Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 03:16 PM EDT

PDB ID	:	2I07
Title	:	Human Complement Component C3b
Authors	:	Janssen, B.J.C.; Christodoulidou, A.; McCarthy, A.; Lambris, J.D.; Gros, P.
Deposited on	:	2006-08-10
Resolution	:	4.00 Å(reported)

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

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

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

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

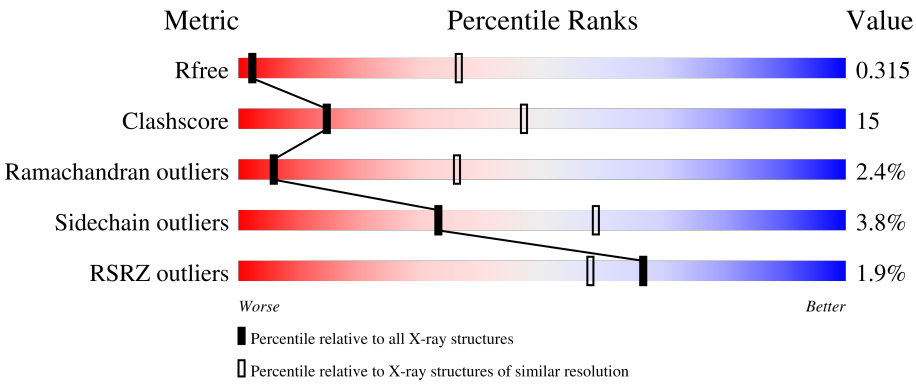
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	645	61% 33% • •
2	B	915	3% 74% 21% • •
3	C	3	33% 33% 33%

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
3	NAG	C	1	X	-	-	-
3	MAN	C	3	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12157 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 Complement C3b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	630	4907	3127	828	937	15	0	0	0

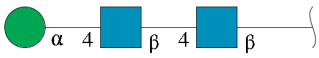
- Molecule 2 is a protein called Complement C3b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	901	7197	4563	1210	1386	38	0	0	0

There is a discrepancy between the modelled and reference sequences:

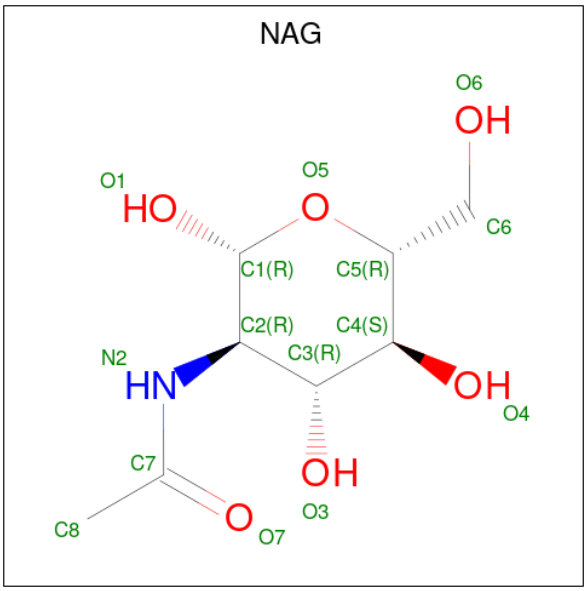
Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	SEE REMARK 999	UNP P01024

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



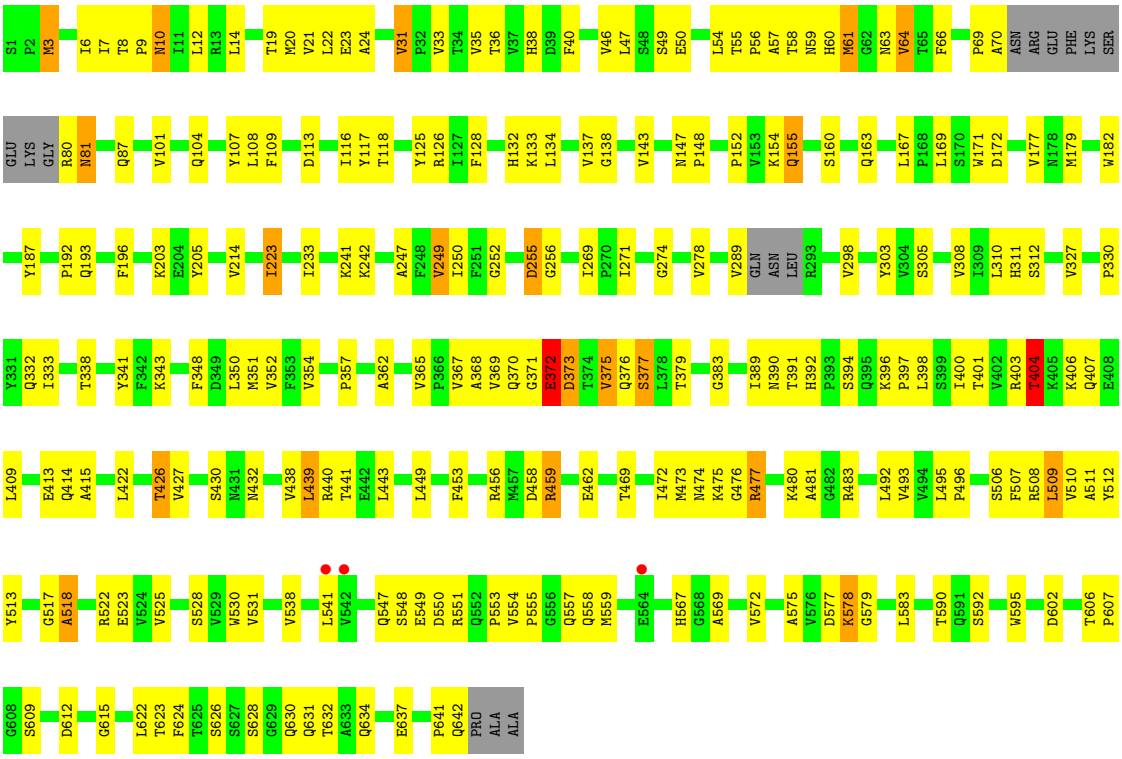
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

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.

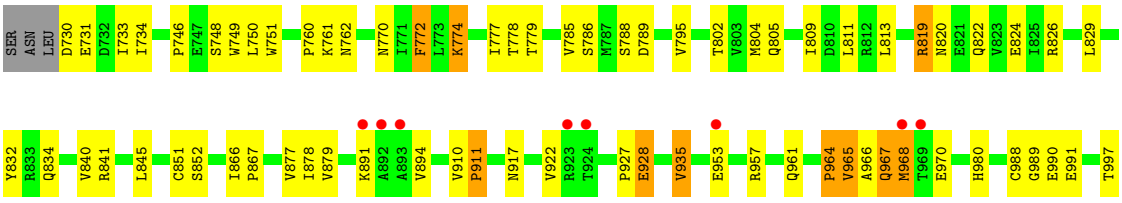
• Molecule 1: Complement C3b

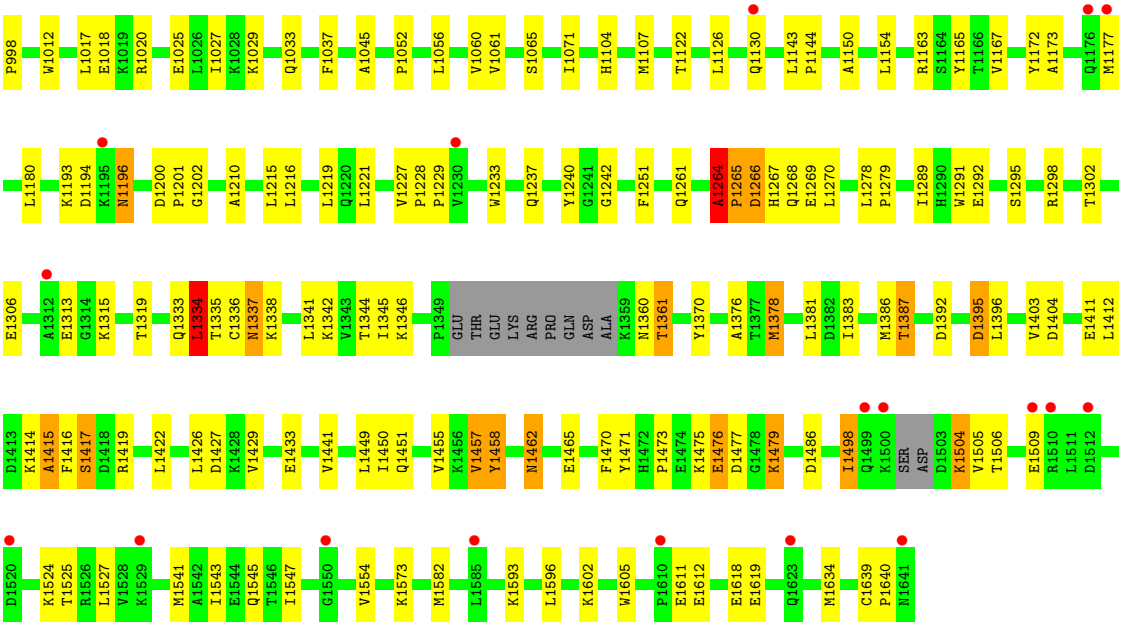
Chain A:



• Molecule 2: Complement C3b

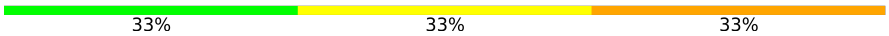
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	123.91Å 128.54Å 147.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 4.00 45.07 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.00-4.00) 99.8 (45.07-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.273 , 0.323 0.283 , 0.315	Depositor DCC
R_{free} test set	1044 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	133.2	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 114.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.054 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	12157	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/5004	0.44	0/6799
2	B	0.24	0/7340	0.43	2/9936 (0.0%)
All	All	0.25	0/12344	0.43	2/16735 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1264	ALA	C-N-CD	-6.46	106.40	120.60
2	B	1264	ALA	C-N-CA	5.43	144.79	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1264	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4907	0	4970	219	0
2	B	7197	0	7124	168	0
3	C	39	0	34	1	0
4	B	14	0	13	0	0
All	All	12157	0	12141	375	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 15.

All (375) 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:A:477:ARG:HG2	1:A:477:ARG:HH11	1.06	1.17
2:B:1264:ALA:HB1	2:B:1265:PRO:O	1.46	1.16
1:A:403:ARG:HB3	1:A:404:THR:HG22	1.24	1.11
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.17	1.09
1:A:69:PRO:HA	1:A:70:ALA:CB	1.77	1.09
1:A:372:GLU:HA	1:A:373:ASP:CB	1.79	1.08
1:A:6:ILE:HD11	1:A:20:MET:HG3	1.34	1.07
1:A:372:GLU:HA	1:A:373:ASP:HB3	1.06	1.05
2:B:819:ARG:HH11	2:B:819:ARG:HG2	1.16	1.04
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.41	1.01
1:A:69:PRO:CA	1:A:70:ALA:HB3	1.90	1.00
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	1.45	0.98
1:A:6:ILE:HD11	1:A:20:MET:CG	1.98	0.93
1:A:372:GLU:CA	1:A:373:ASP:HB3	1.97	0.92
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.84	0.91
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.51	0.91
2:B:819:ARG:HH11	2:B:819:ARG:CG	1.85	0.90
1:A:404:THR:CG2	1:A:414:GLN:HB3	2.02	0.89
2:B:966:ALA:HB1	2:B:1267:HIS:HA	1.55	0.87
1:A:35:VAL:HG21	1:A:64:VAL:HG21	1.56	0.85
1:A:362:ALA:O	1:A:379:THR:HG21	1.75	0.85
2:B:1387:THR:CG2	2:B:1451:GLN:H	1.89	0.84
2:B:927:PRO:O	2:B:928:GLU:HB2	1.78	0.83
1:A:369:VAL:HG12	1:A:370:GLN:H	1.43	0.83
1:A:7:ILE:HA	1:A:623:THR:O	1.78	0.83
1:A:641:PRO:O	1:A:642:GLN:HB2	1.77	0.82
1:A:372:GLU:CA	1:A:373:ASP:CB	2.56	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:HG2	1:A:477:ARG:NH1	1.86	0.81
1:A:404:THR:HG21	1:A:415:ALA:O	1.82	0.80
1:A:55:THR:HG22	1:A:57:ALA:H	1.46	0.79
2:B:966:ALA:O	2:B:967:GLN:HB2	1.83	0.79
1:A:439:LEU:H	1:A:439:LEU:HD12	1.48	0.77
2:B:804:MET:HG2	2:B:805:GLN:H	1.48	0.77
1:A:369:VAL:HG12	1:A:370:GLN:N	2.00	0.76
1:A:403:ARG:HA	1:A:404:THR:HB	1.66	0.76
1:A:403:ARG:CB	1:A:404:THR:HG22	2.12	0.76
2:B:819:ARG:HG2	2:B:819:ARG:NH1	1.91	0.75
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.68	0.75
1:A:549:GLU:HG2	1:A:550:ASP:H	1.52	0.74
2:B:1582:MET:HA	2:B:1605:TRP:O	1.87	0.74
2:B:1334:LEU:HG	2:B:1335:THR:O	1.88	0.74
1:A:510:VAL:HG12	1:A:528:SER:CB	2.17	0.74
2:B:1333:GLN:HB3	2:B:1335:THR:HG22	1.69	0.73
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.70	0.73
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.52	0.73
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.71	0.73
1:A:370:GLN:HG2	1:A:401:THR:HB	1.72	0.71
2:B:1524:LYS:HB3	2:B:1545:GLN:HG2	1.71	0.71
2:B:1465:GLU:O	2:B:1465:GLU:HG3	1.91	0.71
1:A:3:MET:HE2	1:A:628:SER:HB2	1.72	0.70
2:B:910:VAL:HG13	2:B:911:PRO:HD2	1.73	0.70
1:A:549:GLU:HG2	1:A:550:ASP:N	2.06	0.70
2:B:1334:LEU:N	2:B:1335:THR:HA	2.06	0.70
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.74	0.70
1:A:249:VAL:HG11	1:A:278:VAL:HG11	1.74	0.69
1:A:367:VAL:HA	1:A:404:THR:H	1.58	0.68
1:A:404:THR:CG2	1:A:404:THR:O	2.41	0.68
1:A:40:PHE:CE2	2:B:1017:LEU:HD11	2.28	0.68
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.75	0.68
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	1.76	0.67
1:A:8:THR:HB	1:A:9:PRO:CD	2.24	0.67
2:B:1414:LYS:O	2:B:1415:ALA:HB3	1.95	0.67
1:A:474:ASN:C	1:A:476:GLY:H	1.99	0.66
2:B:1386:MET:HG3	2:B:1471:TYR:CE1	2.30	0.66
1:A:368:ALA:N	1:A:403:ARG:O	2.20	0.66
2:B:1334:LEU:H	2:B:1335:THR:HA	1.59	0.66
2:B:1338:LYS:HD3	2:B:1465:GLU:HB2	1.77	0.66
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1411:GLU:CG	2:B:1422:LEU:HD12	2.24	0.65
2:B:1337:ASN:HB2	2:B:1338:LYS:HD2	1.78	0.65
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.62	0.64
2:B:1267:HIS:CE1	2:B:1291:TRP:CZ2	2.86	0.64
1:A:247:ALA:CB	1:A:271:ILE:HD11	2.28	0.64
1:A:247:ALA:HB3	1:A:271:ILE:HD11	1.79	0.64
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.79	0.64
2:B:1267:HIS:HB3	2:B:1268:GLN:O	1.97	0.64
1:A:426:THR:HG21	1:A:432:ASN:H	1.63	0.63
2:B:970:GLU:HB3	2:B:1261:GLN:HE22	1.63	0.63
1:A:143:VAL:O	1:A:155:GLN:HA	1.99	0.63
1:A:551:ARG:H	1:A:551:ARG:HD2	1.64	0.63
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.80	0.63
2:B:1336:CYS:O	2:B:1338:LYS:N	2.26	0.63
2:B:1611:GLU:HG3	2:B:1612:GLU:H	1.62	0.63
2:B:1414:LYS:O	2:B:1415:ALA:CB	2.47	0.62
1:A:474:ASN:O	1:A:476:GLY:N	2.33	0.62
1:A:439:LEU:HD12	1:A:439:LEU:N	2.14	0.61
2:B:1387:THR:HG21	2:B:1451:GLN:H	1.63	0.61
1:A:177:VAL:HG22	1:A:182:TRP:CZ2	2.35	0.61
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.36	0.61
2:B:935:VAL:HG11	2:B:1313:GLU:HG3	1.83	0.61
1:A:548:SER:O	1:A:549:GLU:HB2	1.99	0.61
1:A:179:MET:HG3	1:A:203:LYS:HA	1.82	0.60
1:A:22:LEU:HD13	1:A:33:VAL:HG11	1.81	0.60
1:A:369:VAL:CG1	1:A:370:GLN:H	2.15	0.60
1:A:641:PRO:O	1:A:642:GLN:CB	2.48	0.60
1:A:407:GLN:C	1:A:409:LEU:H	2.04	0.60
1:A:177:VAL:HG22	1:A:182:TRP:HZ2	1.66	0.60
2:B:1462:ASN:ND2	2:B:1465:GLU:H	2.00	0.59
2:B:733:ILE:HG12	2:B:734:ILE:N	2.15	0.59
1:A:624:PHE:H	1:A:632:THR:CG2	2.16	0.59
2:B:1419:ARG:HD3	2:B:1422:LEU:HD13	1.84	0.59
2:B:1462:ASN:HB3	2:B:1465:GLU:HG2	1.85	0.59
1:A:376:GLN:O	1:A:377:SER:HB3	2.03	0.59
2:B:1404:ASP:HA	2:B:1427:ASP:HB2	1.84	0.59
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.84	0.59
2:B:961:GLN:HB3	2:B:1319:THR:HB	1.85	0.58
1:A:439:LEU:H	1:A:439:LEU:CD1	2.15	0.58
2:B:1045:ALA:HB2	2:B:1052:PRO:HA	1.85	0.58
2:B:1386:MET:HB3	2:B:1450:ILE:HD13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1383:ILE:HG12	2:B:1455:VAL:HG22	1.86	0.58
2:B:1376:ALA:HB3	2:B:1429:VAL:HG22	1.87	0.57
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.87	0.57
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.86	0.57
2:B:778:THR:OG1	2:B:779:THR:N	2.37	0.57
1:A:507:PHE:CE1	1:A:531:VAL:HB	2.40	0.57
2:B:968:MET:HB2	2:B:1266:ASP:HA	1.87	0.57
2:B:1392:ASP:HB3	2:B:1395:ASP:HB2	1.87	0.57
2:B:927:PRO:O	2:B:928:GLU:CB	2.52	0.56
2:B:1267:HIS:HE1	2:B:1291:TRP:CZ2	2.22	0.56
1:A:223:ILE:HD12	1:A:223:ILE:H	1.71	0.56
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.88	0.56
2:B:819:ARG:O	2:B:820:ASN:HB2	2.06	0.56
2:B:1267:HIS:CE1	2:B:1291:TRP:CE2	2.94	0.56
2:B:1361:THR:HA	2:B:1441:VAL:O	2.05	0.56
1:A:612:ASP:OD1	1:A:615:GLY:N	2.39	0.55
1:A:250:ILE:HG22	1:A:305:SER:HB3	1.87	0.55
2:B:1386:MET:HG3	2:B:1471:TYR:HE1	1.71	0.55
2:B:804:MET:HG2	2:B:805:GLN:N	2.19	0.55
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.42	0.55
2:B:966:ALA:O	2:B:967:GLN:CB	2.55	0.55
1:A:332:GLN:HE21	1:A:357:PRO:HA	1.71	0.54
2:B:1386:MET:O	2:B:1387:THR:C	2.46	0.54
1:A:472:ILE:HD13	1:A:509:LEU:HD22	1.89	0.54
1:A:474:ASN:C	1:A:476:GLY:N	2.60	0.54
1:A:590:THR:HG22	1:A:592:SER:H	1.71	0.54
1:A:458:ASP:N	1:A:458:ASP:OD1	2.40	0.54
2:B:1412:LEU:O	2:B:1419:ARG:NH2	2.40	0.54
2:B:1457:VAL:O	2:B:1458:TYR:HB3	2.08	0.54
1:A:551:ARG:HD2	1:A:551:ARG:N	2.23	0.53
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.44	0.53
1:A:47:LEU:HD21	1:A:50:GLU:HG2	1.91	0.53
1:A:403:ARG:CA	1:A:404:THR:HB	2.39	0.53
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.90	0.53
1:A:547:GLN:HE22	1:A:559:MET:HB2	1.74	0.53
2:B:877:VAL:H	2:B:1451:GLN:NE2	2.07	0.53
1:A:624:PHE:H	1:A:632:THR:HG23	1.74	0.52
1:A:404:THR:HG23	1:A:404:THR:O	2.09	0.52
1:A:341:TYR:HA	1:A:422:LEU:O	2.09	0.52
1:A:362:ALA:O	1:A:379:THR:CG2	2.51	0.52
1:A:391:THR:HG22	1:A:392:HIS:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:966:ALA:HB2	2:B:1267:HIS:ND1	2.25	0.52
2:B:1498:ILE:HD12	2:B:1605:TRP:HE3	1.74	0.52
2:B:910:VAL:CG1	2:B:911:PRO:HD2	2.37	0.52
2:B:964:PRO:HB3	2:B:1291:TRP:HZ3	1.74	0.52
1:A:577:ASP:O	1:A:579:GLY:N	2.43	0.51
2:B:1278:LEU:HD22	2:B:1302:THR:HG21	1.93	0.51
1:A:214:VAL:O	1:A:214:VAL:HG23	2.10	0.51
1:A:376:GLN:O	1:A:377:SER:CB	2.58	0.51
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.93	0.51
1:A:9:PRO:HD2	1:A:12:LEU:HD21	1.93	0.51
1:A:69:PRO:HA	1:A:70:ALA:HB2	1.82	0.51
1:A:22:LEU:HD11	1:A:64:VAL:HG22	1.93	0.50
1:A:69:PRO:CB	1:A:70:ALA:HB3	2.40	0.50
2:B:819:ARG:CG	2:B:819:ARG:NH1	2.56	0.50
2:B:1193:LYS:O	2:B:1194:ASP:HB2	2.10	0.50
1:A:606:THR:HG23	1:A:607:PRO:HD2	1.93	0.50
1:A:23:GLU:OE2	1:A:512:TYR:OH	2.28	0.50
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.92	0.50
1:A:249:VAL:CG1	1:A:278:VAL:HG21	2.42	0.50
2:B:772:PHE:N	2:B:772:PHE:CD2	2.80	0.50
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.93	0.50
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.94	0.50
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.77	0.50
1:A:55:THR:HB	1:A:58:THR:HG23	1.93	0.50
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.12	0.50
1:A:163:GLN:HA	1:A:163:GLN:NE2	2.27	0.49
1:A:427:VAL:HG21	1:A:523:GLU:HG3	1.94	0.49
2:B:980:HIS:NE2	2:B:1240:TYR:O	2.44	0.49
2:B:1345:ILE:O	2:B:1345:ILE:HG23	2.11	0.49
1:A:558:GLN:NE2	2:B:770:ASN:OD1	2.45	0.49
1:A:333:ILE:HG23	1:A:352:VAL:HG13	1.93	0.49
1:A:370:GLN:CG	1:A:401:THR:HB	2.40	0.49
2:B:777:ILE:HG23	2:B:804:MET:HA	1.94	0.49
2:B:1527:LEU:HD13	2:B:1541:MET:SD	2.52	0.49
1:A:348:PHE:HD2	1:A:389:ILE:HD11	1.77	0.49
2:B:1215:LEU:O	2:B:1219:LEU:HG	2.13	0.49
1:A:187:TYR:CD1	1:A:192:PRO:HA	2.48	0.49
1:A:338:THR:OG1	1:A:351:MET:N	2.42	0.49
1:A:379:THR:CG2	1:A:383:GLY:HA2	2.43	0.49
1:A:567:HIS:HB2	2:B:760:PRO:HB3	1.95	0.49
2:B:789:ASP:OD1	2:B:789:ASP:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.77	0.49
1:A:403:ARG:HB3	1:A:404:THR:CG2	2.17	0.49
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.93	0.49
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.95	0.49
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.43	0.49
1:A:252:GLY:HA3	1:A:303:TYR:CZ	2.47	0.49
2:B:1291:TRP:O	2:B:1292:GLU:HB2	2.12	0.49
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.48	0.49
2:B:1387:THR:HG22	2:B:1451:GLN:N	2.22	0.49
2:B:1289:ILE:HG12	2:B:1298:ARG:HE	1.78	0.48
1:A:104:GLN:O	1:A:132:HIS:CE1	2.66	0.48
2:B:1061:VAL:O	2:B:1065:SER:OG	2.27	0.48
1:A:104:GLN:O	1:A:132:HIS:HE1	1.97	0.48
1:A:575:ALA:O	2:B:748:SER:HA	2.14	0.48
1:A:595:TRP:CE3	1:A:595:TRP:HA	2.48	0.48
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.14	0.48
2:B:1270:LEU:HD12	2:B:1291:TRP:HE3	1.79	0.48
1:A:8:THR:HB	1:A:9:PRO:HD2	1.95	0.48
1:A:80:ARG:O	1:A:81:ASN:HB2	2.12	0.48
2:B:964:PRO:HB3	2:B:1291:TRP:CZ3	2.49	0.48
2:B:1150:ALA:O	2:B:1154:LEU:HG	2.14	0.48
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.79	0.48
2:B:1381:LEU:CD2	2:B:1457:VAL:HG13	2.43	0.48
2:B:991:GLU:HG2	2:B:1104:HIS:NE2	2.29	0.48
1:A:3:MET:HE3	1:A:522:ARG:CG	2.43	0.47
1:A:255:ASP:HA	1:A:256:GLY:HA2	1.62	0.47
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.96	0.47
2:B:1334:LEU:H	2:B:1335:THR:HG22	1.79	0.47
2:B:746:PRO:CG	2:B:774:LYS:HG3	2.44	0.47
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.49	0.47
1:A:14:LEU:HD21	1:A:101:VAL:HG11	1.97	0.47
1:A:553:PRO:HD2	2:B:802:THR:O	2.14	0.47
1:A:628:SER:CB	1:A:630:GLN:OE1	2.63	0.47
1:A:404:THR:HG22	1:A:404:THR:O	2.14	0.47
2:B:1012:TRP:HB3	2:B:1017:LEU:CD1	2.44	0.47
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.97	0.46
1:A:109:PHE:HB2	1:A:128:PHE:HB2	1.98	0.46
2:B:761:LYS:O	2:B:762:ASN:HB2	2.16	0.46
2:B:1200:ASP:O	2:B:1202:GLY:N	2.48	0.46
2:B:1344:THR:HG21	2:B:1346:LYS:HE2	1.98	0.46
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.49	0.46
2:B:1475:LYS:O	2:B:1476:GLU:C	2.53	0.46
1:A:152:PRO:O	2:B:957:ARG:NH2	2.49	0.46
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.97	0.46
1:A:113:ASP:OD1	1:A:113:ASP:N	2.47	0.46
2:B:840:VAL:HG12	2:B:841:ARG:N	2.30	0.46
2:B:1025:GLU:O	2:B:1029:LYS:HB2	2.15	0.46
2:B:1416:PHE:O	2:B:1417:SER:C	2.54	0.46
1:A:310:LEU:C	1:A:312:SER:H	2.17	0.46
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.98	0.46
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.98	0.45
2:B:1504:LYS:HD3	2:B:1504:LYS:N	2.30	0.45
2:B:1333:GLN:HG3	2:B:1334:LEU:HD23	1.98	0.45
1:A:6:ILE:HD12	1:A:7:ILE:H	1.81	0.45
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.98	0.45
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.97	0.45
2:B:988:CYS:O	2:B:990:GLU:N	2.49	0.45
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.46	0.45
1:A:472:ILE:HG12	1:A:480:LYS:O	2.17	0.45
2:B:730:ASP:HB3	2:B:731:GLU:H	1.62	0.45
2:B:1465:GLU:O	2:B:1465:GLU:CG	2.64	0.45
1:A:310:LEU:O	1:A:312:SER:N	2.49	0.45
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.98	0.45
1:A:6:ILE:HD12	1:A:21:VAL:O	2.16	0.44
1:A:247:ALA:HB2	1:A:271:ILE:HD11	1.99	0.44
1:A:392:HIS:C	1:A:394:SER:H	2.21	0.44
1:A:481:ALA:H	3:C:1:NAG:H81	1.82	0.44
2:B:1334:LEU:H	2:B:1335:THR:CA	2.29	0.44
1:A:50:GLU:HG3	1:A:66:PHE:HB3	1.99	0.44
1:A:403:ARG:HA	1:A:404:THR:CB	2.43	0.44
1:A:177:VAL:CG2	1:A:182:TRP:CZ2	3.00	0.44
1:A:47:LEU:HD23	1:A:47:LEU:O	2.18	0.44
1:A:133:LYS:O	1:A:134:LEU:HB2	2.17	0.44
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.52	0.44
2:B:1126:LEU:HD21	2:B:1177:MET:CE	2.47	0.44
1:A:404:THR:CG2	1:A:415:ALA:O	2.61	0.44
1:A:469:THR:O	1:A:511:ALA:HA	2.17	0.44
2:B:1291:TRP:CD1	2:B:1292:GLU:HG3	2.52	0.44
2:B:819:ARG:O	2:B:820:ASN:CB	2.66	0.44
2:B:966:ALA:CB	2:B:1267:HIS:HA	2.38	0.44
2:B:1403:VAL:O	2:B:1404:ASP:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:O	1:A:375:VAL:N	2.41	0.44
1:A:624:PHE:O	1:A:631:GLN:HA	2.18	0.44
2:B:1378:MET:HA	2:B:1426:LEU:O	2.18	0.44
2:B:829:LEU:N	2:B:829:LEU:HD12	2.33	0.43
2:B:1196:ASN:HD22	2:B:1196:ASN:N	2.15	0.43
1:A:6:ILE:CD1	1:A:20:MET:HE3	2.49	0.43
2:B:1122:THR:O	2:B:1126:LEU:HB2	2.19	0.43
2:B:1126:LEU:O	2:B:1130:GLN:HG3	2.19	0.43
2:B:1462:ASN:HD22	2:B:1465:GLU:H	1.65	0.43
1:A:310:LEU:C	1:A:312:SER:N	2.72	0.43
1:A:365:VAL:H	1:A:379:THR:HB	1.83	0.43
1:A:379:THR:HG23	1:A:383:GLY:HA2	2.01	0.43
1:A:372:GLU:N	1:A:372:GLU:OE1	2.52	0.43
1:A:453:PHE:O	1:A:492:LEU:HA	2.17	0.43
1:A:606:THR:CG2	1:A:607:PRO:HD2	2.48	0.43
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.19	0.43
2:B:1506:THR:OG1	2:B:1509:GLU:HG2	2.18	0.43
1:A:443:LEU:HD11	1:A:449:LEU:HD13	2.01	0.43
2:B:1593:LYS:HG2	2:B:1596:LEU:HD11	2.00	0.43
1:A:36:THR:HG21	1:A:38:HIS:CE1	2.54	0.43
1:A:406:LYS:O	1:A:414:GLN:NE2	2.52	0.43
1:A:517:GLY:O	1:A:518:ALA:C	2.57	0.43
2:B:1618:GLU:O	2:B:1619:GLU:HG3	2.18	0.43
1:A:249:VAL:HA	1:A:305:SER:O	2.19	0.42
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.49	0.42
2:B:964:PRO:O	2:B:965:VAL:C	2.57	0.42
1:A:343:LYS:HD2	1:A:343:LYS:N	2.35	0.42
2:B:785:VAL:HG22	2:B:795:VAL:HG22	2.00	0.42
1:A:409:LEU:HG	1:A:413:GLU:HB2	2.02	0.42
1:A:577:ASP:C	1:A:579:GLY:N	2.72	0.42
2:B:1029:LYS:HG2	2:B:1033:GLN:OE1	2.20	0.42
1:A:407:GLN:C	1:A:409:LEU:N	2.72	0.42
2:B:1404:ASP:CA	2:B:1427:ASP:HB2	2.49	0.42
1:A:330:PRO:HG2	1:A:409:LEU:HD11	2.01	0.42
1:A:440:ARG:HA	1:A:440:ARG:HD2	1.82	0.42
2:B:811:LEU:HG	2:B:813:LEU:CD1	2.49	0.42
1:A:19:THR:CG2	1:A:63:ASN:OD1	2.68	0.42
1:A:137:VAL:HG22	1:A:138:GLY:N	2.34	0.42
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.89	0.42
2:B:749:TRP:O	2:B:750:LEU:HB3	2.20	0.42
2:B:1381:LEU:HD23	2:B:1457:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1396:LEU:HD23	2:B:1396:LEU:HA	1.94	0.42
1:A:6:ILE:HD12	1:A:7:ILE:N	2.35	0.42
2:B:822:GLN:OE1	2:B:1479:LYS:HA	2.19	0.42
2:B:1360:ASN:O	2:B:1361:THR:O	2.37	0.42
1:A:108:LEU:HB2	1:A:196:PHE:CG	2.54	0.41
1:A:477:ARG:CG	1:A:477:ARG:NH1	2.54	0.41
2:B:988:CYS:HA	2:B:1037:PHE:CZ	2.55	0.41
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.41
2:B:1547:ILE:HG22	2:B:1634:MET:HB3	2.02	0.41
1:A:19:THR:HG22	1:A:63:ASN:OD1	2.21	0.41
1:A:205:TYR:CD1	1:A:205:TYR:C	2.94	0.41
1:A:233:ILE:HG13	1:A:269:ILE:HD11	2.02	0.41
1:A:459:ARG:HA	1:A:462:GLU:HG2	2.02	0.41
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.85	0.41
1:A:247:ALA:HB3	1:A:269:ILE:HG13	2.01	0.41
2:B:1267:HIS:CB	2:B:1268:GLN:CA	2.99	0.41
2:B:1279:PRO:HG2	2:B:1306:GLU:OE1	2.20	0.41
1:A:113:ASP:OD1	1:A:117:TYR:OH	2.35	0.41
2:B:866:ILE:HA	2:B:867:PRO:HD3	1.85	0.41
1:A:7:ILE:HG22	1:A:622:LEU:HD22	2.03	0.41
1:A:403:ARG:CA	1:A:404:THR:CB	2.99	0.41
2:B:824:GLU:OE1	2:B:826:ARG:NH1	2.53	0.41
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.61	0.41
1:A:125:TYR:CZ	1:A:169:LEU:HB3	2.56	0.41
1:A:241:LYS:HG3	2:B:832:TYR:CZ	2.55	0.41
1:A:369:VAL:CG1	1:A:370:GLN:N	2.70	0.41
1:A:55:THR:HG23	1:A:56:PRO:HD2	2.02	0.41
1:A:59:ASN:O	1:A:60:HIS:HB2	2.21	0.41
1:A:333:ILE:HG12	1:A:354:VAL:HG22	2.02	0.41
2:B:1525:THR:HG22	2:B:1543:ILE:HA	2.03	0.41
1:A:3:MET:HE1	1:A:626:SER:CB	2.50	0.41
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.56	0.41
1:A:371:GLY:O	1:A:372:GLU:O	2.39	0.41
1:A:578:LYS:HE2	1:A:578:LYS:HB3	1.93	0.41
2:B:964:PRO:O	2:B:965:VAL:O	2.38	0.41
2:B:1012:TRP:CE2	2:B:1020:ARG:HD2	2.56	0.41
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.21	0.41
2:B:1341:LEU:HD21	2:B:1455:VAL:HG12	2.02	0.41
1:A:12:LEU:O	1:A:101:VAL:HA	2.21	0.41
1:A:160:SER:HA	1:A:167:LEU:HD21	2.03	0.41
1:A:249:VAL:HG11	1:A:278:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:TYR:CZ	1:A:525:VAL:HB	2.55	0.41
2:B:997:THR:HG23	2:B:1251:PHE:HB2	2.03	0.41
2:B:1470:PHE:HB2	2:B:1477:ASP:O	2.21	0.41
1:A:10:ASN:HD22	1:A:10:ASN:HA	1.57	0.40
1:A:163:GLN:CA	1:A:163:GLN:HE21	2.34	0.40
1:A:396:LYS:HG3	1:A:397:PRO:HD2	2.02	0.40
1:A:87:GLN:HE21	1:A:87:GLN:HB2	1.65	0.40
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.57	0.40
1:A:223:ILE:HG12	1:A:298:VAL:HG22	2.02	0.40
1:A:430:SER:OG	1:A:523:GLU:OE1	2.34	0.40
2:B:1639:CYS:HA	2:B:1640:PRO:HD3	1.92	0.40
1:A:242:LYS:HB3	1:A:274:GLY:HA3	2.03	0.40
1:A:554:VAL:O	1:A:557:GLN:HB2	2.22	0.40
2:B:774:LYS:HA	2:B:774:LYS:HD3	1.95	0.40
1:A:107:TYR:HA	1:A:196:PHE:CZ	2.57	0.40
1:A:528:SER:OG	1:A:609:SER:N	2.55	0.40
2:B:1104:HIS:O	2:B:1107:MET:HG2	2.21	0.40
1:A:249:VAL:HG13	1:A:278:VAL:HG21	2.03	0.40
2:B:845:LEU:HD21	2:B:891:LYS:HE3	2.04	0.40
2:B:997:THR:HB	2:B:998:PRO:CD	2.52	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	624/645 (97%)	567 (91%)	45 (7%)	12 (2%)	8 40
2	B	895/915 (98%)	805 (90%)	65 (7%)	25 (3%)	5 33
All	All	1519/1560 (97%)	1372 (90%)	110 (7%)	37 (2%)	6 36

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	372	GLU
1	A	377	SER
1	A	475	LYS
2	B	928	GLU
2	B	965	VAL
2	B	967	GLN
2	B	1265	PRO
2	B	1361	THR
2	B	1415	ALA
2	B	1476	GLU
2	B	1505	VAL
1	A	373	ASP
1	A	375	VAL
1	A	404	THR
1	A	518	ALA
2	B	935	VAL
2	B	989	GLY
2	B	1266	ASP
2	B	1417	SER
1	A	578	LYS
2	B	911	PRO
2	B	964	PRO
2	B	1334	LEU
2	B	1337	ASN
2	B	1387	THR
2	B	1458	TYR
1	A	311	HIS
2	B	1295	SER
1	A	81	ASN
1	A	255	ASP
2	B	774	LYS
2	B	1201	PRO
2	B	1486	ASP
2	B	1449	LEU
2	B	1498	ILE
2	B	1242	GLY

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	555/567 (98%)	526 (95%)	29 (5%)	23	51
2	B	797/810 (98%)	774 (97%)	23 (3%)	42	65
All	All	1352/1377 (98%)	1300 (96%)	52 (4%)	33	59

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	10	ASN
1	A	31	VAL
1	A	46	VAL
1	A	61	MET
1	A	64	VAL
1	A	155	GLN
1	A	172	ASP
1	A	193	GLN
1	A	223	ILE
1	A	249	VAL
1	A	289	VAL
1	A	327	VAL
1	A	372	GLU
1	A	390	ASN
1	A	398	LEU
1	A	404	THR
1	A	426	THR
1	A	439	LEU
1	A	441	THR
1	A	456	ARG
1	A	459	ARG
1	A	477	ARG
1	A	509	LEU
1	A	538	VAL
1	A	583	LEU
1	A	602	ASP
1	A	634	GLN
1	A	637	GLU
2	B	772	PHE
2	B	809	ILE
2	B	819	ARG
2	B	834	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	917	ASN
2	B	922	VAL
2	B	953	GLU
2	B	968	MET
2	B	1018	GLU
2	B	1196	ASN
2	B	1269	GLU
2	B	1315	LYS
2	B	1334	LEU
2	B	1342	LYS
2	B	1378	MET
2	B	1395	ASP
2	B	1433	GLU
2	B	1457	VAL
2	B	1462	ASN
2	B	1479	LYS
2	B	1504	LYS
2	B	1573	LYS
2	B	1602	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	132	HIS
1	A	144	ASN
1	A	155	GLN
1	A	161	GLN
1	A	163	GLN
1	A	332	GLN
1	A	334	HIS
1	A	390	ASN
1	A	490	GLN
1	A	558	GLN
1	A	587	ASN
1	A	634	GLN
2	B	738	ASN
2	B	752	ASN
2	B	762	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	860	HIS
2	B	961	GLN
2	B	967	GLN
2	B	1076	GLN
2	B	1114	ASN
2	B	1141	ASN
2	B	1160	ASN
2	B	1196	ASN
2	B	1204	GLN
2	B	1261	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1333	GLN
2	B	1401	ASN
2	B	1451	GLN
2	B	1462	ASN
2	B	1499	GLN
2	B	1620	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)

3 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.59	0	17,19,21	1.07	1 (5%)
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	0.64	0
3	MAN	C	3	3	11,11,12	0.58	0	15,15,17	1.26	2 (13%)

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
3	NAG	C	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	MAN	C1-C2-C3	3.13	113.52	109.67
3	C	1	NAG	C4-C3-C2	2.62	114.86	111.02
3	C	3	MAN	C1-O5-C5	2.12	115.07	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1	NAG	C1
3	C	3	MAN	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6

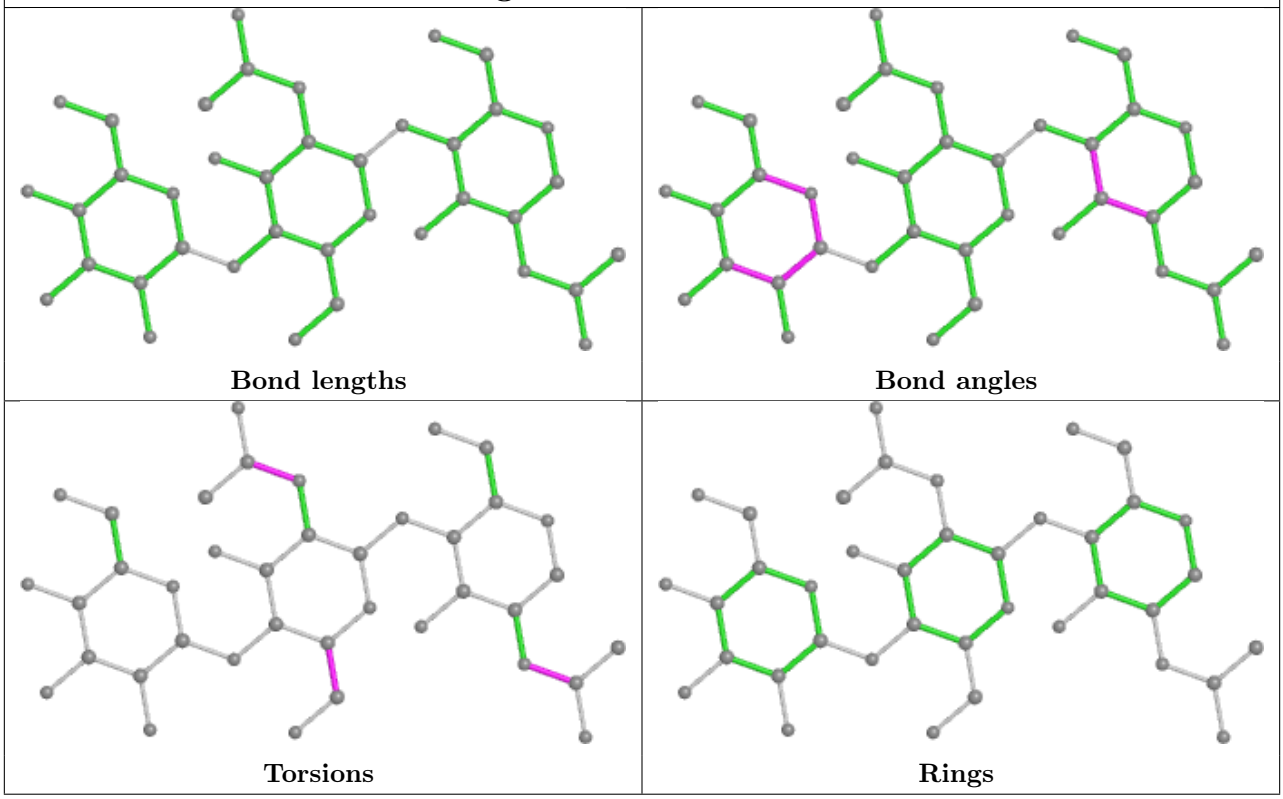
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	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



5.6 Ligand geometry (i)

1 ligand is 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	NAG	B	1	2	14,14,15	0.55	0	17,19,21	0.67	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	NAG	B	1	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2

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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	630/645 (97%)	-0.30	3 (0%)	91	85	85, 132, 184, 224	0
2	B	901/915 (98%)	0.02	26 (2%)	51	41	99, 201, 275, 319	0
All	All	1531/1560 (98%)	-0.11	29 (1%)	66	58	85, 164, 262, 319	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1500	LYS	6.0
2	B	1195	LYS	3.9
2	B	968	MET	3.8
2	B	953	GLU	3.4
2	B	1641	ASN	3.2
2	B	1312	ALA	3.1
2	B	1130	GLN	3.0
1	A	564	GLU	3.0
2	B	924	THR	2.9
2	B	1499	GLN	2.8
2	B	1177	MET	2.8
2	B	1509	GLU	2.6
2	B	923	ARG	2.4
2	B	1550	GLY	2.4
2	B	1230	VAL	2.4
2	B	1610	PRO	2.4
2	B	1520	ASP	2.4
2	B	1512	ASP	2.4
2	B	892	ALA	2.4
2	B	1176	GLN	2.3
2	B	893	ALA	2.3
2	B	1585	LEU	2.3
1	A	541	LEU	2.2
2	B	1529	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	891	LYS	2.1
1	A	542	VAL	2.0
2	B	969	THR	2.0
2	B	1510	ARG	2.0
2	B	1623	GLN	2.0

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

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

6.3 Carbohydrates (i)

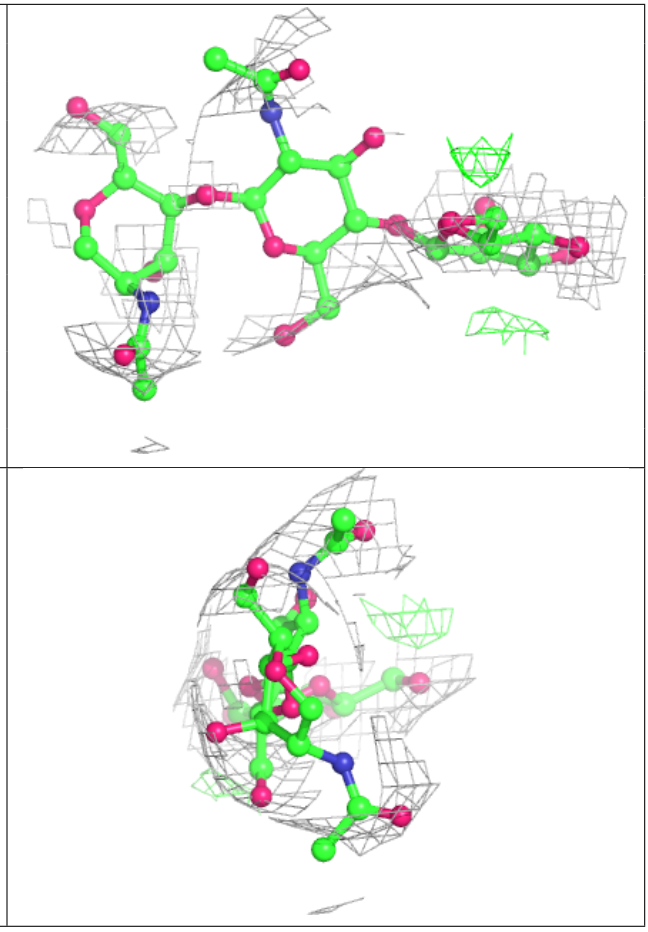
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	C	3	11/12	0.72	0.34	203,216,241,248	0
3	NAG	C	2	14/15	0.86	0.20	171,183,203,204	0
3	NAG	C	1	14/15	0.96	0.18	133,148,163,164	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)



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	1	14/15	0.83	0.39	203,215,226,226	0

6.5 Other polymers (i)

There are no such residues in this entry.