Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 09:21 AM EDT

PDB ID	:	3VTA
Title	:	Crystal Structure of cucumisin, a subtilisin-like endoprotease from Cucumis melo L
Authors	:	Murayama, K.; Kato-Murayama, M.; Hosaka, T.; Sotokawauchi, A.; Shirouzu, M.; Arima, K.; Yokoyama, S.
Deposited on	:	2012-05-23
Resolution	:	2.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

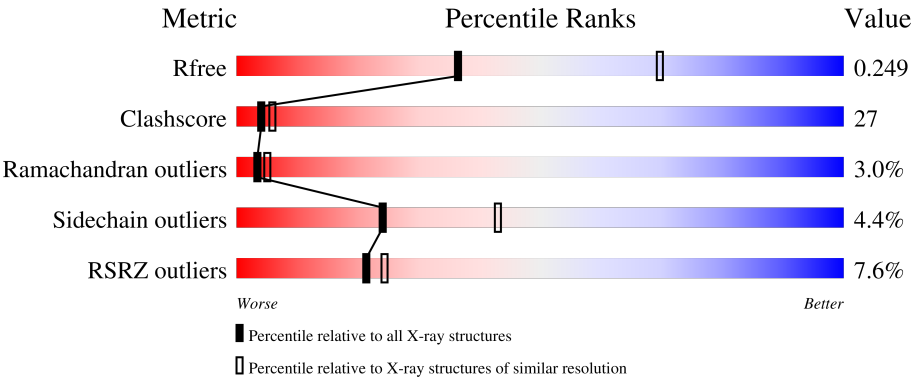
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	3%, 57%, 34%, ·, 5%
1	B	621	12%, 50%, 42%, ·, ·
2	C	5	20%, 40%, 40%
2	D	5	60%, 20%, 20%
3	E	3	33%, 67%

2 Entry composition

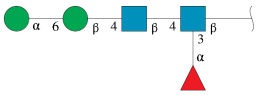
There are 5 unique types of molecules in this entry. The entry contains 9322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cucumisin.

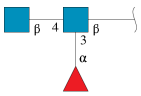
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4455	2818	773	851	13			
1	B	594	Total	C	N	O	S	0	0	0
			4483	2839	777	854	13			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



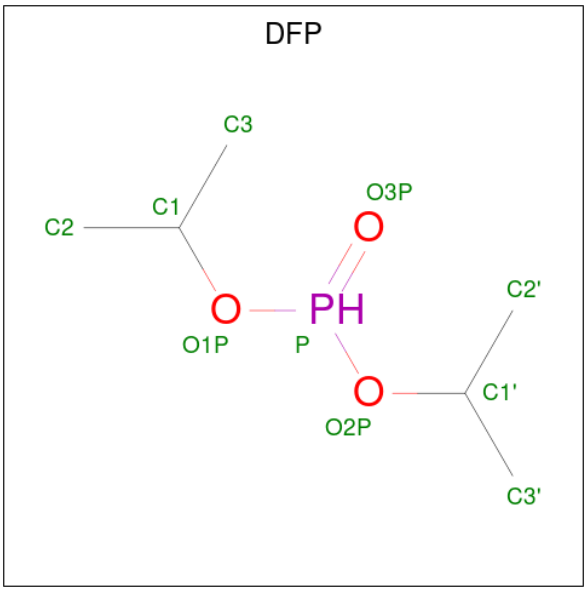
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			60	34	2	24			
2	D	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula: $C_6H_{15}O_3P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 10 6 3 1	0	0
4	B	1	Total C O P 10 6 3 1	0	0

- Molecule 5 is water.

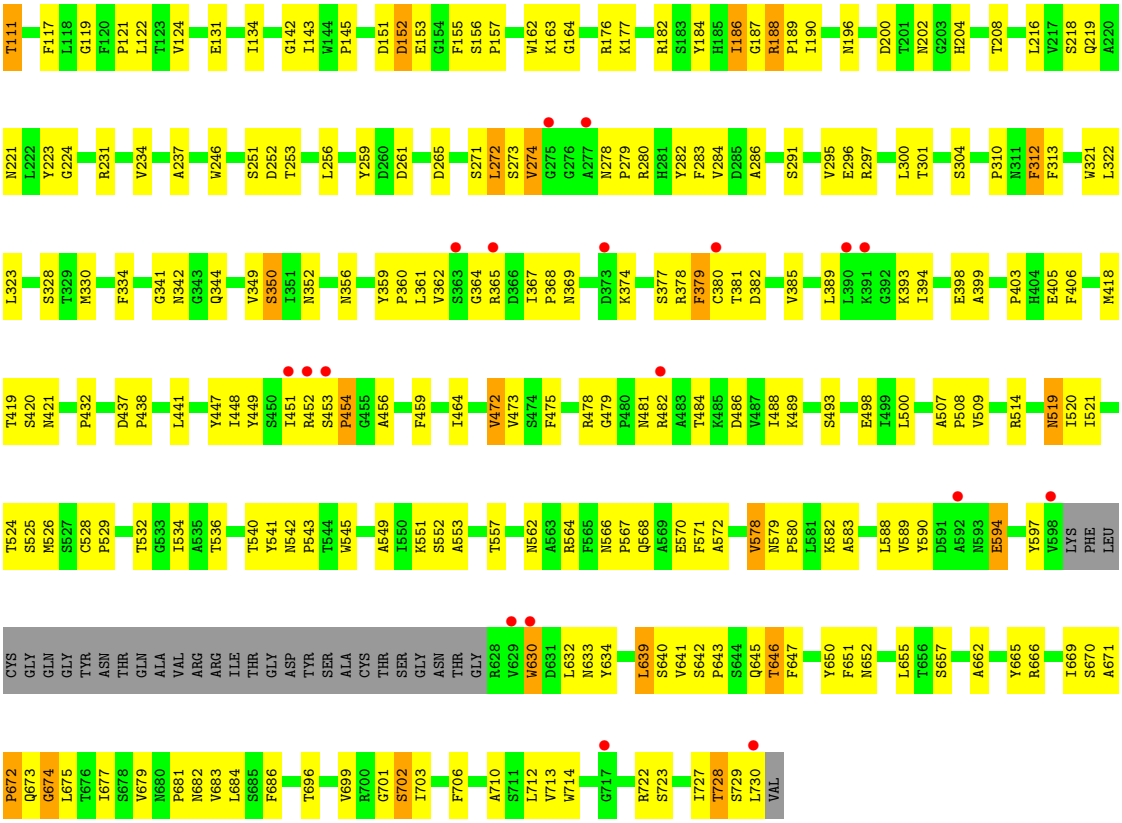
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	129	Total O 129 129	0	0
5	B	77	Total O 77 77	0	0

3 Residue-property plots (i)

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

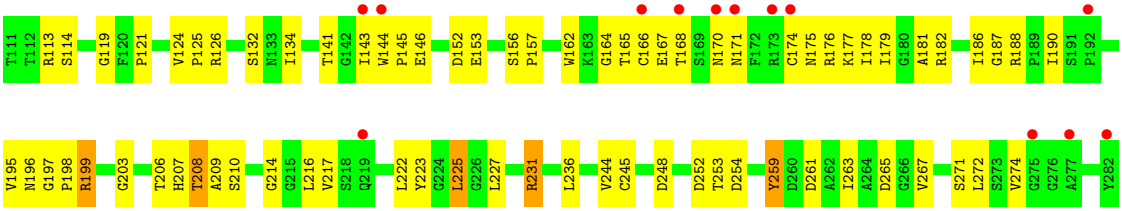
• Molecule 1: Cucumisin

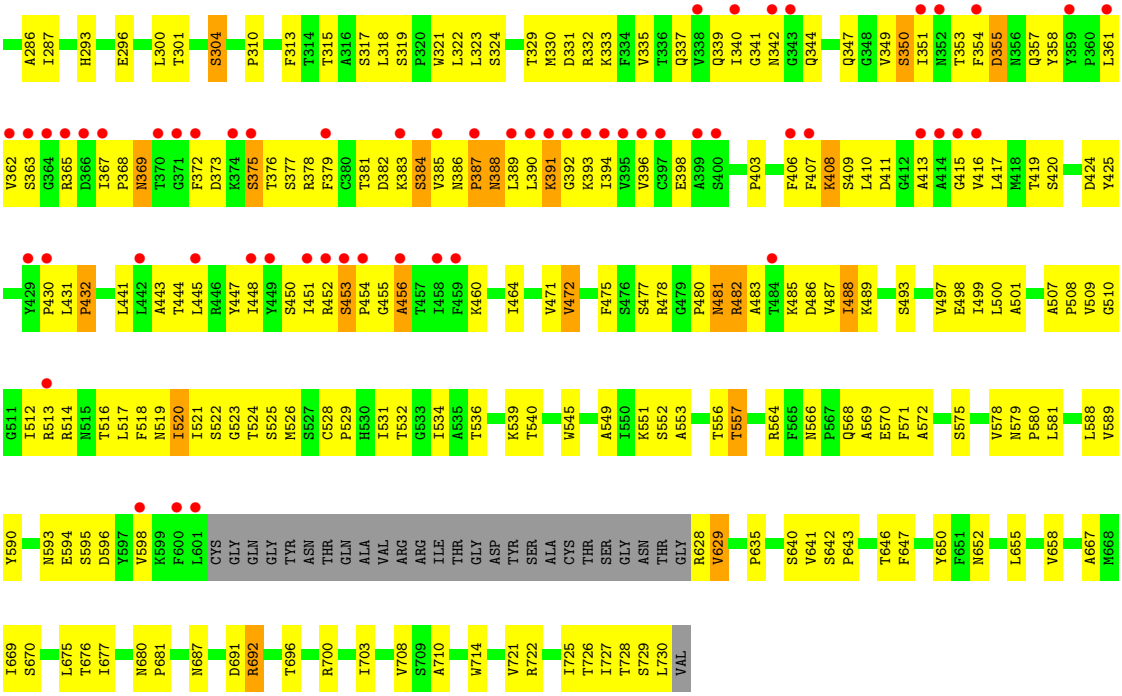
Chain A:



• Molecule 1: Cucumisin

Chain B:





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

Chain C:

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

Chain D:

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

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	149.48Å 149.48Å 218.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.64 – 2.75 44.64 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.64-2.75) 99.9 (44.64-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.262 0.204 , 0.249	Depositor DCC
R_{free} test set	2331 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9322	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/4570	0.65	0/6241
1	B	0.37	0/4599	0.63	0/6279
All	All	0.38	0/9169	0.64	0/12520

There are no bond length outliers.

There are no bond angle outliers.

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	4455	0	4358	224	0
1	B	4483	0	4389	266	0
2	C	60	0	52	3	0
2	D	60	0	52	3	0
3	E	38	0	34	3	0
4	A	10	0	14	0	0
4	B	10	0	14	0	0
5	A	129	0	0	6	0
5	B	77	0	0	11	0
All	All	9322	0	8913	491	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 (491) 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:361:LEU:HB3	1:B:454:PRO:HB2	1.30	1.08
1:A:221:ASN:HD22	1:A:224:GLY:H	1.02	0.99
1:A:488:ILE:HD11	1:A:570:GLU:HB3	1.40	0.98
1:A:342:ASN:HD22	1:A:344:GLN:HE21	1.14	0.96
1:B:363:SER:HB3	1:B:448:ILE:HD13	1.48	0.94
1:B:545:TRP:CZ2	1:B:658:VAL:HG11	2.03	0.94
1:A:296:GLU:HG2	1:A:594:GLU:HG2	1.50	0.92
1:A:278:ASN:HD21	1:A:280:ARG:HB2	1.37	0.90
1:A:374:LYS:H	1:A:374:LYS:HD2	1.37	0.88
1:A:221:ASN:ND2	1:A:224:GLY:H	1.73	0.87
1:B:545:TRP:HZ2	1:B:658:VAL:HG11	1.39	0.86
1:B:165:THR:HG22	1:B:182:ARG:HH21	1.41	0.85
1:A:478:ARG:HD3	1:A:568:GLN:NE2	1.92	0.85
1:A:364:GLY:O	1:A:377:SER:HB3	1.77	0.84
1:B:570:GLU:HG3	1:B:726:THR:OG1	1.77	0.84
1:A:342:ASN:ND2	1:A:344:GLN:HE21	1.76	0.83
1:A:300:LEU:HD12	1:A:301:THR:H	1.43	0.83
1:B:641:VAL:HG22	1:B:642:SER:H	1.46	0.81
1:A:557:THR:HG21	1:A:583:ALA:HA	1.62	0.81
1:B:225:LEU:HD12	1:B:225:LEU:H	1.43	0.81
1:A:280:ARG:HG3	1:A:482:ARG:HH11	1.46	0.80
1:B:696:THR:OG1	3:E:1:NAG:H82	1.81	0.79
1:A:464:ILE:HA	1:B:670:SER:HB2	1.65	0.78
1:A:278:ASN:ND2	1:A:280:ARG:HB2	1.98	0.76
1:A:365:ARG:HE	1:A:378:ARG:HG2	1.50	0.76
1:A:712:LEU:HD21	1:A:714:TRP:HE1	1.48	0.76
1:A:553:ALA:O	1:A:557:THR:HG22	1.85	0.76
1:A:323:LEU:HD13	1:A:551:LYS:HG3	1.68	0.76
1:A:472:VAL:H	1:A:566:ASN:HD21	1.33	0.75
1:A:478:ARG:HD3	1:A:568:GLN:HE22	1.51	0.75
1:B:430:PRO:O	1:B:512:ILE:HD11	1.88	0.74
1:B:340:ILE:HG23	1:B:342:ASN:H	1.52	0.74
1:A:202:ASN:ND2	1:A:204:HIS:HB2	2.03	0.74
1:B:464:ILE:HD11	2:D:1:NAG:H81	1.70	0.74
1:B:335:VAL:HG11	1:B:347:GLN:HG3	1.69	0.73
1:A:488:ILE:CD1	1:A:570:GLU:HB3	2.17	0.73
1:A:341:GLY:HA3	1:A:447:TYR:OH	1.89	0.73
1:A:380:CYS:HB2	1:A:385:VAL:HG21	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:PHE:O	1:B:411:ASP:HB2	1.87	0.73
1:B:362:VAL:HG21	1:B:393:LYS:HD3	1.70	0.73
1:B:313:PHE:CE2	1:B:480:PRO:HG2	2.25	0.72
1:B:199:ARG:HH11	1:B:199:ARG:HB2	1.53	0.72
1:A:671:ALA:HB2	1:A:677:ILE:HD12	1.72	0.72
1:B:669:ILE:HD13	1:B:677:ILE:HG22	1.72	0.72
1:B:367:ILE:HG22	1:B:369:ASN:ND2	2.05	0.72
1:A:703:ILE:HD13	1:A:727:ILE:HG22	1.71	0.71
1:B:121:PRO:O	1:B:124:VAL:HG23	1.90	0.71
1:B:271:SER:HB2	1:B:532:THR:HG21	1.71	0.71
1:A:313:PHE:HB3	1:A:482:ARG:HH21	1.55	0.71
1:A:552:SER:HB3	1:A:589:VAL:HG13	1.73	0.71
1:B:482:ARG:HA	1:B:482:ARG:HH11	1.55	0.71
1:B:358:TYR:HE1	1:B:456:ALA:H	1.38	0.70
1:A:231:ARG:HD2	5:A:918:HOH:O	1.90	0.70
1:A:478:ARG:HB2	1:A:571:PHE:O	1.92	0.70
1:B:369:ASN:HD22	1:B:386:ASN:H	1.39	0.70
1:B:481:ASN:C	1:B:481:ASN:HD22	1.95	0.69
1:A:421:ASN:O	2:C:3:BMA:H2	1.92	0.69
1:B:367:ILE:HG23	1:B:389:LEU:HD12	1.75	0.69
1:B:692:ARG:HH11	1:B:692:ARG:HB3	1.57	0.69
1:A:452:ARG:C	1:A:454:PRO:HD3	2.13	0.69
1:B:641:VAL:HG22	1:B:642:SER:N	2.07	0.69
1:B:486:ASP:HB2	1:B:629:VAL:HG11	1.73	0.69
1:B:552:SER:HB3	1:B:589:VAL:HG13	1.75	0.69
1:A:679:VAL:HG12	1:A:681:PRO:O	1.93	0.69
1:B:313:PHE:CD2	1:B:482:ARG:HD2	2.28	0.69
1:B:144:TRP:CZ3	1:B:146:GLU:HB2	2.28	0.68
1:B:333:LYS:HD3	2:D:1:NAG:H82	1.74	0.68
1:B:441:LEU:C	1:B:443:ALA:H	1.95	0.68
1:A:182:ARG:HG2	5:A:912:HOH:O	1.94	0.67
1:A:472:VAL:HG13	1:A:566:ASN:ND2	2.09	0.67
1:B:216:LEU:HD23	1:B:231:ARG:CB	2.24	0.67
1:A:500:LEU:HD23	1:A:500:LEU:C	2.14	0.67
1:A:669:ILE:HD13	1:A:677:ILE:HG22	1.76	0.67
1:B:403:PRO:O	1:B:406:PHE:HB2	1.93	0.67
1:B:497:VAL:HG12	1:B:498:GLU:HG3	1.75	0.67
1:A:641:VAL:HG12	1:A:642:SER:N	2.09	0.67
1:A:134:ILE:HD12	1:A:540:THR:HG22	1.76	0.67
1:A:478:ARG:CD	1:A:568:GLN:HE22	2.08	0.67
1:B:341:GLY:HA3	1:B:447:TYR:OH	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:VAL:HG13	1:A:519:ASN:ND2	2.10	0.67
1:B:394:ILE:HA	1:B:415:GLY:O	1.93	0.66
1:B:667:ALA:HB2	1:B:714:TRP:CZ3	2.30	0.66
1:A:221:ASN:HD22	1:A:224:GLY:N	1.86	0.66
1:A:399:ALA:O	1:A:418:MET:HB3	1.96	0.65
1:B:692:ARG:HH11	1:B:692:ARG:CB	2.08	0.65
1:B:369:ASN:HB3	1:B:386:ASN:HD22	1.61	0.65
1:B:481:ASN:ND2	1:B:483:ALA:H	1.94	0.65
1:B:628:ARG:HG2	1:B:629:VAL:H	1.61	0.65
1:A:509:VAL:HG13	1:A:519:ASN:HD21	1.60	0.65
1:B:199:ARG:HB2	1:B:199:ARG:NH1	2.11	0.65
1:A:188:ARG:HB3	1:A:189:PRO:CD	2.27	0.64
1:A:208:THR:HG23	1:A:529:PRO:HG3	1.78	0.64
1:A:156:SER:HB2	1:A:157:PRO:HD2	1.80	0.64
1:B:369:ASN:ND2	1:B:386:ASN:H	1.96	0.64
1:B:385:VAL:HG12	1:B:390:LEU:HD11	1.80	0.64
1:B:594:GLU:O	1:B:598:VAL:HG23	1.98	0.64
1:A:352:ASN:HD21	1:A:432:PRO:HA	1.62	0.63
1:A:528:CYS:HB3	1:A:529:PRO:HD3	1.80	0.63
1:B:444:THR:O	1:B:448:ILE:HG13	1.98	0.63
1:A:683:VAL:O	1:A:684:LEU:HD23	1.99	0.62
1:B:643:PRO:HG3	1:B:729:SER:HB2	1.80	0.62
1:B:406:PHE:CD2	1:B:430:PRO:HD2	2.34	0.62
1:B:223:TYR:H	1:B:225:LEU:HD12	1.62	0.62
1:A:310:PRO:O	1:A:478:ARG:HD2	2.00	0.61
1:B:408:LYS:HG2	1:B:409:SER:N	2.15	0.61
1:B:488:ILE:HG12	1:B:489:LYS:N	2.15	0.61
1:A:272:LEU:CD2	1:A:274:VAL:HG22	2.30	0.61
1:A:594:GLU:HA	1:A:597:TYR:HD1	1.65	0.61
1:A:328:SER:HA	1:A:472:VAL:HA	1.83	0.61
1:B:539:LYS:HE3	5:B:970:HOH:O	2.01	0.61
1:B:549:ALA:HA	1:B:589:VAL:HG11	1.83	0.61
1:A:361:LEU:HB2	1:A:454:PRO:HB2	1.83	0.61
1:B:478:ARG:HG3	1:B:568:GLN:OE1	2.00	0.61
1:B:368:PRO:HB3	1:B:372:PHE:O	2.02	0.60
1:A:419:THR:OG1	1:A:441:LEU:HD22	2.01	0.60
1:B:132:SER:HA	1:B:236:LEU:O	2.01	0.60
1:A:342:ASN:HD22	1:A:344:GLN:NE2	1.93	0.60
1:B:362:VAL:HG11	1:B:389:LEU:O	2.00	0.60
1:A:283:PHE:CD1	1:A:284:VAL:HG13	2.37	0.59
1:A:283:PHE:HD1	1:A:284:VAL:HG13	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASP:OD1	1:B:176:ARG:HB2	2.02	0.59
1:B:481:ASN:HD21	1:B:483:ALA:HB3	1.67	0.59
1:B:526:MET:O	1:B:529:PRO:HD2	2.01	0.59
1:A:280:ARG:HG3	1:A:482:ARG:HD3	1.84	0.59
1:B:134:ILE:HD12	1:B:540:THR:HG22	1.84	0.59
1:A:304:SER:HB3	1:A:524:THR:O	2.03	0.59
1:A:252:ASP:O	1:A:256:LEU:HG	2.02	0.59
1:B:143:ILE:HG21	1:B:178:ILE:HD13	1.84	0.59
1:B:386:ASN:HB2	1:B:388:ASN:ND2	2.18	0.59
1:B:464:ILE:HD11	2:D:1:NAG:C8	2.32	0.59
1:A:359:TYR:HB2	1:A:394:ILE:HG13	1.85	0.59
1:A:381:THR:HG22	1:A:382:ASP:N	2.17	0.59
1:A:557:THR:HG21	1:A:583:ALA:CA	2.32	0.58
1:B:526:MET:C	1:B:529:PRO:HD2	2.24	0.58
1:A:639:LEU:HD22	1:A:641:VAL:HG23	1.86	0.58
1:B:217:VAL:HG11	1:B:518:PHE:CZ	2.38	0.58
1:B:361:LEU:HA	1:B:394:ILE:CG2	2.34	0.58
1:B:367:ILE:HD13	1:B:389:LEU:HB2	1.85	0.58
1:B:387:PRO:O	1:B:391:LYS:HG3	2.03	0.58
1:B:383:LYS:HA	1:B:409:SER:HB3	1.86	0.58
1:B:369:ASN:CG	1:B:388:ASN:HD22	2.06	0.58
1:A:271:SER:HB2	1:A:532:THR:HG21	1.85	0.58
1:B:335:VAL:HG11	1:B:347:GLN:CG	2.33	0.58
1:A:549:ALA:HA	1:A:589:VAL:HG11	1.85	0.58
1:A:131:GLU:CG	1:A:234:VAL:HG13	2.34	0.58
1:B:362:VAL:HG21	1:B:393:LYS:CD	2.34	0.58
1:B:392:GLY:H	1:B:413:ALA:HA	1.68	0.58
1:A:300:LEU:HD12	1:A:301:THR:N	2.16	0.57
1:A:682:ASN:OD1	1:A:683:VAL:HG23	2.04	0.57
1:B:430:PRO:O	1:B:431:LEU:HD23	2.04	0.57
1:B:528:CYS:HB3	1:B:529:PRO:HD3	1.87	0.57
1:B:216:LEU:HD23	1:B:231:ARG:HB3	1.85	0.57
1:B:646:THR:HG22	1:B:647:PHE:N	2.20	0.57
1:B:680:ASN:HD22	1:B:681:PRO:HA	1.70	0.57
1:A:234:VAL:HG12	1:A:234:VAL:O	2.05	0.57
1:B:430:PRO:HG3	1:B:510:GLY:O	2.05	0.57
1:A:291:SER:O	1:A:295:VAL:HG23	2.05	0.57
1:B:222:LEU:HB3	1:B:225:LEU:HD13	1.86	0.57
1:B:377:SER:HA	1:B:384:SER:HB3	1.86	0.57
1:A:706:PHE:HA	1:A:729:SER:OG	2.05	0.56
1:B:658:VAL:HG12	1:B:658:VAL:O	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:SER:O	1:A:578:VAL:HG22	2.04	0.56
1:B:373:ASP:O	1:B:377:SER:HB2	2.06	0.56
1:A:398:GLU:HG2	1:A:441:LEU:HD21	1.88	0.56
1:B:304:SER:HB3	1:B:524:THR:O	2.05	0.56
1:B:519:ASN:ND2	1:B:520:ILE:H	2.04	0.56
1:B:475:PHE:CE1	1:B:523:GLY:HA2	2.41	0.56
1:B:337:GLN:HB3	5:B:966:HOH:O	2.05	0.56
1:A:684:LEU:HG	1:A:714:TRP:CZ3	2.41	0.55
1:B:304:SER:HB2	1:B:524:THR:OG1	2.07	0.55
1:B:340:ILE:HD11	1:B:444:THR:HA	1.88	0.55
1:B:598:VAL:HG12	1:B:598:VAL:O	2.06	0.55
1:B:480:PRO:HB3	1:B:571:PHE:CE1	2.41	0.55
1:B:593:ASN:ND2	1:B:595:SER:HB3	2.21	0.55
1:B:361:LEU:CB	1:B:454:PRO:HB2	2.20	0.55
1:A:448:ILE:HA	1:A:454:PRO:HG2	1.88	0.55
1:B:488:ILE:HG22	5:B:922:HOH:O	2.07	0.55
1:B:553:ALA:O	1:B:557:THR:HB	2.07	0.54
1:A:231:ARG:NH2	5:A:945:HOH:O	2.40	0.54
1:B:658:VAL:O	1:B:658:VAL:CG1	2.54	0.54
1:A:646:THR:HA	1:A:702:SER:HB3	1.88	0.54
1:B:509:VAL:HB	1:B:514:ARG:HG3	1.90	0.54
1:A:451:ILE:O	1:A:452:ARG:HB2	2.08	0.54
1:B:728:THR:HG22	1:B:730:LEU:H	1.72	0.54
1:A:218:SER:O	1:A:219:GLN:HB2	2.06	0.54
1:A:349:VAL:O	1:A:350:SER:HB3	2.08	0.54
1:B:165:THR:HG22	1:B:182:ARG:NH2	2.19	0.54
1:A:453:SER:N	1:A:454:PRO:HD3	2.23	0.54
1:A:478:ARG:CB	1:A:571:PHE:O	2.56	0.54
1:B:186:ILE:HD12	1:B:253:THR:HG22	1.88	0.54
1:B:569:ALA:HB1	1:B:570:GLU:OE2	2.08	0.54
1:B:319:SER:HB3	1:B:321:TRP:CE2	2.43	0.54
1:A:639:LEU:HD22	1:A:641:VAL:CG2	2.39	0.53
1:B:680:ASN:ND2	1:B:681:PRO:HA	2.23	0.53
1:A:712:LEU:HD21	1:A:714:TRP:NE1	2.21	0.53
1:B:481:ASN:HD22	1:B:483:ALA:H	1.56	0.53
1:A:632:LEU:O	1:A:634:TYR:N	2.38	0.53
1:A:119:GLY:C	1:A:121:PRO:HD3	2.29	0.53
1:B:341:GLY:HA3	1:B:447:TYR:CZ	2.43	0.53
1:B:329:THR:HG23	1:B:471:VAL:O	2.08	0.53
1:A:162:TRP:C	1:A:163:LYS:HD2	2.29	0.53
1:A:669:ILE:HG22	1:A:670:SER:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLY:C	1:A:200:ASP:HB2	2.28	0.53
1:B:188:ARG:NH2	1:B:254:ASP:OD2	2.42	0.53
1:A:322:LEU:O	1:A:489:LYS:NZ	2.42	0.53
1:B:556:THR:HA	1:B:722:ARG:O	2.08	0.53
1:A:557:THR:HG23	5:A:907:HOH:O	2.09	0.53
1:A:570:GLU:C	1:A:572:ALA:H	2.12	0.53
1:B:488:ILE:HG23	5:B:903:HOH:O	2.09	0.53
1:B:512:ILE:HG22	1:B:513:ARG:N	2.24	0.53
1:A:594:GLU:HA	1:A:597:TYR:CD1	2.43	0.52
1:A:641:VAL:HG12	1:A:642:SER:H	1.74	0.52
1:B:272:LEU:CD1	1:B:274:VAL:HG12	2.40	0.52
1:B:385:VAL:CG1	1:B:390:LEU:HD11	2.38	0.52
1:A:186:ILE:HD12	1:A:253:THR:HG22	1.90	0.52
1:A:448:ILE:HA	1:A:454:PRO:CG	2.38	0.52
1:A:256:LEU:HD21	1:A:286:ALA:HB1	1.92	0.52
1:A:481:ASN:HB3	1:A:484:THR:O	2.09	0.52
1:A:567:PRO:HG2	2:C:4:MAN:O4	2.09	0.52
1:B:170:ASN:HD22	1:B:197:GLY:HA3	1.73	0.52
1:A:374:LYS:HD2	1:A:374:LYS:N	2.15	0.52
1:A:117:PHE:CE2	1:A:330:MET:HA	2.45	0.52
1:B:354:PHE:CD1	1:B:432:PRO:HD3	2.45	0.52
1:B:323:LEU:HD13	1:B:551:LYS:HG3	1.91	0.52
1:B:441:LEU:C	1:B:443:ALA:N	2.62	0.52
1:B:119:GLY:C	1:B:121:PRO:HD3	2.30	0.52
1:B:223:TYR:H	1:B:225:LEU:CD1	2.23	0.52
1:A:273:SER:HB3	1:A:525:SER:HB2	1.92	0.52
1:A:486:ASP:OD1	1:A:639:LEU:HA	2.10	0.51
1:B:167:GLU:OE1	1:B:198:PRO:HD3	2.11	0.51
1:B:692:ARG:HH11	1:B:692:ARG:CG	2.23	0.51
1:A:451:ILE:O	1:A:451:ILE:HG22	2.10	0.51
1:A:374:LYS:H	1:A:374:LYS:CD	2.15	0.51
1:A:665:TYR:HD2	1:A:714:TRP:O	1.94	0.51
1:A:272:LEU:HD21	1:A:274:VAL:HG22	1.91	0.51
1:B:340:ILE:CD1	1:B:444:THR:HA	2.40	0.51
1:A:362:VAL:HG13	1:A:393:LYS:HD3	1.92	0.51
1:A:641:VAL:CG1	1:A:642:SER:N	2.74	0.51
1:B:575:SER:HA	5:B:918:HOH:O	2.09	0.51
1:B:182:ARG:HH11	1:B:261:ASP:HB3	1.74	0.51
1:B:355:ASP:O	1:B:357:GLN:HG3	2.11	0.51
1:B:519:ASN:HD22	1:B:520:ILE:H	1.59	0.51
1:A:646:THR:HA	1:A:701:GLY:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:LYS:HE3	1:B:640:SER:OG	2.11	0.50
1:B:549:ALA:HA	1:B:589:VAL:CG1	2.41	0.50
1:A:312:PHE:O	1:A:479:GLY:O	2.28	0.50
1:A:728:THR:HG22	1:A:730:LEU:H	1.76	0.50
1:B:141:THR:HG22	1:B:245:CYS:HB2	1.93	0.50
1:B:416:VAL:O	1:B:417:LEU:HD23	2.12	0.50
1:B:588:LEU:HD13	1:B:655:LEU:HD13	1.94	0.50
1:A:360:PRO:HB2	1:A:393:LYS:HG2	1.93	0.50
1:A:119:GLY:O	1:A:121:PRO:HD3	2.11	0.50
1:A:472:VAL:N	1:A:566:ASN:HD21	2.07	0.50
1:A:521:ILE:HG13	1:A:526:MET:HE3	1.94	0.50
1:A:641:VAL:HG11	1:A:647:PHE:CD2	2.47	0.50
1:B:497:VAL:CG1	1:B:498:GLU:HG3	2.41	0.50
1:A:184:TYR:OH	1:A:261:ASP:OD1	2.26	0.49
1:B:272:LEU:HG	1:B:274:VAL:HG12	1.94	0.49
1:B:340:ILE:HG22	1:B:344:GLN:HB2	1.94	0.49
1:B:646:THR:CG2	1:B:647:PHE:N	2.74	0.49
1:B:222:LEU:HB3	1:B:225:LEU:CD1	2.43	0.49
1:B:481:ASN:HD22	1:B:482:ARG:N	2.09	0.49
1:B:318:LEU:HD22	1:B:481:ASN:ND2	2.27	0.49
1:B:472:VAL:HG11	1:B:572:ALA:HB1	1.94	0.49
1:A:202:ASN:HD22	1:A:204:HIS:HB2	1.73	0.49
1:A:639:LEU:HD23	1:A:640:SER:N	2.28	0.49
1:A:706:PHE:O	1:A:728:THR:HA	2.12	0.49
1:B:195:VAL:HG12	1:B:196:ASN:O	2.13	0.49
1:B:383:LYS:C	1:B:385:VAL:H	2.17	0.49
1:A:379:PHE:CD1	1:A:379:PHE:N	2.81	0.48
1:B:164:GLY:HA2	1:B:265:ASP:OD1	2.13	0.48
1:B:165:THR:CG2	1:B:182:ARG:HH21	2.20	0.48
1:B:641:VAL:HG21	1:B:647:PHE:CD2	2.48	0.48
1:A:403:PRO:O	1:A:406:PHE:HB2	2.14	0.48
1:B:259:TYR:O	1:B:263:ILE:HG13	2.14	0.48
1:B:441:LEU:O	1:B:445:LEU:HG	2.13	0.48
1:B:676:THR:HB	1:B:700:ARG:HG2	1.95	0.48
1:B:453:SER:N	1:B:454:PRO:HD3	2.29	0.48
1:A:111:THR:HB	1:A:500:LEU:O	2.13	0.48
1:A:500:LEU:HB2	1:A:520:ILE:HG12	1.96	0.48
1:A:570:GLU:CD	1:A:570:GLU:H	2.17	0.48
1:B:162:TRP:NE1	1:B:179:ILE:O	2.44	0.48
1:A:367:ILE:HG22	1:A:367:ILE:O	2.13	0.48
1:B:710:ALA:HB3	1:B:725:ILE:HB	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:HD21	1:A:204:HIS:HB2	1.79	0.48
1:A:131:GLU:CD	1:A:234:VAL:HG13	2.34	0.48
1:A:304:SER:HB2	1:A:524:THR:OG1	2.14	0.47
1:B:447:TYR:OH	1:B:455:GLY:N	2.40	0.47
1:B:641:VAL:CG2	1:B:642:SER:N	2.77	0.47
1:B:650:TYR:HE1	1:B:652:ASN:OD1	1.97	0.47
1:B:317:SER:OG	1:B:322:LEU:HD23	2.14	0.47
1:B:389:LEU:O	1:B:390:LEU:HD23	2.14	0.47
1:A:473:VAL:HG11	1:A:475:PHE:CZ	2.50	0.47
1:B:225:LEU:HD11	1:B:353:THR:HG22	1.97	0.47
1:B:354:PHE:CB	1:B:432:PRO:HG3	2.44	0.47
1:B:551:LYS:HD3	5:B:950:HOH:O	2.13	0.47
1:A:729:SER:O	1:A:730:LEU:HB3	2.14	0.47
1:A:378:ARG:HD2	1:A:379:PHE:CE1	2.50	0.47
1:B:166:CYS:HA	1:B:181:ALA:O	2.15	0.47
1:B:641:VAL:CG2	1:B:642:SER:H	2.21	0.47
1:A:164:GLY:HA2	1:A:265:ASP:OD1	2.14	0.47
1:A:374:LYS:HA	1:A:377:SER:HB2	1.97	0.47
1:B:481:ASN:C	1:B:481:ASN:ND2	2.67	0.47
1:B:340:ILE:HD11	1:B:444:THR:HG23	1.97	0.47
1:A:367:ILE:HG21	1:A:389:LEU:HB2	1.96	0.46
1:B:369:ASN:HB3	1:B:386:ASN:ND2	2.29	0.46
1:B:493:SER:O	1:B:578:VAL:HG23	2.15	0.46
1:B:252:ASP:HB3	1:B:286:ALA:HB2	1.97	0.46
1:B:349:VAL:O	1:B:350:SER:HB3	2.15	0.46
1:A:472:VAL:H	1:A:566:ASN:ND2	2.06	0.46
1:B:188:ARG:NH1	1:B:248:ASP:OD2	2.48	0.46
1:B:367:ILE:N	1:B:368:PRO:HD3	2.30	0.46
1:A:367:ILE:CG2	1:A:389:LEU:HB2	2.46	0.46
1:A:202:ASN:HD22	1:A:204:HIS:CB	2.29	0.46
1:B:272:LEU:HD11	1:B:274:VAL:HG12	1.98	0.46
1:B:378:ARG:HD2	1:B:398:GLU:OE2	2.16	0.46
1:A:342:ASN:ND2	1:A:344:GLN:NE2	2.54	0.46
1:B:287:ILE:HG13	5:B:917:HOH:O	2.15	0.46
1:B:703:ILE:HD13	1:B:727:ILE:HG22	1.96	0.46
1:B:520:ILE:O	1:B:520:ILE:CG1	2.64	0.46
1:A:381:THR:HG22	1:A:382:ASP:H	1.78	0.46
1:A:662:ALA:HA	1:A:686:PHE:O	2.16	0.46
1:B:156:SER:HB2	1:B:157:PRO:CD	2.46	0.46
1:B:174:CYS:HB2	1:B:178:ILE:O	2.16	0.46
1:B:203:GLY:O	1:B:206:THR:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ASN:ND2	1:B:483:ALA:N	2.63	0.46
1:B:181:ALA:HB1	1:B:198:PRO:HB3	1.97	0.45
1:B:507:ALA:HA	1:B:508:PRO:HD3	1.83	0.45
1:B:590:TYR:CZ	1:B:655:LEU:HD21	2.51	0.45
1:B:114:SER:HA	1:B:330:MET:HE2	1.97	0.45
1:A:280:ARG:CG	1:A:482:ARG:HH11	2.21	0.45
1:A:362:VAL:CG1	1:A:393:LYS:HD3	2.47	0.45
1:B:486:ASP:CB	1:B:629:VAL:HG11	2.45	0.45
1:B:409:SER:O	1:B:410:LEU:HD23	2.17	0.45
1:A:334:PHE:HD1	1:A:498:GLU:OE1	1.99	0.45
1:B:365:ARG:HB3	1:B:378:ARG:HB3	1.99	0.45
1:B:367:ILE:CG2	1:B:369:ASN:ND2	2.76	0.45
1:A:534:ILE:CD1	1:A:580:PRO:HG3	2.47	0.45
1:B:351:ILE:HD13	1:B:520:ILE:CG1	2.46	0.45
1:B:488:ILE:HA	5:B:913:HOH:O	2.17	0.45
1:B:536:THR:O	1:B:540:THR:HG23	2.16	0.45
1:B:628:ARG:CG	1:B:629:VAL:H	2.28	0.45
1:A:641:VAL:CG1	1:A:642:SER:H	2.30	0.45
1:A:500:LEU:HA	1:A:519:ASN:O	2.17	0.45
1:B:487:VAL:HG23	1:B:629:VAL:HG13	1.98	0.45
1:B:568:GLN:HG3	5:B:948:HOH:O	2.17	0.45
1:A:163:LYS:HD2	1:A:163:LYS:N	2.32	0.44
1:A:438:PRO:O	1:A:441:LEU:HB3	2.18	0.44
1:B:358:TYR:OH	1:B:455:GLY:HA2	2.17	0.44
1:B:198:PRO:O	1:B:199:ARG:C	2.56	0.44
1:B:488:ILE:HG21	5:B:928:HOH:O	2.17	0.44
1:A:542:ASN:N	1:A:543:PRO:HD3	2.32	0.44
1:A:647:PHE:HE1	1:A:699:VAL:HG12	1.81	0.44
1:A:729:SER:O	1:A:730:LEU:CB	2.66	0.44
1:B:315:THR:CA	1:B:477:SER:HB3	2.47	0.44
1:A:121:PRO:HD2	1:A:124:VAL:CG1	2.48	0.44
1:A:361:LEU:HD11	1:A:456:ALA:HB2	1.99	0.44
1:A:365:ARG:HH21	1:A:378:ARG:HD3	1.83	0.44
1:A:381:THR:HG23	1:A:405:GLU:CD	2.37	0.44
1:A:645:GLN:O	1:A:646:THR:C	2.56	0.44
1:B:168:THR:O	1:B:168:THR:HG22	2.17	0.44
1:B:315:THR:HA	1:B:477:SER:HB3	1.98	0.44
1:A:234:VAL:CG1	1:A:237:ALA:HB2	2.47	0.44
1:B:210:SER:O	1:B:214:GLY:N	2.46	0.44
1:B:375:SER:C	1:B:377:SER:H	2.20	0.44
1:B:628:ARG:HG2	1:B:629:VAL:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PRO:HB2	1:B:391:LYS:HE3	1.99	0.44
1:B:647:PHE:CZ	1:B:727:ILE:HD13	2.53	0.44
1:B:650:TYR:HH	3:E:1:NAG:HO6	1.65	0.44
1:A:188:ARG:CB	1:A:189:PRO:CD	2.95	0.44
1:A:562:ASN:OD1	1:A:564:ARG:HB3	2.18	0.44
1:A:673:GLN:C	1:A:675:LEU:H	2.20	0.44
1:B:351:ILE:CD1	1:B:520:ILE:HD11	2.47	0.44
1:A:551:LYS:HD3	5:A:946:HOH:O	2.18	0.44
1:A:177:LYS:HE3	5:A:985:HOH:O	2.18	0.43
1:A:507:ALA:HA	1:A:508:PRO:HD3	1.90	0.43
1:A:672:PRO:HD3	1:A:710:ALA:HB2	1.99	0.43
1:B:339:GLN:O	1:B:456:ALA:HA	2.18	0.43
1:B:522:SER:O	1:B:526:MET:CE	2.66	0.43
1:A:341:GLY:HA3	1:A:447:TYR:CZ	2.52	0.43
1:A:666:ARG:NH1	1:A:666:ARG:HB2	2.32	0.43
1:B:190:ILE:HD11	1:B:196:ASN:OD1	2.18	0.43
1:A:419:THR:HG21	1:A:438:PRO:HA	2.01	0.43
1:A:669:ILE:CG2	1:A:670:SER:N	2.81	0.43
1:B:519:ASN:ND2	1:B:520:ILE:N	2.66	0.43
1:B:534:ILE:HD13	1:B:578:VAL:HG11	1.99	0.43
1:A:279:PRO:O	1:A:282:TYR:HD2	2.02	0.43
1:B:339:GLN:HG3	1:B:344:GLN:O	2.19	0.43
1:B:728:THR:HG22	1:B:730:LEU:N	2.33	0.43
3:E:1:NAG:O7	3:E:2:FUC:C1	2.67	0.43
1:A:155:PHE:CE2	1:A:177:LYS:HD3	2.53	0.43
1:A:699:VAL:HG11	1:A:727:ILE:HD11	2.00	0.43
1:B:208:THR:HG22	1:B:209:ALA:N	2.33	0.43
1:B:416:VAL:HG12	1:B:417:LEU:N	2.34	0.43
1:B:482:ARG:HH11	1:B:482:ARG:CA	2.28	0.43
1:A:190:ILE:HD12	1:A:246:TRP:CZ3	2.53	0.43
1:A:234:VAL:HG11	1:A:237:ALA:HB2	2.01	0.43
1:B:272:LEU:HD11	1:B:274:VAL:CG1	2.49	0.43
1:B:315:THR:HG22	1:B:478:ARG:O	2.18	0.43
1:A:121:PRO:O	1:A:124:VAL:HG13	2.18	0.43
1:A:500:LEU:C	1:A:500:LEU:CD2	2.87	0.43
1:A:552:SER:CB	1:A:589:VAL:HG13	2.45	0.43
1:A:650:TYR:HE1	1:A:652:ASN:ND2	2.17	0.43
1:B:381:THR:HG22	1:B:382:ASP:N	2.34	0.43
1:A:280:ARG:HG3	1:A:482:ARG:CD	2.49	0.43
1:B:175:ASN:OD1	1:B:177:LYS:N	2.49	0.43
1:B:497:VAL:O	1:B:499:ILE:HD12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:HD2	1:A:124:VAL:HG12	2.01	0.43
1:A:280:ARG:HG3	1:A:482:ARG:NH1	2.25	0.43
1:A:541:TYR:C	1:A:543:PRO:HD3	2.39	0.43
1:B:217:VAL:HG11	1:B:518:PHE:HZ	1.82	0.42
1:A:223:TYR:CE1	1:A:514:ARG:HB3	2.54	0.42
1:A:295:VAL:HG21	1:A:321:TRP:HB2	2.00	0.42
1:B:453:SER:H	1:B:454:PRO:HD3	1.84	0.42
1:A:208:THR:HG23	1:A:529:PRO:CG	2.46	0.42
1:B:472:VAL:HG13	1:B:566:ASN:CG	2.39	0.42
1:A:545:TRP:HZ3	1:A:553:ALA:HB2	1.85	0.42
1:B:351:ILE:HD13	1:B:520:ILE:HG12	2.00	0.42
1:A:557:THR:OG1	1:A:582:LYS:HB3	2.19	0.42
1:B:390:LEU:O	1:B:391:LYS:C	2.57	0.42
1:A:728:THR:HG22	1:A:730:LEU:N	2.34	0.42
1:B:675:LEU:HD11	1:B:708:VAL:HG11	2.02	0.42
1:A:588:LEU:HD23	1:A:657:SER:HA	2.02	0.42
1:B:378:ARG:HG3	1:B:379:PHE:CD1	2.54	0.42
1:A:589:VAL:HG12	1:A:590:TYR:N	2.35	0.42
1:B:207:HIS:CE1	1:B:501:ALA:HB3	2.55	0.42
1:B:424:ASP:O	1:B:425:TYR:HB3	2.20	0.42
1:B:588:LEU:HB2	1:B:721:VAL:HG21	2.02	0.42
1:A:151:ASP:OD1	1:A:152:ASP:N	2.52	0.42
1:A:155:PHE:CZ	1:A:177:LYS:HD3	2.55	0.42
2:C:2:NAG:O5	2:C:5:FUC:H5	2.20	0.42
1:A:356:ASN:OD1	1:A:459:PHE:HA	2.20	0.42
1:A:419:THR:HG22	1:A:420:SER:N	2.35	0.42
1:A:449:TYR:CG	1:A:449:TYR:O	2.73	0.42
1:B:522:SER:C	1:B:526:MET:HE3	2.39	0.42
1:B:676:THR:HB	1:B:700:ARG:CG	2.50	0.42
1:A:509:VAL:CG1	1:A:519:ASN:ND2	2.81	0.41
1:A:674:GLY:O	1:A:675:LEU:HD23	2.20	0.41
1:A:713:VAL:HG22	1:A:722:ARG:CB	2.50	0.41
1:B:430:PRO:HA	1:B:512:ILE:CD1	2.50	0.41
1:A:152:ASP:O	1:A:153:GLU:C	2.58	0.41
1:A:369:ASN:HB2	1:A:385:VAL:C	2.40	0.41
1:A:650:TYR:HD1	1:A:696:THR:CG2	2.34	0.41
1:B:113:ARG:HA	1:B:113:ARG:HD2	1.90	0.41
1:B:361:LEU:HD11	1:B:396:VAL:CG2	2.51	0.41
1:B:375:SER:C	1:B:377:SER:N	2.74	0.41
1:B:500:LEU:C	1:B:500:LEU:HD23	2.41	0.41
1:A:367:ILE:N	1:A:368:PRO:HD3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ARG:CG	1:A:568:GLN:HE22	2.33	0.41
1:B:408:LYS:CG	1:B:409:SER:N	2.81	0.41
1:A:134:ILE:HG21	1:A:536:THR:HG23	2.03	0.41
1:A:536:THR:O	1:A:540:THR:HG23	2.20	0.41
1:B:293:HIS:O	1:B:296:GLU:HB3	2.20	0.41
1:B:386:ASN:O	1:B:388:ASN:N	2.53	0.41
1:B:455:GLY:O	1:B:456:ALA:HB2	2.21	0.41
1:A:381:THR:CG2	1:A:382:ASP:N	2.83	0.41
1:B:207:HIS:ND1	1:B:501:ALA:HB3	2.35	0.41
1:A:364:GLY:HA3	1:A:377:SER:O	2.21	0.41
1:A:630:TRP:HB3	1:A:651:PHE:CE2	2.55	0.41
1:B:125:PRO:O	1:B:126:ARG:HG3	2.20	0.41
1:B:318:LEU:HD22	1:B:481:ASN:CG	2.41	0.41
1:A:143:ILE:O	1:A:145:PRO:HD3	2.21	0.41
1:A:488:ILE:CD1	1:A:570:GLU:CB	2.96	0.41
1:B:324:SER:OG	1:B:489:LYS:HE3	2.21	0.41
1:B:516:THR:OG1	1:B:517:LEU:N	2.54	0.41
1:B:531:ILE:HD11	1:B:578:VAL:HG21	2.02	0.41
1:A:475:PHE:CD1	1:A:475:PHE:C	2.95	0.41
1:A:650:TYR:HE1	1:A:652:ASN:HD21	1.69	0.41
1:B:354:PHE:HD1	1:B:432:PRO:CD	2.34	0.41
1:B:520:ILE:O	1:B:520:ILE:HG13	2.18	0.41
1:B:596:ASP:HB3	5:B:909:HOH:O	2.20	0.41
1:B:687:ASN:HB2	1:B:691:ASP:OD2	2.21	0.41
1:A:304:SER:HB2	1:A:524:THR:CB	2.51	0.40
1:A:590:TYR:CZ	1:A:655:LEU:HD21	2.57	0.40
1:B:379:PHE:HD1	1:B:379:PHE:H	1.69	0.40
1:B:448:ILE:HG22	1:B:448:ILE:O	2.21	0.40
1:B:499:ILE:O	1:B:520:ILE:HA	2.21	0.40
1:A:156:SER:O	1:A:176:ARG:HD3	2.20	0.40
1:A:188:ARG:HB3	1:A:189:PRO:HD2	2.02	0.40
1:A:272:LEU:HD23	1:A:274:VAL:HG13	2.02	0.40
1:B:124:VAL:HG13	1:B:581:LEU:HD21	2.03	0.40
1:B:165:THR:OG1	1:B:166:CYS:N	2.53	0.40
1:B:187:GLY:O	1:B:188:ARG:HB3	2.21	0.40
1:B:419:THR:CG2	1:B:420:SER:N	2.84	0.40
1:A:643:PRO:HG3	1:A:729:SER:HB2	2.02	0.40
1:B:272:LEU:CG	1:B:274:VAL:HG12	2.51	0.40
1:B:300:LEU:HG	1:B:301:THR:N	2.37	0.40
1:B:354:PHE:CD1	1:B:432:PRO:CD	3.05	0.40
1:B:369:ASN:HD22	1:B:386:ASN:N	2.12	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:CYS:N	1:A:529:PRO:CD	2.85	0.40
1:B:419:THR:HG22	1:B:420:SER:N	2.35	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	587/621 (94%)	527 (90%)	50 (8%)	10 (2%)	7 13
1	B	590/621 (95%)	497 (84%)	68 (12%)	25 (4%)	2 2
All	All	1177/1242 (95%)	1024 (87%)	118 (10%)	35 (3%)	3 5

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	633	ASN
1	B	375	SER
1	B	388	ASN
1	B	391	LYS
1	B	408	LYS
1	B	450	SER
1	A	187	GLY
1	A	454	PRO
1	B	171	ASN
1	B	267	VAL
1	B	355	ASP
1	B	369	ASN
1	B	451	ILE
1	B	452	ARG
1	B	453	SER
1	B	629	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	312	PHE
1	A	646	THR
1	A	702	SER
1	B	153	GLU
1	B	350	SER
1	B	456	ALA
1	A	350	SER
1	B	384	SER
1	B	145	PRO
1	B	199	ARG
1	B	376	THR
1	B	387	PRO
1	B	635	PRO
1	A	186	ILE
1	A	672	PRO
1	B	432	PRO
1	B	580	PRO
1	A	674	GLY
1	B	244	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/512 (96%)	467 (96%)	22 (4%)	23	42
1	B	492/512 (96%)	471 (96%)	21 (4%)	25	44
All	All	981/1024 (96%)	938 (96%)	43 (4%)	24	43

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	A	122	LEU
1	A	152	ASP
1	A	188	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	ASN
1	A	216	LEU
1	A	251	SER
1	A	259	TYR
1	A	272	LEU
1	A	274	VAL
1	A	297	ARG
1	A	379	PHE
1	A	437	ASP
1	A	472	VAL
1	A	519	ASN
1	A	578	VAL
1	A	579	ASN
1	A	594	GLU
1	A	630	TRP
1	A	639	LEU
1	A	723	SER
1	A	728	THR
1	B	208	THR
1	B	225	LEU
1	B	227	LEU
1	B	231	ARG
1	B	259	TYR
1	B	304	SER
1	B	310	PRO
1	B	331	ASP
1	B	332	ARG
1	B	460	LYS
1	B	472	VAL
1	B	481	ASN
1	B	482	ARG
1	B	488	ILE
1	B	520	ILE
1	B	521	ILE
1	B	525	SER
1	B	557	THR
1	B	564	ARG
1	B	579	ASN
1	B	692	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	221	ASN
1	A	278	ASN
1	A	303	ASN
1	A	339	GLN
1	A	342	ASN
1	A	352	ASN
1	A	386	ASN
1	A	519	ASN
1	A	566	ASN
1	A	568	GLN
1	A	652	ASN
1	A	719	HIS
1	B	311	ASN
1	B	369	ASN
1	B	386	ASN
1	B	388	ASN
1	B	481	ASN
1	B	519	ASN
1	B	577	HIS
1	B	579	ASN
1	B	680	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)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	1	2,1	14,14,15	0.50	0	17,19,21	0.66	0
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	0.91	1 (5%)
2	BMA	C	3	2	11,11,12	0.43	0	15,15,17	0.44	0
2	MAN	C	4	2	11,11,12	0.46	0	15,15,17	0.86	1 (6%)
2	FUC	C	5	2	10,10,11	0.55	0	14,14,16	0.33	0
2	NAG	D	1	2,1	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
2	NAG	D	2	2	14,14,15	0.60	0	17,19,21	0.71	0
2	BMA	D	3	2	11,11,12	0.60	0	15,15,17	0.61	0
2	MAN	D	4	2	11,11,12	0.56	0	15,15,17	0.84	1 (6%)
2	FUC	D	5	2	10,10,11	0.52	0	14,14,16	0.33	0
3	NAG	E	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	1.04	0
3	FUC	E	2	3	10,10,11	0.85	0	14,14,16	0.95	1 (7%)
3	NAG	E	3	3	14,14,15	1.01	1 (7%)	17,19,21	0.69	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	FUC	C	5	2	-	-	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	FUC	D	5	2	-	-	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	NAG	C1-C2	2.06	1.55	1.52
3	E	1	NAG	C1-C2	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	FUC	C1-C2-C3	2.82	113.75	109.64
2	D	4	MAN	C1-O5-C5	2.76	115.88	112.19
2	D	1	NAG	C2-N2-C7	-2.59	119.44	122.90
2	C	4	MAN	C1-O5-C5	2.50	115.54	112.19
2	C	2	NAG	C2-N2-C7	-2.47	119.59	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

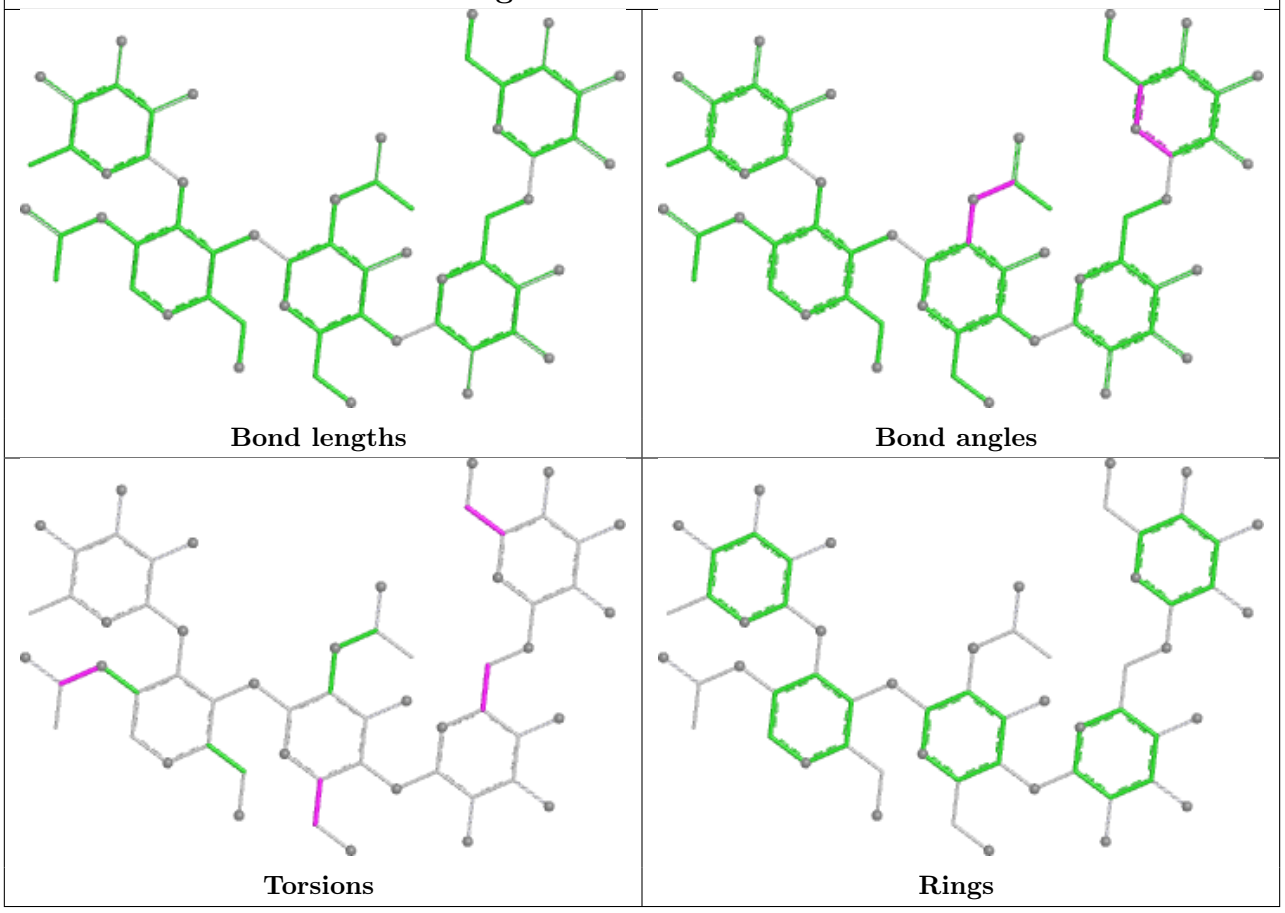
There are no ring outliers.

7 monomers are involved in 9 short contacts:

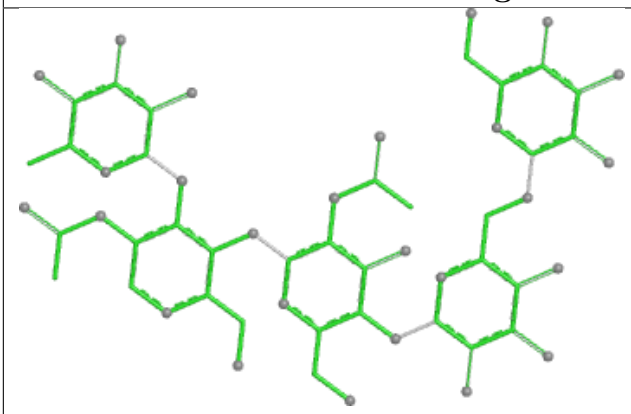
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
3	E	1	NAG	3	0
3	E	2	FUC	1	0
2	C	5	FUC	1	0
2	C	4	MAN	1	0
2	C	3	BMA	1	0
2	C	2	NAG	1	0

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

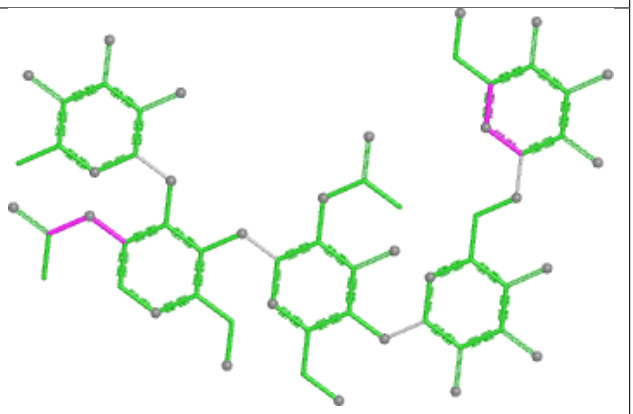
Oligosaccharide Chain C



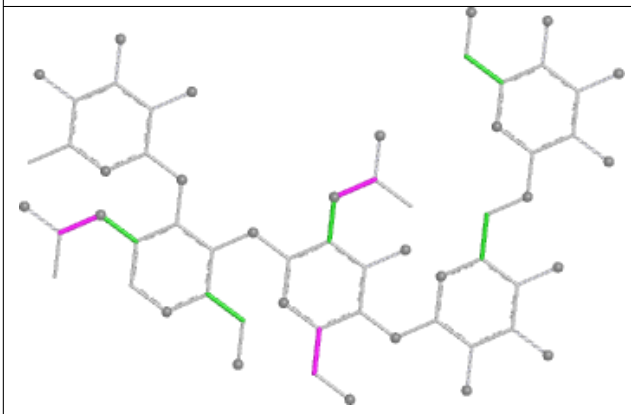
Oligosaccharide Chain D



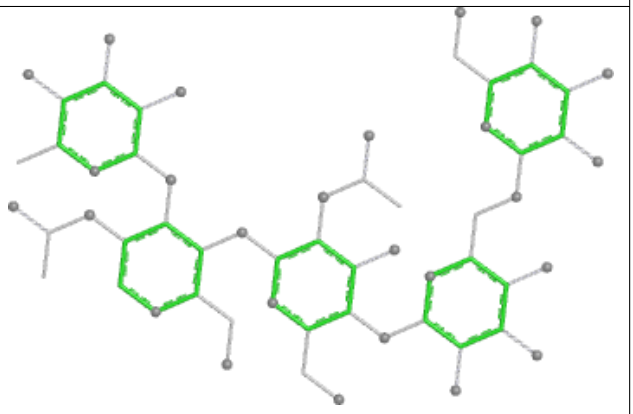
Bond lengths



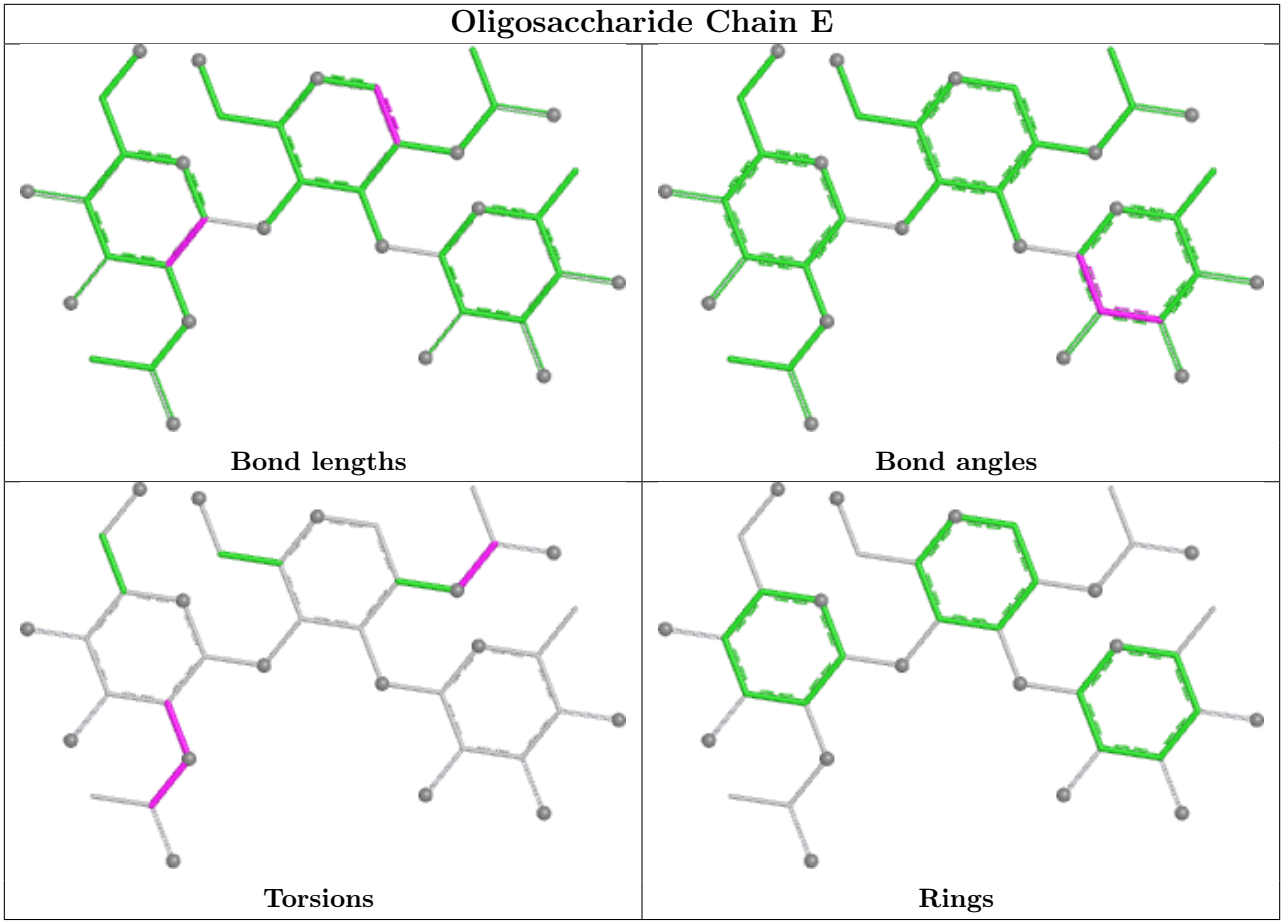
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
4	DFP	A	801	1	6,9,9	1.02	0	6,11,11	0.50	0
4	DFP	B	801	1	6,9,9	0.85	0	6,11,11	0.43	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
4	DFP	A	801	1	-	0/4/8/8	-
4	DFP	B	801	1	-	0/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	591/621 (95%)	0.07	18 (3%) 52 54	13, 38, 78, 97	0
1	B	594/621 (95%)	0.52	72 (12%) 10 12	22, 45, 116, 140	0
All	All	1185/1242 (95%)	0.30	90 (7%) 21 24	13, 41, 98, 140	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	PHE	6.0
1	B	363	SER	5.1
1	B	451	ILE	5.1
1	B	414	ALA	5.0
1	B	370	THR	4.4
1	B	372	PHE	4.4
1	B	166	CYS	4.2
1	B	389	LEU	4.0
1	B	396	VAL	3.9
1	B	445	LEU	3.9
1	B	406	PHE	3.8
1	A	451	ILE	3.6
1	B	366	ASP	3.6
1	A	598	VAL	3.6
1	B	413	ALA	3.5
1	A	629	VAL	3.5
1	B	394	ILE	3.5
1	B	601	LEU	3.5
1	B	144	TRP	3.4
1	B	173	ARG	3.3
1	B	174	CYS	3.3
1	B	415	GLY	3.3
1	B	392	GLY	3.2
1	B	275	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	453	SER	3.2
1	B	383	LYS	3.1
1	B	170	ASN	3.1
1	B	362	VAL	3.1
1	B	397	CYS	3.0
1	B	458	ILE	2.8
1	B	364	GLY	2.8
1	B	456	ALA	2.7
1	B	407	PHE	2.7
1	A	630	TRP	2.7
1	B	429	TYR	2.7
1	B	393	LYS	2.7
1	A	730	LEU	2.7
1	A	380	CYS	2.7
1	A	277	ALA	2.6
1	B	454	PRO	2.6
1	B	385	VAL	2.6
1	B	452	ARG	2.6
1	A	363	SER	2.5
1	B	192	PRO	2.5
1	B	374	LYS	2.5
1	B	359	TYR	2.5
1	B	459	PHE	2.5
1	A	275	GLY	2.5
1	B	399	ALA	2.4
1	B	143	ILE	2.4
1	B	352	ASN	2.4
1	B	168	THR	2.4
1	B	390	LEU	2.3
1	B	171	ASN	2.3
1	B	598	VAL	2.3
1	B	400	SER	2.3
1	A	390	LEU	2.3
1	B	391	LYS	2.3
1	B	351	ILE	2.3
1	B	343	GLY	2.3
1	B	282	TYR	2.3
1	B	416	VAL	2.3
1	B	379	PHE	2.3
1	B	367	ILE	2.3
1	B	277	ALA	2.3
1	B	375	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	354	PHE	2.2
1	B	448	ILE	2.2
1	B	442	LEU	2.2
1	A	452	ARG	2.2
1	B	365	ARG	2.2
1	B	430	PRO	2.2
1	B	342	ASN	2.2
1	B	340	ILE	2.2
1	B	361	LEU	2.2
1	A	365	ARG	2.2
1	B	371	GLY	2.2
1	B	219	GLN	2.1
1	A	592	ALA	2.1
1	A	373	ASP	2.1
1	B	395	VAL	2.1
1	A	482	ARG	2.1
1	B	387	PRO	2.1
1	A	391	LYS	2.1
1	B	449	TYR	2.0
1	A	717	GLY	2.0
1	B	484	THR	2.0
1	B	338	VAL	2.0
1	B	453	SER	2.0
1	B	513	ARG	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	3	14/15	0.48	0.18	81,84,85,86	0
3	FUC	E	2	10/11	0.52	0.16	78,80,81,81	0
3	NAG	E	1	14/15	0.63	0.18	70,75,80,80	0
2	MAN	D	4	11/12	0.66	0.19	80,83,84,85	0

Continued on next page...

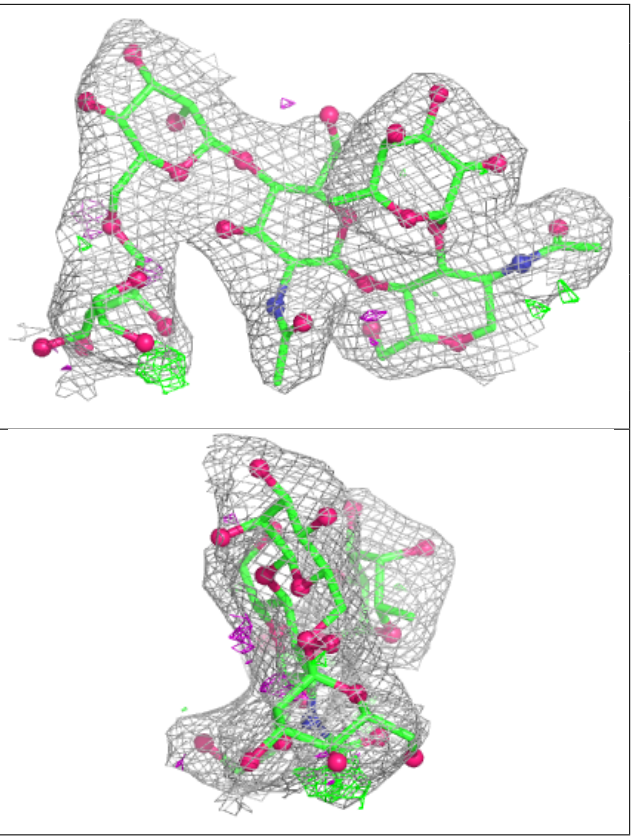
Continued from previous page...

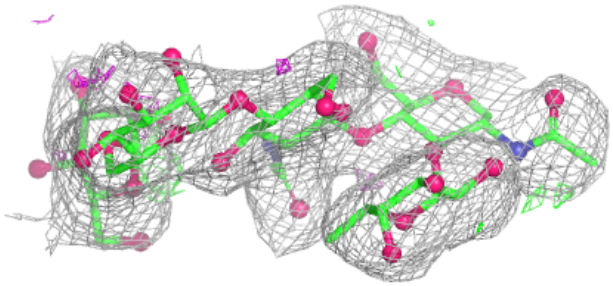
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	4	11/12	0.74	0.17	77,79,82,83	0
2	BMA	C	3	11/12	0.83	0.11	60,65,68,72	0
2	BMA	D	3	11/12	0.85	0.10	65,68,73,77	0
2	FUC	D	5	10/11	0.90	0.10	57,59,61,62	0
2	NAG	C	2	14/15	0.92	0.09	40,49,53,55	0
2	FUC	C	5	10/11	0.92	0.09	42,47,48,49	0
2	NAG	D	2	14/15	0.92	0.10	54,57,62,62	0
2	NAG	C	1	14/15	0.93	0.09	34,39,43,44	0
2	NAG	D	1	14/15	0.94	0.10	47,51,56,57	0

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

Electron density around Chain C:

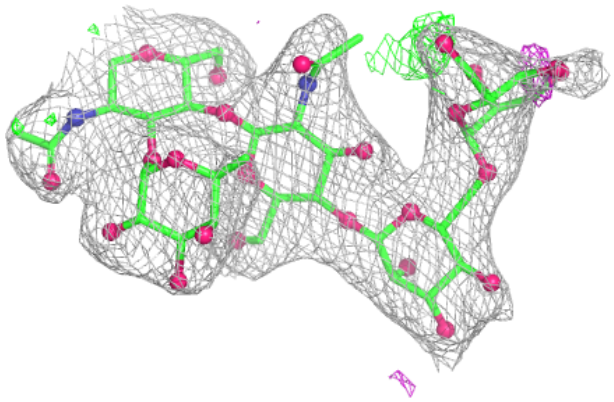
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

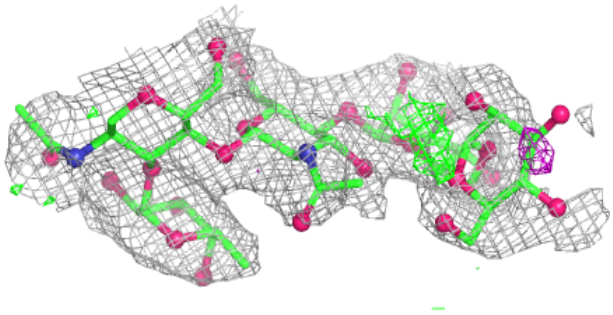


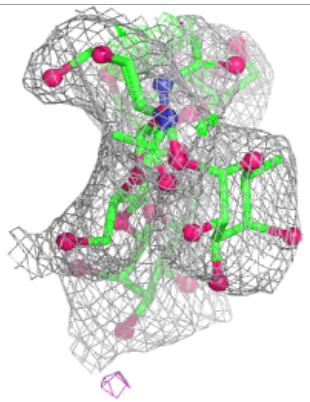


Electron density around Chain D:

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

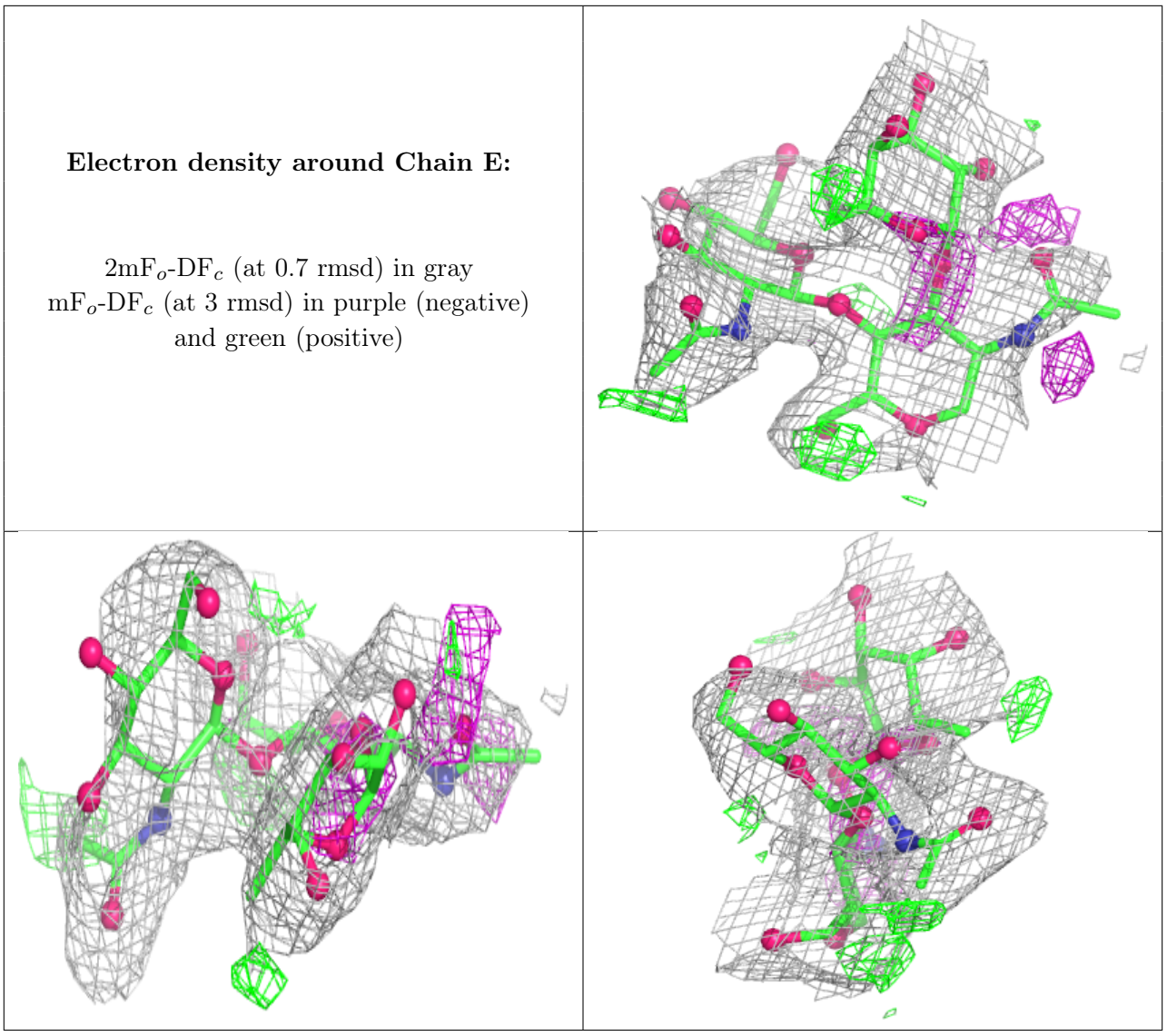






Electron density around Chain E:

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



6.4 Ligands

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DFP	B	801	10/10	0.89	0.20	53,57,63,64	0
4	DFP	A	801	10/10	0.94	0.16	34,38,44,46	0

6.5 Other polymers

There are no such residues in this entry.