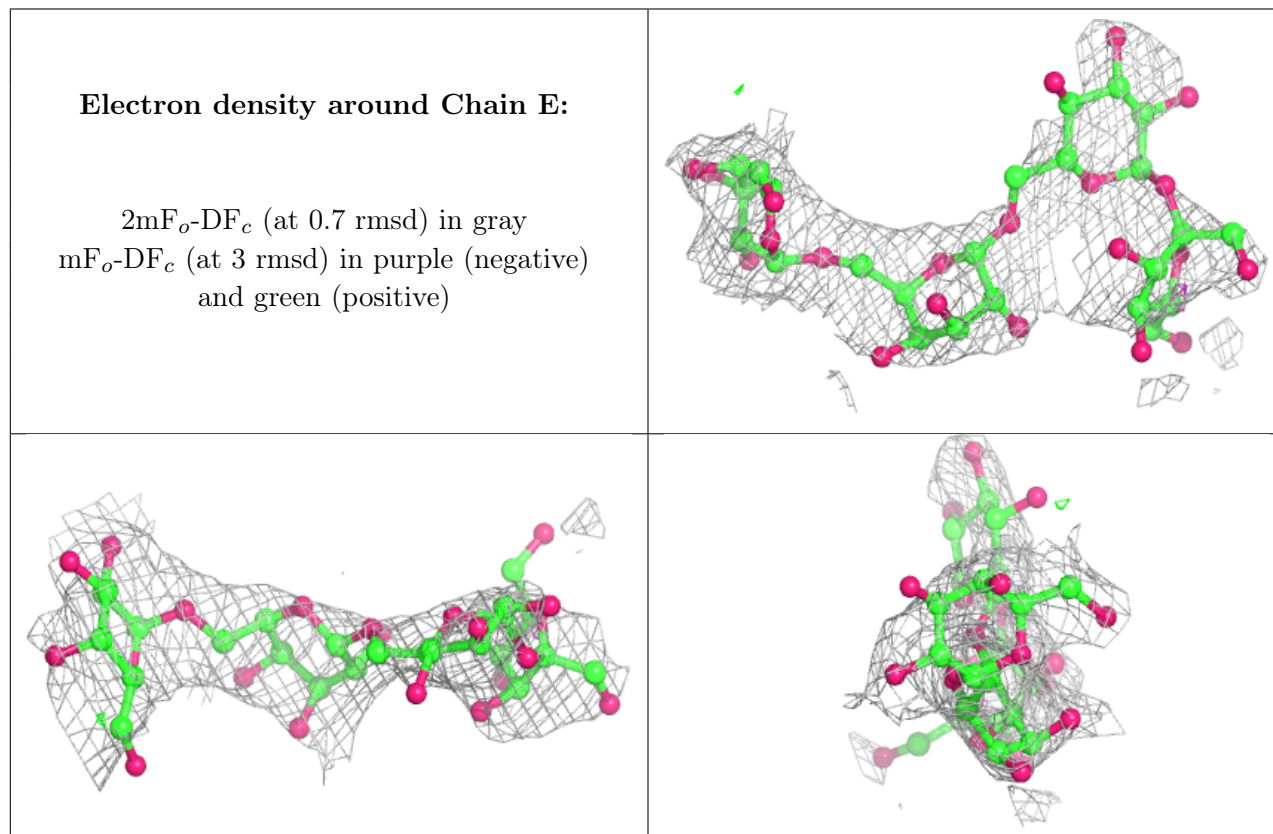
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FRU	G	4	12/12	0.68	0.52	99,131,142,146	0

*Continued on next page...*

Continued from previous page...

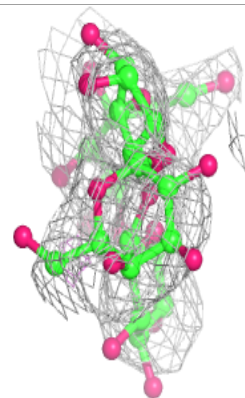
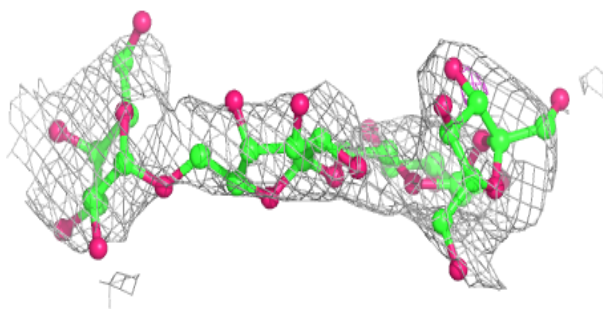
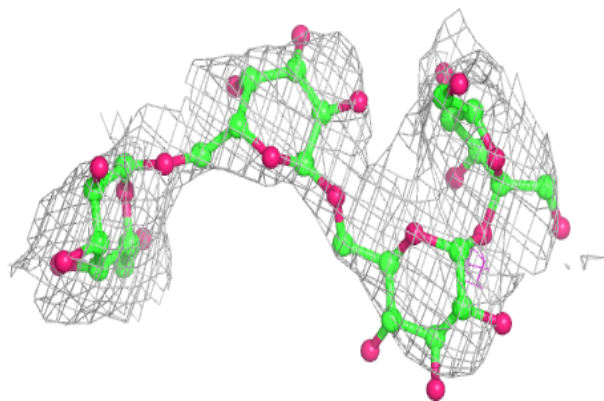
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FRU	E	4	12/12	0.70	0.50	117,138,149,157	0
2	GLC	G	3	11/12	0.73	0.63	124,139,148,150	0
2	GLC	H	3	11/12	0.73	0.34	109,129,137,138	0
2	FRU	F	4	12/12	0.81	0.38	104,131,137,140	0
2	GLA	E	2	11/12	0.81	0.30	106,116,119,121	0
2	GLC	E	3	11/12	0.82	0.45	125,141,146,151	0
2	GLA	G	1	11/12	0.85	0.25	114,119,123,125	0
2	GLA	F	2	11/12	0.87	0.28	104,109,124,127	0
2	GLA	E	1	11/12	0.87	0.26	105,123,130,131	0
2	FRU	H	4	12/12	0.87	0.30	102,121,135,143	0
2	GLC	F	3	11/12	0.88	0.39	122,129,136,138	0
2	GLA	G	2	11/12	0.88	0.27	99,110,115,119	0
2	GLA	F	1	11/12	0.89	0.23	95,103,109,110	0
2	GLA	H	2	11/12	0.91	0.18	94,102,110,110	0
2	GLA	H	1	11/12	0.93	0.19	87,98,102,103	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.

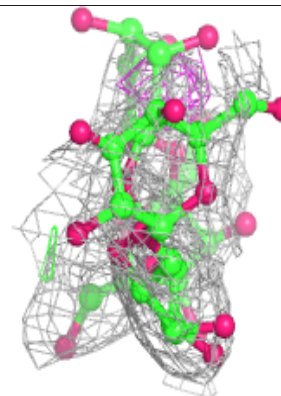
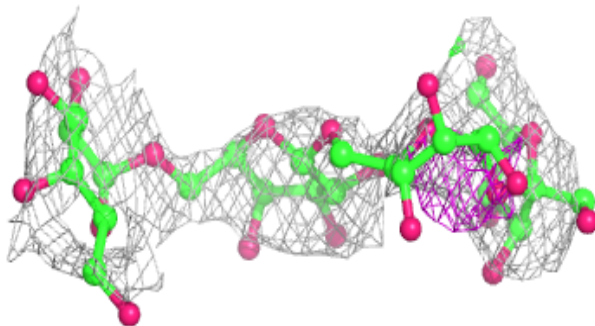
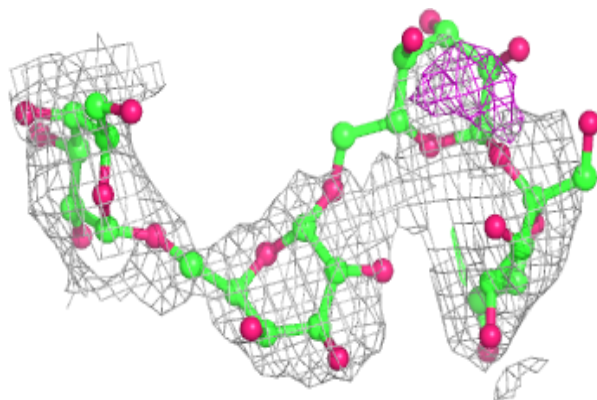


**Electron density around Chain F:**

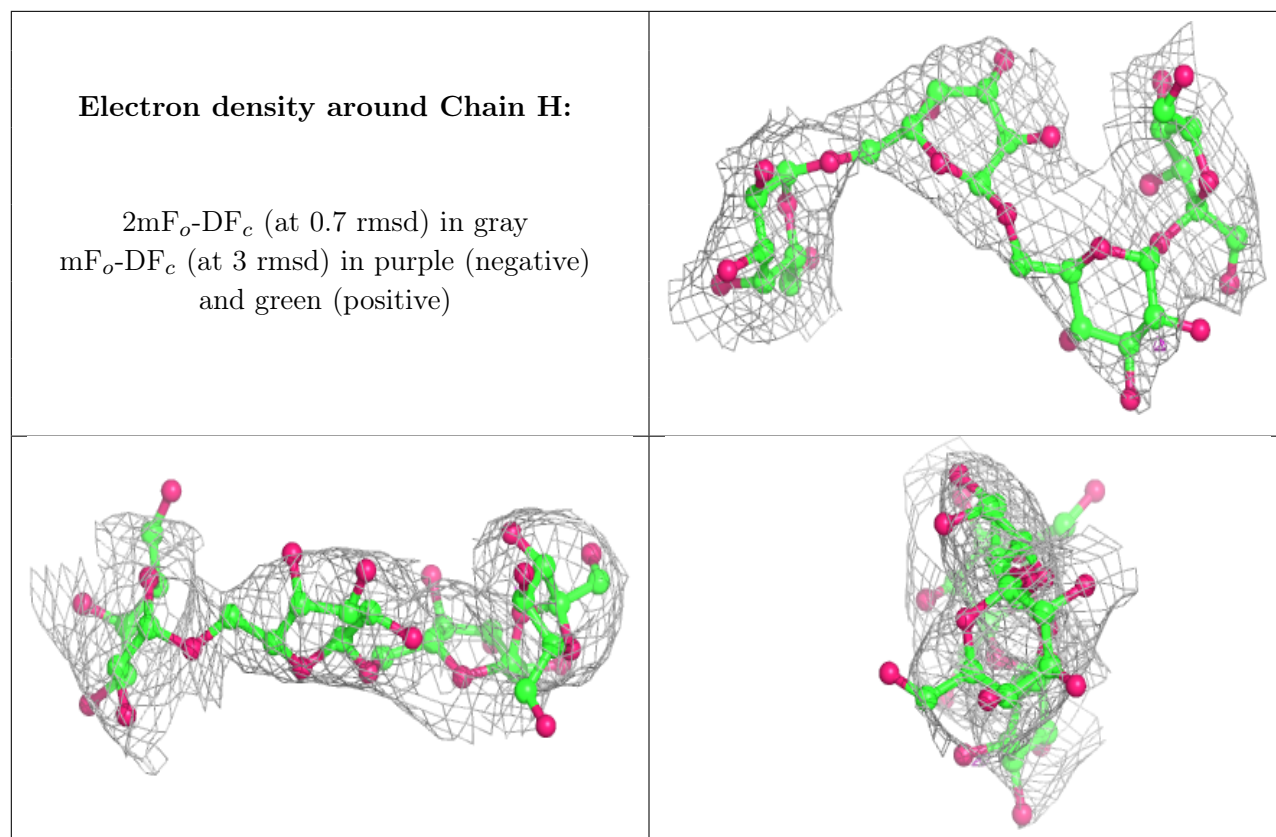
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain G:**

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







## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.