



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 2ICF / pdb_00002icf
Title : CRIG bound to C3b
Authors : Wiesmann, C.
Deposited on : 2006-09-12
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

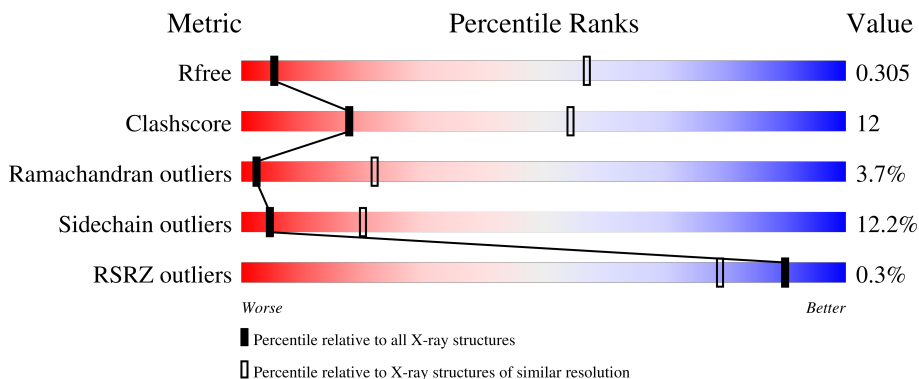
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	642	 61% 32% 7%
2	B	915	 67% 27% 5% ..
3	S	119	 72% 25% .
4	C	4	 25% 75%

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
4	NAG	C	1	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13236 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 C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	642	5008	3188	848	957	15	0	0	0

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	903	7213	4572	1213	1390	38	1161	0	0

- Molecule 3 is a protein called V-set and immunoglobulin domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S	119	950	595	169	183	3	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-beta-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			
4	C	4	50	28	2	20	0	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

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

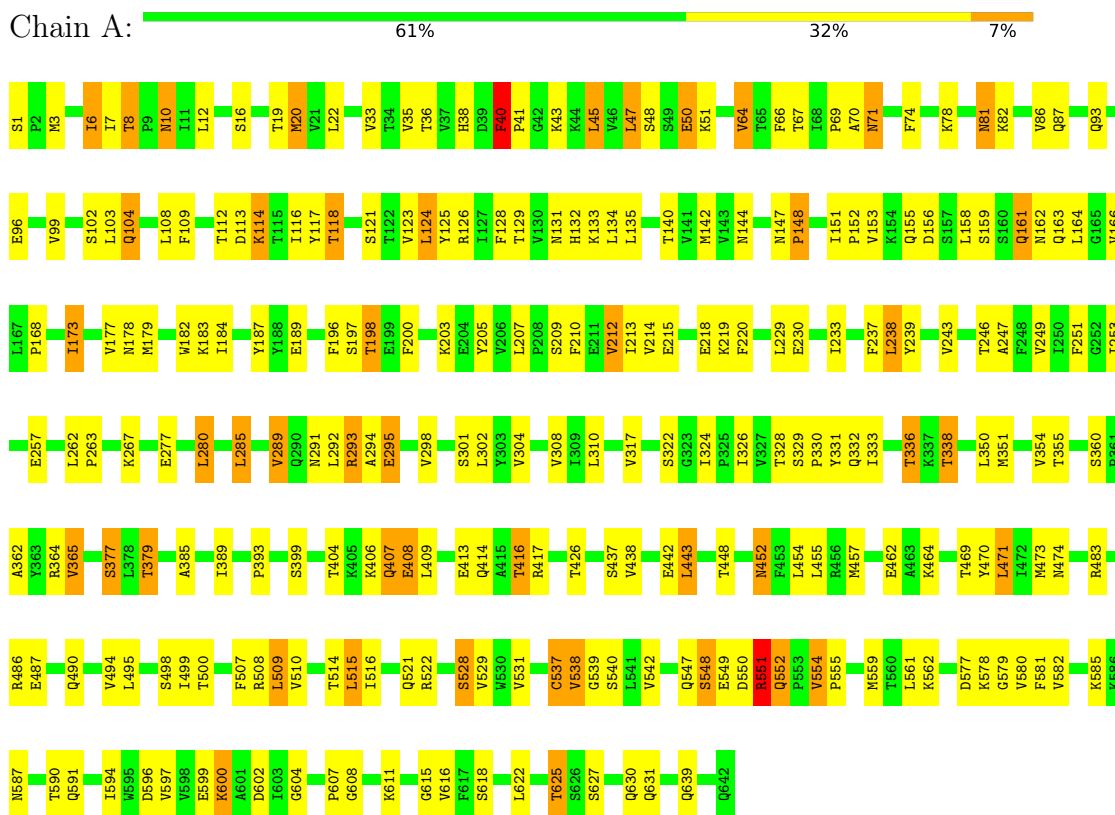


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0

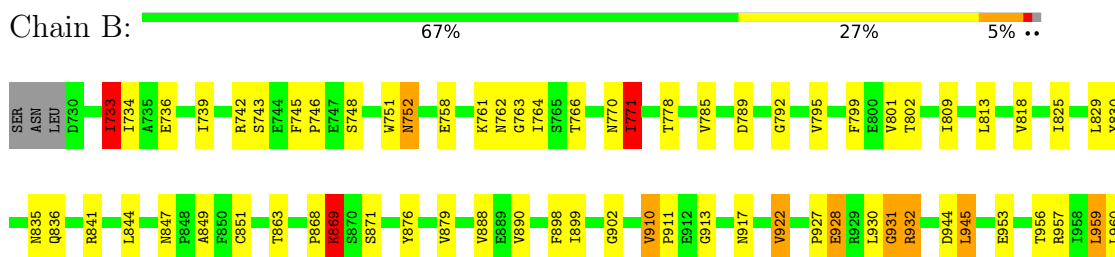
3 Residue-property plots i

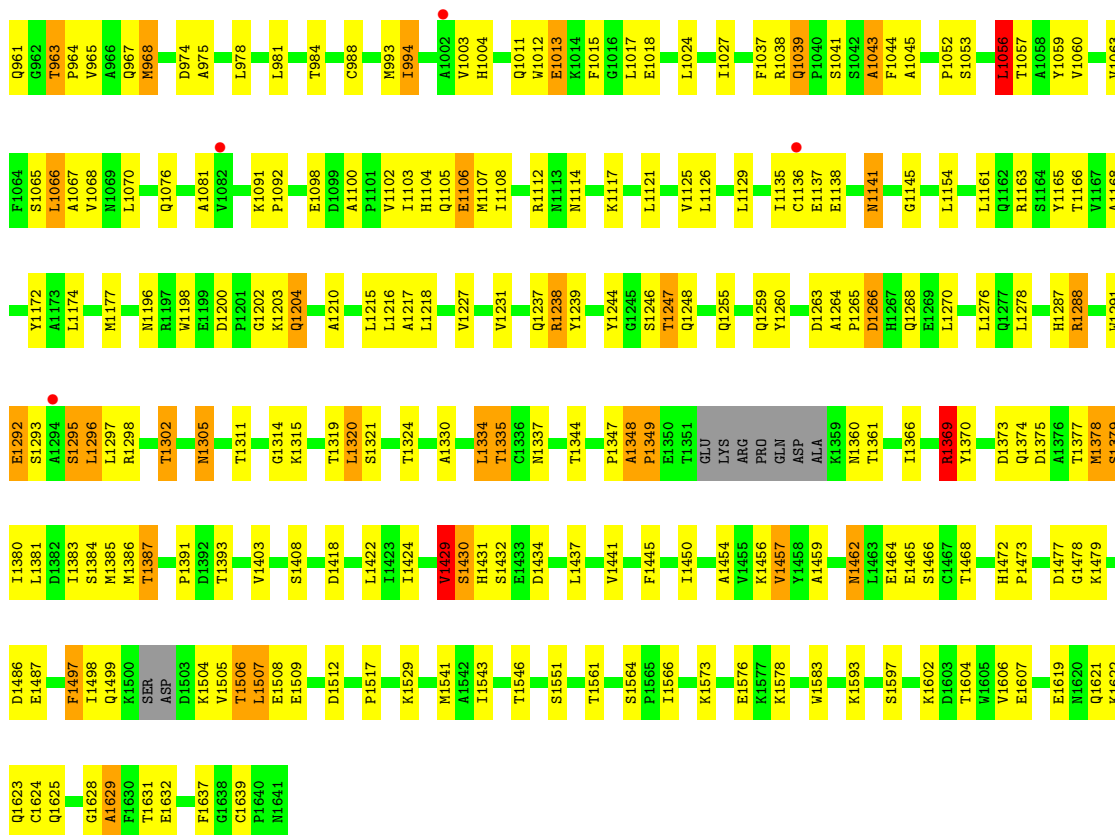
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 C3 beta chain



- Molecule 2: Complement C3 alpha chain





- Molecule 3: V-set and immunoglobulin domain-containing protein 4

Chain S: 72% 25%



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

Chain C: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.61Å 255.75Å 180.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 20.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-4.10) 95.0 (20.00-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 4.07Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.252 , 0.330 0.236 , 0.305	Depositor DCC
R_{free} test set	875 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	157.2	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 118.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13236	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, 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	0.74	0/5108	0.95	10/6939 (0.1%)
2	B	0.72	7/7356 (0.1%)	1.16	15/9958 (0.2%)
3	S	0.76	0/972	0.88	0/1323
All	All	0.73	7/13436 (0.1%)	1.06	25/18220 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	7
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1041	SER	CB-OG	8.09	1.58	1.42
2	B	1043	ALA	C-O	6.26	1.32	1.23
2	B	1607	GLU	CD-OE2	5.88	1.36	1.25
2	B	1056	LEU	C-N	5.65	1.40	1.33
2	B	1043	ALA	C-N	5.24	1.40	1.33
2	B	922	VAL	CA-CB	5.08	1.59	1.53
2	B	1039	GLN	CD-NE2	5.03	1.43	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1497	PHE	O-C-N	-72.79	43.45	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1499	GLN	N-CA-C	7.10	120.55	107.99
2	B	1629	ALA	N-CA-C	-6.96	104.78	113.55
2	B	931	GLY	N-CA-C	-6.72	103.78	113.86
1	A	336	THR	N-CA-C	-6.68	104.08	111.36
2	B	910	VAL	CA-C-N	6.44	127.89	119.84
2	B	910	VAL	C-N-CA	6.44	127.89	119.84
1	A	407	GLN	N-CA-C	-6.31	102.03	110.55
2	B	1296	LEU	N-CA-C	-6.24	102.64	111.24
1	A	173	ILE	CB-CA-C	-6.18	105.19	110.94
1	A	40	PHE	CA-C-N	-6.08	113.26	119.83
1	A	40	PHE	C-N-CA	-6.08	113.26	119.83
1	A	538	VAL	N-CA-C	-6.07	104.93	110.82
1	A	600	LYS	N-CA-C	-6.03	105.00	112.90
2	B	771	ILE	N-CA-C	5.80	116.22	108.27
1	A	8	THR	CB-CA-C	-5.64	102.64	110.37
2	B	1379	SER	N-CA-C	5.64	117.64	109.07
1	A	78	LYS	N-CA-C	5.62	117.46	108.41
2	B	1335	THR	N-CA-C	5.45	117.48	108.49
2	B	1348	ALA	CA-C-N	5.34	126.51	119.84
2	B	1348	ALA	C-N-CA	5.34	126.51	119.84
2	B	770	ASN	N-CA-C	-5.31	101.88	110.32
2	B	945	LEU	N-CA-C	5.27	117.61	111.02
1	A	562	LYS	N-CA-C	-5.24	102.15	109.96
2	B	752	ASN	N-CA-C	5.20	116.43	108.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	PHE	Peptide
1	A	599	GLU	Peptide
2	B	1056	LEU	Mainchain
2	B	1335	THR	Peptide
2	B	1347	PRO	Peptide
2	B	1369	ARG	Peptide
2	B	1430	SER	Peptide
2	B	1497	PHE	Mainchain
2	B	930	LEU	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	5008	0	5071	154	0
2	B	7213	0	7141	136	99
3	S	950	0	935	15	0
4	C	50	0	43	0	0
5	A	1	0	0	0	0
6	B	14	0	13	0	0
All	All	13236	0	13203	298	99

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1370:TYR:N	2:B:1430:SER:O	2.13	0.81
1:A:507:PHE:CE1	1:A:531:VAL:HB	2.20	0.77
1:A:329:SER:OG	1:A:413:GLU:O	2.04	0.76
2:B:1383:ILE:HD11	2:B:1424:ILE:HD11	1.69	0.73
1:A:214:VAL:HG12	1:A:233:ILE:HD13	1.70	0.73
2:B:1330:ALA:HB1	2:B:1334:LEU:HD21	1.74	0.69
2:B:1385:MET:HE1	2:B:1441:VAL:HG12	1.74	0.69
3:S:4:LEU:HD22	3:S:22:CYS:SG	2.33	0.69
1:A:487:GLU:O	1:A:490:GLN:NE2	2.26	0.69
2:B:993:MET:HE2	2:B:1060:VAL:HG22	1.74	0.69
1:A:123:VAL:HG23	1:A:173:ILE:HD11	1.73	0.68
2:B:1059:TYR:O	2:B:1063:VAL:HG23	1.94	0.68
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.29	0.67
1:A:6:ILE:HD11	1:A:20:MET:HE3	1.77	0.67
2:B:785:VAL:HG22	2:B:795:VAL:HG22	1.75	0.66
1:A:302:LEU:HG	1:A:326:ILE:HD11	1.77	0.66
1:A:362:ALA:O	1:A:379:THR:HG21	1.96	0.66
2:B:956:THR:HG23	2:B:1324:THR:CG2	2.29	0.63
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.34	0.62
1:A:443:LEU:HD22	1:A:499:ILE:HG21	1.82	0.62
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:HD21	1:A:155:GLN:HE21	1.46	0.61
2:B:1385:MET:HE3	2:B:1391:PRO:HG3	1.81	0.61
1:A:117:TYR:CD1	1:A:123:VAL:HG22	2.36	0.61
2:B:1369:ARG:HG2	2:B:1430:SER:O	2.01	0.61
1:A:229:LEU:HD21	1:A:324:ILE:HD13	1.82	0.60
1:A:293:ARG:O	1:A:293:ARG:HG2	2.02	0.60
1:A:302:LEU:CG	1:A:326:ILE:HD11	2.32	0.60
1:A:262:LEU:O	1:A:263:PRO:C	2.44	0.60
1:A:197:SER:O	1:A:198:THR:OG1	2.14	0.60
1:A:45:LEU:HD12	1:A:48:SER:HB2	1.82	0.59
1:A:210:PHE:CE2	1:A:310:LEU:HD21	2.38	0.59
2:B:956:THR:HA	2:B:1324:THR:HG22	1.85	0.59
2:B:1348:ALA:HB1	2:B:1349:PRO:CD	2.33	0.59
1:A:220:PHE:CE2	1:A:330:PRO:HB3	2.38	0.59
3:S:6:VAL:HG22	3:S:22:CYS:HA	1.84	0.58
1:A:6:ILE:CD1	1:A:20:MET:HE3	2.34	0.58
1:A:40:PHE:CD2	1:A:41:PRO:HD3	2.38	0.58
2:B:868:PRO:O	2:B:869:LYS:C	2.47	0.58
1:A:142:MET:HB2	1:A:187:TYR:CE1	2.38	0.57
2:B:1381:LEU:HB2	2:B:1424:ILE:HB	1.87	0.57
2:B:1297:LEU:HD23	2:B:1298:ARG:N	2.20	0.56
1:A:522:ARG:HB3	1:A:630:GLN:HE22	1.69	0.56
2:B:1126:LEU:HD21	2:B:1177:MET:CE	2.35	0.56
2:B:1348:ALA:HB1	2:B:1349:PRO:HD2	1.86	0.56
1:A:253:ILE:HD12	1:A:253:ILE:N	2.21	0.56
1:A:470:TYR:CZ	1:A:495:LEU:HD21	2.41	0.56
3:S:63:TYR:O	3:S:64:GLN:C	2.48	0.56
1:A:338:THR:OG1	1:A:351:MET:N	2.38	0.56
1:A:509:LEU:O	1:A:528:SER:HA	2.05	0.56
2:B:1377:THR:O	2:B:1378:MET:O	2.24	0.55
1:A:131:ASN:O	1:A:134:LEU:N	2.39	0.55
2:B:968:MET:HE2	2:B:968:MET:HA	1.88	0.55
1:A:22:LEU:HD13	1:A:33:VAL:HG11	1.89	0.55
2:B:1472:HIS:ND1	2:B:1473:PRO:HD2	2.21	0.55
2:B:742:ARG:N	2:B:902:GLY:O	2.38	0.55
1:A:125:TYR:CD1	1:A:184:ILE:HD13	2.42	0.54
1:A:36:THR:HB	1:A:87:GLN:HB3	1.90	0.54
1:A:40:PHE:CG	1:A:41:PRO:HD3	2.42	0.54
2:B:733:ILE:HG23	2:B:734:ILE:N	2.23	0.54
2:B:978:LEU:HB3	2:B:981:LEU:HD12	1.89	0.54
2:B:927:PRO:O	2:B:928:GLU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.89	0.54
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.43	0.53
2:B:898:PHE:O	2:B:899:ILE:HD13	2.08	0.53
2:B:1464:GLU:O	2:B:1466:SER:N	2.41	0.53
2:B:1276:LEU:N	2:B:1276:LEU:HD12	2.23	0.53
2:B:1320:LEU:C	2:B:1320:LEU:HD12	2.33	0.53
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.90	0.53
2:B:1456:LYS:HB2	2:B:1468:THR:HG23	1.91	0.53
2:B:1237:GLN:O	2:B:1239:TYR:N	2.42	0.53
1:A:113:ASP:CG	1:A:124:LEU:HD12	2.35	0.52
1:A:452:ASN:N	1:A:452:ASN:HD22	2.08	0.52
2:B:1385:MET:HE1	2:B:1441:VAL:CG1	2.38	0.52
1:A:522:ARG:O	1:A:630:GLN:NE2	2.41	0.52
1:A:469:THR:HG23	1:A:483:ARG:HD3	1.89	0.52
2:B:1477:ASP:O	2:B:1479:LYS:N	2.42	0.52
1:A:81:ASN:N	1:A:81:ASN:HD22	2.05	0.52
2:B:1369:ARG:HG3	2:B:1429:VAL:HG23	1.92	0.52
1:A:285:LEU:C	1:A:285:LEU:HD12	2.36	0.51
1:A:596:ASP:O	1:A:600:LYS:N	2.44	0.51
1:A:591:GLN:O	1:A:594:ILE:HB	2.10	0.51
2:B:1288:ARG:O	2:B:1298:ARG:NH1	2.43	0.51
1:A:118:THR:O	1:A:121:SER:OG	2.20	0.51
1:A:237:PHE:O	1:A:239:TYR:N	2.43	0.51
2:B:1053:SER:HA	2:B:1100:ALA:HB3	1.93	0.51
2:B:1237:GLN:O	2:B:1238:ARG:C	2.54	0.51
2:B:1295:SER:OG	2:B:1297:LEU:N	2.42	0.50
1:A:102:SER:HB2	1:A:104:GLN:HE21	1.76	0.50
2:B:1154:LEU:HB2	2:B:1174:LEU:HD21	1.94	0.50
3:S:24:TYR:OH	3:S:32:GLN:NE2	2.42	0.50
1:A:443:LEU:CD2	1:A:499:ILE:HG21	2.41	0.50
2:B:1126:LEU:HD21	2:B:1177:MET:HE1	1.93	0.50
1:A:289:VAL:HG13	1:A:291:ASN:HB2	1.93	0.50
1:A:602:ASP:OD2	1:A:604:GLY:N	2.32	0.50
1:A:331:TYR:CE1	1:A:365:VAL:HG21	2.47	0.50
1:A:377:SER:OG	1:A:385:ALA:HB1	2.12	0.50
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.93	0.49
1:A:86:VAL:O	1:A:96:GLU:HA	2.13	0.49
1:A:594:ILE:O	1:A:597:VAL:N	2.45	0.49
2:B:961:GLN:HB3	2:B:1319:THR:HB	1.94	0.49
2:B:830:TYR:CD1	2:B:871:SER:HB3	2.47	0.49
2:B:1098:GLU:HB2	2:B:1121:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1369:ARG:HD3	2:B:1434:ASP:HA	1.95	0.49
2:B:1105:GLN:NE2	2:B:1108:ILE:HD13	2.28	0.49
1:A:220:PHE:CZ	1:A:330:PRO:HB3	2.48	0.49
1:A:45:LEU:HD23	1:A:45:LEU:H	1.78	0.49
1:A:289:VAL:HG12	1:A:289:VAL:O	2.12	0.49
2:B:1165:TYR:CD1	2:B:1210:ALA:HB2	2.48	0.49
3:S:37:TRP:CE3	3:S:93:THR:O	2.66	0.49
2:B:1168:ALA:HB2	2:B:1198:TRP:CD1	2.48	0.48
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.94	0.48
2:B:1107:MET:O	2:B:1248:GLN:HG2	2.13	0.48
1:A:561:LEU:HD13	2:B:771:ILE:HD11	1.95	0.48
2:B:1369:ARG:HB3	2:B:1431:HIS:HA	1.95	0.48
1:A:295:GLU:N	1:A:295:GLU:OE1	2.45	0.48
3:S:83:THR:HG22	3:S:83:THR:O	2.14	0.48
2:B:1011:GLN:O	2:B:1012:TRP:C	2.56	0.48
2:B:1141:ASN:HD22	2:B:1141:ASN:N	2.11	0.48
2:B:965:VAL:O	2:B:1268:GLN:HB2	2.14	0.48
1:A:416:THR:OG1	1:A:417:ARG:N	2.47	0.48
1:A:548:SER:O	1:A:550:ASP:N	2.47	0.48
2:B:1330:ALA:HB1	2:B:1334:LEU:CD2	2.43	0.48
2:B:1293:SER:O	2:B:1293:SER:OG	2.32	0.48
1:A:437:SER:OG	1:A:452:ASN:HB2	2.14	0.47
1:A:151:ILE:CG2	2:B:1297:LEU:HD13	2.43	0.47
2:B:931:GLY:O	2:B:932:ARG:HB2	2.13	0.47
1:A:486:ARG:HG3	1:A:490:GLN:NE2	2.30	0.47
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.95	0.47
1:A:40:PHE:HB3	1:A:41:PRO:HD3	1.96	0.47
1:A:177:VAL:HG22	1:A:178:ASN:N	2.29	0.47
1:A:550:ASP:O	1:A:551:ARG:HG2	2.15	0.47
2:B:844:LEU:HB2	2:B:876:TYR:CE1	2.50	0.47
2:B:1373:ASP:OD1	2:B:1430:SER:OG	2.24	0.47
1:A:123:VAL:CG2	1:A:173:ILE:HD11	2.43	0.47
1:A:212:VAL:O	1:A:213:ILE:HG13	2.14	0.47
2:B:1266:ASP:OD1	2:B:1266:ASP:N	2.47	0.47
1:A:257:GLU:N	1:A:257:GLU:CD	2.73	0.46
1:A:515:LEU:HD12	1:A:516:ILE:C	2.41	0.46
1:A:625:THR:HG23	1:A:631:GLN:CB	2.45	0.46
1:A:590:THR:O	1:A:591:GLN:C	2.58	0.46
2:B:1057:THR:HG22	2:B:1081:ALA:HB1	1.96	0.46
1:A:7:ILE:HD12	1:A:7:ILE:N	2.30	0.46
1:A:74:PHE:O	1:A:82:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:743:SER:O	2:B:745:PHE:CD2	2.68	0.46
2:B:1098:GLU:HB2	2:B:1121:LEU:CD2	2.46	0.46
2:B:1291:TRP:O	2:B:1292:GLU:CB	2.64	0.46
1:A:164:LEU:O	1:A:166:VAL:HG23	2.15	0.46
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.98	0.45
1:A:218:GLU:C	1:A:220:PHE:H	2.24	0.45
1:A:537:CYS:HB3	1:A:539:GLY:O	2.16	0.45
1:A:551:ARG:HA	1:A:551:ARG:NH1	2.31	0.45
1:A:577:ASP:O	1:A:578:LYS:C	2.59	0.45
2:B:1172:TYR:HA	2:B:1217:ALA:HB2	1.98	0.45
1:A:114:LYS:N	1:A:117:TYR:OH	2.48	0.45
2:B:1045:ALA:HB2	2:B:1052:PRO:HA	1.98	0.45
1:A:151:ILE:HG21	2:B:1297:LEU:HD13	1.99	0.45
1:A:333:ILE:HD12	1:A:416:THR:HA	1.99	0.45
2:B:1004:HIS:CD2	2:B:1066:LEU:HD11	2.51	0.45
2:B:927:PRO:O	2:B:928:GLU:CB	2.63	0.45
1:A:470:TYR:CE1	1:A:495:LEU:HD21	2.51	0.45
2:B:829:LEU:N	2:B:829:LEU:HD12	2.32	0.45
2:B:851:CYS:CB	2:B:879:VAL:HB	2.47	0.45
2:B:945:LEU:HD12	2:B:1305:ASN:HD22	1.81	0.45
1:A:293:ARG:O	1:A:295:GLU:N	2.50	0.45
2:B:1102:VAL:HG22	2:B:1105:GLN:HE21	1.82	0.45
2:B:1370:TYR:O	2:B:1431:HIS:HB2	2.16	0.45
3:S:67:LEU:HD21	3:S:79:LEU:HD11	1.98	0.45
1:A:406:LYS:N	1:A:414:GLN:HE22	2.14	0.45
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.99	0.45
2:B:1278:LEU:HD12	2:B:1278:LEU:H	1.82	0.45
2:B:959:LEU:HB3	2:B:1321:SER:OG	2.17	0.44
2:B:1003:VAL:HG21	2:B:1027:ILE:HD11	1.99	0.44
1:A:40:PHE:CB	1:A:41:PRO:HD3	2.47	0.44
1:A:407:GLN:O	1:A:408:GLU:CB	2.65	0.44
1:A:551:ARG:O	1:A:552:GLN:CB	2.65	0.44
1:A:69:PRO:O	1:A:71:ASN:N	2.50	0.44
1:A:547:GLN:OE1	1:A:559:MET:HA	2.17	0.44
2:B:1381:LEU:HD23	2:B:1457:VAL:HG13	1.99	0.44
1:A:182:TRP:HB3	1:A:200:PHE:CE2	2.53	0.44
1:A:197:SER:O	1:A:198:THR:CB	2.66	0.44
1:A:302:LEU:HB2	1:A:324:ILE:HB	2.00	0.44
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.52	0.44
2:B:1215:LEU:HD11	2:B:1231:VAL:HG23	1.99	0.44
3:S:37:TRP:HB2	3:S:49:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD11	1:A:285:LEU:HB2	1.98	0.44
2:B:736:GLU:HA	2:B:739:ILE:HD12	2.00	0.44
2:B:961:GLN:HE21	2:B:963:THR:HG23	1.82	0.44
1:A:135:LEU:HA	2:B:792:GLY:HA2	2.00	0.44
1:A:455:LEU:HD11	1:A:457:MET:HE3	1.99	0.44
1:A:251:PHE:CD1	1:A:304:VAL:HG22	2.53	0.44
1:A:93:GLN:HE21	1:A:627:SER:HB2	1.82	0.44
2:B:1360:ASN:C	2:B:1360:ASN:HD22	2.26	0.44
3:S:99:GLN:HG2	3:S:105:GLN:HG2	1.99	0.44
1:A:50:GLU:HB3	1:A:64:VAL:HG22	2.00	0.43
1:A:528:SER:OG	1:A:608:GLY:HA2	2.18	0.43
2:B:1384:SER:OG	2:B:1454:ALA:N	2.51	0.43
2:B:1437:LEU:C	2:B:1437:LEU:HD12	2.42	0.43
1:A:237:PHE:O	1:A:238:LEU:C	2.60	0.43
1:A:365:VAL:H	1:A:379:THR:HG22	1.83	0.43
2:B:1037:PHE:O	2:B:1039:GLN:N	2.52	0.43
1:A:81:ASN:N	1:A:81:ASN:ND2	2.66	0.43
2:B:761:LYS:O	2:B:762:ASN:HB2	2.19	0.43
2:B:945:LEU:HD12	2:B:1305:ASN:ND2	2.33	0.43
2:B:1231:VAL:HG21	2:B:1260:TYR:CE1	2.53	0.43
1:A:40:PHE:CG	1:A:41:PRO:CD	3.02	0.43
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.19	0.43
1:A:12:LEU:HD11	1:A:99:VAL:HG11	2.01	0.43
1:A:126:ARG:HG3	2:B:751:TRP:HZ2	1.82	0.43
1:A:551:ARG:HA	1:A:551:ARG:CZ	2.48	0.43
2:B:994:ILE:HG13	2:B:1107:MET:HE3	1.99	0.43
1:A:295:GLU:O	1:A:298:VAL:HG23	2.19	0.43
1:A:529:VAL:O	1:A:529:VAL:HG13	2.19	0.43
2:B:745:PHE:N	2:B:746:PRO:CD	2.81	0.43
3:S:67:LEU:CG	3:S:79:LEU:HD11	2.49	0.43
1:A:16:SER:O	1:A:67:THR:HA	2.19	0.43
1:A:507:PHE:CD1	1:A:531:VAL:HB	2.53	0.43
2:B:1043:ALA:C	2:B:1044:PHE:CD1	2.97	0.43
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.84	0.43
1:A:625:THR:HG23	1:A:631:GLN:HB2	2.01	0.43
2:B:1369:ARG:CZ	2:B:1430:SER:H	2.32	0.43
2:B:1067:ALA:HA	2:B:1070:LEU:HG	2.01	0.43
1:A:20:MET:HE2	1:A:35:VAL:CG2	2.49	0.42
1:A:152:PRO:CG	2:B:1295:SER:HA	2.49	0.42
2:B:1065:SER:O	2:B:1068:VAL:HG13	2.18	0.42
2:B:1366:ILE:HD12	2:B:1437:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:VAL:HG13	1:A:555:PRO:HD2	2.01	0.42
2:B:1377:THR:O	2:B:1378:MET:C	2.61	0.42
1:A:109:PHE:CE1	1:A:594:ILE:HG23	2.54	0.42
1:A:128:PHE:CD1	1:A:166:VAL:HG22	2.53	0.42
1:A:581:PHE:O	1:A:582:VAL:C	2.62	0.42
1:A:615:GLY:O	1:A:616:VAL:C	2.62	0.42
1:A:407:GLN:O	1:A:408:GLU:HB2	2.19	0.42
1:A:471:LEU:HD12	1:A:510:VAL:O	2.19	0.42
2:B:799:PHE:CE2	2:B:801:VAL:CG2	3.02	0.42
2:B:1293:SER:OG	2:B:1296:LEU:HD23	2.20	0.42
1:A:117:TYR:CG	1:A:123:VAL:HG22	2.54	0.42
1:A:161:GLN:HE21	1:A:161:GLN:HB2	1.73	0.42
1:A:597:VAL:O	1:A:600:LYS:N	2.47	0.42
2:B:1264:ALA:O	2:B:1265:PRO:C	2.63	0.42
2:B:1380:ILE:O	2:B:1457:VAL:HG12	2.20	0.42
2:B:1462:ASN:HD22	2:B:1462:ASN:HA	1.65	0.42
3:S:20:LEU:HD12	3:S:79:LEU:HD23	2.02	0.42
2:B:799:PHE:CE2	2:B:801:VAL:HG22	2.54	0.42
2:B:1125:VAL:O	2:B:1129:LEU:HG	2.20	0.42
2:B:1293:SER:O	2:B:1296:LEU:HG	2.19	0.42
1:A:108:LEU:HD23	1:A:129:THR:HA	2.02	0.41
1:A:116:ILE:HD11	1:A:203:LYS:HB3	2.00	0.41
1:A:166:VAL:O	1:A:168:PRO:HD3	2.21	0.41
1:A:237:PHE:CD2	1:A:243:VAL:HG22	2.55	0.41
1:A:579:GLY:O	1:A:580:VAL:C	2.61	0.41
2:B:1011:GLN:O	2:B:1013:GLU:N	2.53	0.41
2:B:1204:GLN:HE21	2:B:1204:GLN:HB3	1.71	0.41
2:B:1218:LEU:HB3	2:B:1227:VAL:HG22	2.01	0.41
1:A:113:ASP:HB3	1:A:124:LEU:HB2	2.02	0.41
2:B:1068:VAL:HG11	2:B:1135:ILE:HD11	2.02	0.41
2:B:847:ASN:ND2	2:B:849:ALA:HB3	2.36	0.41
1:A:507:PHE:CE1	1:A:531:VAL:CB	3.00	0.41
1:A:355:THR:HB	1:A:360:SER:O	2.20	0.41
2:B:763:GLY:O	2:B:764:ILE:HD13	2.20	0.41
2:B:1091:LYS:HB3	2:B:1092:PRO:HD2	2.03	0.41
2:B:1246:SER:O	2:B:1247:THR:C	2.63	0.41
2:B:1287:HIS:CE1	2:B:1298:ARG:HB3	2.55	0.41
3:S:3:ILE:HD12	3:S:3:ILE:N	2.36	0.41
3:S:34:LEU:HD12	3:S:51:ARG:O	2.21	0.41
3:S:38:LEU:N	3:S:38:LEU:HD12	2.36	0.41
1:A:10:ASN:HD22	1:A:10:ASN:HA	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HE1	1:A:189:GLU:OE2	2.21	0.41
2:B:745:PHE:N	2:B:746:PRO:HD3	2.36	0.41
1:A:19:THR:HG22	1:A:20:MET:N	2.36	0.41
1:A:237:PHE:CE2	1:A:243:VAL:HG22	2.56	0.41
1:A:253:ILE:HD11	1:A:262:LEU:HD21	2.03	0.41
1:A:332:GLN:HB3	1:A:355:THR:OG1	2.20	0.41
1:A:596:ASP:O	1:A:597:VAL:C	2.61	0.41
2:B:1161:LEU:HD13	2:B:1166:THR:HB	2.02	0.41
2:B:1291:TRP:O	2:B:1292:GLU:HB2	2.20	0.41
3:S:69:VAL:HG22	3:S:79:LEU:HD12	2.02	0.41
2:B:813:LEU:HD21	2:B:888:VAL:HB	2.03	0.41
2:B:1369:ARG:HD3	2:B:1434:ASP:CA	2.51	0.41
1:A:131:ASN:O	1:A:133:LYS:N	2.54	0.40
2:B:964:PRO:HB3	2:B:1270:LEU:HD11	2.02	0.40
1:A:362:ALA:O	1:A:379:THR:CG2	2.68	0.40
2:B:1379:SER:OG	2:B:1459:ALA:HA	2.21	0.40
1:A:10:ASN:ND2	1:A:622:LEU:O	2.53	0.40
1:A:38:HIS:CD2	1:A:43:LYS:HB3	2.57	0.40
1:A:473:MET:O	1:A:507:PHE:HA	2.21	0.40
2:B:956:THR:HB	2:B:1302:THR:HB	2.03	0.40
2:B:1012:TRP:HB3	2:B:1017:LEU:HD12	2.02	0.40
2:B:1057:THR:CG2	2:B:1081:ALA:HB1	2.51	0.40
2:B:1107:MET:O	2:B:1247:THR:HB	2.21	0.40
2:B:1385:MET:HE3	2:B:1391:PRO:CG	2.51	0.40
1:A:117:TYR:CE1	1:A:123:VAL:HG22	2.57	0.40
1:A:302:LEU:HG	1:A:326:ILE:CD1	2.50	0.40
1:A:515:LEU:HD12	1:A:516:ILE:N	2.36	0.40
1:A:578:LYS:O	1:A:579:GLY:C	2.64	0.40
2:B:975:ALA:HB1	2:B:1015:PHE:HB2	2.03	0.40
2:B:1386:MET:O	2:B:1387:THR:C	2.64	0.40
2:B:960:LEU:HD23	2:B:960:LEU:HA	1.92	0.40

All (99) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1105:GLN:N	2:B:1508:GLU:CD[5_445]	0.40	1.80
2:B:1203:LYS:NZ	2:B:1622:LYS:C[5_445]	0.42	1.78
2:B:1203:LYS:C	2:B:1622:LYS:NZ[5_445]	0.70	1.50
2:B:1202:GLY:CA	2:B:1621:GLN:CG[5_445]	0.83	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1203:LYS:CG	2:B:1622:LYS:CB[5_445]	0.90	1.30
2:B:1202:GLY:CA	2:B:1621:GLN:CB[5_445]	1.01	1.19
2:B:1105:GLN:N	2:B:1508:GLU:OE1[5_445]	1.03	1.17
2:B:1202:GLY:N	2:B:1621:GLN:CD[5_445]	1.05	1.15
2:B:1203:LYS:NZ	2:B:1623:GLN:N[5_445]	1.07	1.13
2:B:1104:HIS:C	2:B:1508:GLU:CD[5_445]	1.08	1.12
2:B:1104:HIS:CA	2:B:1508:GLU:CG[5_445]	1.09	1.11
2:B:1203:LYS:CG	2:B:1622:LYS:CG[5_445]	1.09	1.11
2:B:1203:LYS:CD	2:B:1622:LYS:CB[5_445]	1.10	1.10
2:B:1203:LYS:O	2:B:1622:LYS:NZ[5_445]	1.13	1.07
2:B:1203:LYS:CB	2:B:1622:LYS:CD[5_445]	1.17	1.03
2:B:1203:LYS:CE	2:B:1622:LYS:C[5_445]	1.18	1.02
2:B:1105:GLN:N	2:B:1508:GLU:OE2[5_445]	1.22	0.98
2:B:1104:HIS:N	2:B:1508:GLU:CG[5_445]	1.24	0.96
2:B:1117:LYS:NZ	2:B:1632:GLU:OE1[5_445]	1.26	0.94
2:B:1203:LYS:CB	2:B:1622:LYS:CG[5_445]	1.29	0.91
2:B:1103:ILE:CG2	2:B:1512:ASP:OD2[5_445]	1.30	0.90
2:B:1103:ILE:O	2:B:1508:GLU:CB[5_445]	1.33	0.87
2:B:1114:ASN:OD1	2:B:1632:GLU:OE2[5_445]	1.34	0.86
2:B:1203:LYS:CE	2:B:1622:LYS:O[5_445]	1.35	0.85
2:B:1112:ARG:NH1	2:B:1507:LEU:N[5_445]	1.38	0.82
2:B:1105:GLN:CA	2:B:1508:GLU:OE2[5_445]	1.41	0.79
2:B:1203:LYS:CA	2:B:1622:LYS:NZ[5_445]	1.41	0.79
2:B:1203:LYS:NZ	2:B:1622:LYS:CA[5_445]	1.45	0.75
2:B:1114:ASN:OD1	2:B:1632:GLU:CB[5_445]	1.49	0.71
2:B:1202:GLY:O	2:B:1621:GLN:NE2[5_445]	1.50	0.70
2:B:1202:GLY:N	2:B:1621:GLN:CG[5_445]	1.51	0.69
2:B:1203:LYS:CE	2:B:1622:LYS:CA[5_445]	1.51	0.69
2:B:1112:ARG:O	2:B:1629:ALA:CB[5_445]	1.53	0.67
2:B:1202:GLY:CA	2:B:1621:GLN:CD[5_445]	1.54	0.66
2:B:1203:LYS:CG	2:B:1622:LYS:CA[5_445]	1.54	0.66
2:B:1098:GLU:O	2:B:1637:PHE:CZ[5_445]	1.55	0.65
2:B:1106:GLU:CB	2:B:1506:THR:CG2[5_445]	1.56	0.64
2:B:1103:ILE:CG2	2:B:1512:ASP:CG[5_445]	1.57	0.63
2:B:1104:HIS:C	2:B:1508:GLU:CG[5_445]	1.58	0.62
2:B:1103:ILE:O	2:B:1508:GLU:CA[5_445]	1.59	0.61
2:B:1203:LYS:C	2:B:1622:LYS:CE[5_445]	1.62	0.58
2:B:1104:HIS:C	2:B:1508:GLU:OE1[5_445]	1.63	0.57
2:B:1203:LYS:NZ	2:B:1622:LYS:O[5_445]	1.64	0.56
2:B:1203:LYS:CA	2:B:1622:LYS:CE[5_445]	1.65	0.55
2:B:1103:ILE:CG2	2:B:1512:ASP:OD1[5_445]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1114:ASN:OD1	2:B:1632:GLU:CD[5_445]	1.70	0.50
2:B:1202:GLY:C	2:B:1621:GLN:CB[5_445]	1.70	0.50
2:B:1203:LYS:CD	2:B:1622:LYS:CA[5_445]	1.71	0.49
2:B:1114:ASN:O	2:B:1632:GLU:OE2[5_445]	1.72	0.48
2:B:1202:GLY:N	2:B:1621:GLN:OE1[5_445]	1.75	0.45
2:B:1106:GLU:CD	2:B:1506:THR:CB[5_445]	1.79	0.41
2:B:1105:GLN:CA	2:B:1508:GLU:CD[5_445]	1.81	0.39
2:B:1114:ASN:CB	2:B:1628:GLY:O[5_445]	1.81	0.39
2:B:1114:ASN:OD1	2:B:1632:GLU:CG[5_445]	1.82	0.38
2:B:1203:LYS:CB	2:B:1622:LYS:CE[5_445]	1.82	0.38
2:B:1202:GLY:C	2:B:1621:GLN:NE2[5_445]	1.83	0.37
2:B:1202:GLY:N	2:B:1621:GLN:NE2[5_445]	1.84	0.36
2:B:1105:GLN:CA	2:B:1508:GLU:OE1[5_445]	1.86	0.34
2:B:1106:GLU:OE1	2:B:1507:LEU:N[5_445]	1.86	0.34
2:B:1202:GLY:C	2:B:1621:GLN:CG[5_445]	1.86	0.34
2:B:1103:ILE:C	2:B:1508:GLU:CG[5_445]	1.87	0.33
2:B:1105:GLN:N	2:B:1508:GLU:CG[5_445]	1.89	0.31
2:B:1103:ILE:C	2:B:1508:GLU:CB[5_445]	1.90	0.30
2:B:1104:HIS:CA	2:B:1508:GLU:CB[5_445]	1.90	0.30
2:B:1104:HIS:C	2:B:1508:GLU:OE2[5_445]	1.90	0.30
2:B:1202:GLY:C	2:B:1621:GLN:CD[5_445]	1.90	0.30
2:B:1244:TYR:OH	2:B:1509:GLU:CD[5_445]	1.91	0.29
2:B:1114:ASN:ND2	2:B:1632:GLU:N[5_445]	1.92	0.28
2:B:1244:TYR:CE2	2:B:1506:THR:OG1[5_445]	1.92	0.28
2:B:1204:GLN:N	2:B:1622:LYS:NZ[5_445]	1.94	0.26
2:B:1202:GLY:CA	2:B:1621:GLN:NE2[5_445]	1.95	0.25
2:B:1106:GLU:CG	2:B:1506:THR:CG2[5_445]	1.98	0.22
2:B:1204:GLN:N	2:B:1622:LYS:CE[5_445]	1.98	0.22
2:B:1106:GLU:OE2	2:B:1506:THR:CB[5_445]	1.99	0.21
2:B:1112:ARG:NH1	2:B:1506:THR:C[5_445]	1.99	0.21
2:B:1203:LYS:CB	2:B:1622:LYS:NZ[5_445]	1.99	0.21
2:B:1114:ASN:CG	2:B:1632:GLU:CB[5_445]	2.00	0.20
2:B:1112:ARG:CZ	2:B:1507:LEU:N[5_445]	2.01	0.19
2:B:1200:ASP:O	2:B:1621:GLN:OE1[5_445]	2.05	0.15
2:B:1244:TYR:OH	2:B:1509:GLU:OE2[5_445]	2.06	0.14
2:B:1104:HIS:CA	2:B:1508:GLU:CD[5_445]	2.08	0.12
2:B:1106:GLU:N	2:B:1508:GLU:OE1[5_445]	2.09	0.11
2:B:1117:LYS:NZ	2:B:1632:GLU:CD[5_445]	2.09	0.11
2:B:1203:LYS:CA	2:B:1622:LYS:CG[5_445]	2.09	0.11
2:B:1103:ILE:CG1	2:B:1512:ASP:OD1[5_445]	2.10	0.10
2:B:1163:ARG:NH2	2:B:1625:GLN:NE2[5_445]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1104:HIS:N	2:B:1508:GLU:CB[5_445]	2.12	0.08
2:B:1114:ASN:ND2	2:B:1632:GLU:CB[5_445]	2.12	0.08
2:B:1104:HIS:O	2:B:1508:GLU:CD[5_445]	2.13	0.07
2:B:1114:ASN:CG	2:B:1632:GLU:OE2[5_445]	2.13	0.07
2:B:1203:LYS:CE	2:B:1622:LYS:CB[5_445]	2.13	0.07
2:B:1203:LYS:CG	2:B:1622:LYS:N[5_445]	2.14	0.06
2:B:1103:ILE:CB	2:B:1512:ASP:OD1[5_445]	2.15	0.05
2:B:1106:GLU:OE2	2:B:1509:GLU:CG[5_445]	2.15	0.05
2:B:1105:GLN:C	2:B:1508:GLU:OE1[5_445]	2.18	0.02
2:B:1112:ARG:CZ	2:B:1507:LEU:CA[5_445]	2.18	0.02
2:B:1203:LYS:CA	2:B:1622:LYS:CD[5_445]	2.18	0.02
2:B:1103:ILE:O	2:B:1508:GLU:C[5_445]	2.19	0.01
2:B:1203:LYS:CG	2:B:1622:LYS:CD[5_445]	2.19	0.01

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	640/642 (100%)	526 (82%)	93 (14%)	21 (3%)	3	24
2	B	897/915 (98%)	748 (83%)	112 (12%)	37 (4%)	2	20
3	S	117/119 (98%)	99 (85%)	15 (13%)	3 (3%)	4	28
All	All	1654/1676 (99%)	1373 (83%)	220 (13%)	61 (4%)	2	22

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	198	THR
1	A	294	ALA
1	A	549	GLU
1	A	552	GLN
2	B	733	ILE

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Mol	Chain	Res	Type
2	B	928	GLU
2	B	1238	ARG
2	B	1247	THR
2	B	1378	MET
2	B	1429	VAL
2	B	1450	ILE
2	B	1465	GLU
2	B	1498	ILE
2	B	1602	LYS
1	A	40	PHE
1	A	292	LEU
1	A	293	ARG
1	A	548	SER
1	A	551	ARG
2	B	869	LYS
2	B	932	ARG
2	B	1038	ARG
2	B	1106	GLU
2	B	1292	GLU
2	B	1334	LEU
2	B	1375	ASP
2	B	1478	GLY
2	B	1517	PRO
2	B	1619	GLU
3	S	103	GLY
1	A	132	HIS
1	A	393	PRO
1	A	442	GLU
2	B	967	GLN
2	B	1013	GLU
2	B	1196	ASN
2	B	1486	ASP
2	B	1551	SER
2	B	1573	LYS
2	B	1583	TRP
3	S	64	GLN
1	A	70	ALA
1	A	408	GLU
1	A	607	PRO
2	B	911	PRO
2	B	944	ASP
2	B	988	CYS

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Mol	Chain	Res	Type
2	B	1576	GLU
1	A	50	GLU
1	A	364	ARG
2	B	778	THR
2	B	1314	GLY
2	B	1315	LYS
1	A	148	PRO
1	A	219	LYS
1	A	238	LEU
2	B	1349	PRO
3	S	20	LEU
2	B	1145	GLY
2	B	913	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	566/566 (100%)	481 (85%)	85 (15%)	3	15
2	B	799/810 (99%)	716 (90%)	83 (10%)	7	24
3	S	109/109 (100%)	97 (89%)	12 (11%)	6	23
All	All	1474/1485 (99%)	1294 (88%)	180 (12%)	5	20

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	8	THR
1	A	10	ASN
1	A	20	MET
1	A	45	LEU
1	A	47	LEU
1	A	51	LYS
1	A	64	VAL
1	A	71	ASN

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Mol	Chain	Res	Type
1	A	81	ASN
1	A	103	LEU
1	A	104	GLN
1	A	112	THR
1	A	114	LYS
1	A	118	THR
1	A	124	LEU
1	A	140	THR
1	A	153	VAL
1	A	156	ASP
1	A	158	LEU
1	A	159	SER
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	179	MET
1	A	183	LYS
1	A	207	LEU
1	A	209	SER
1	A	212	VAL
1	A	215	GLU
1	A	230	GLU
1	A	246	THR
1	A	249	VAL
1	A	267	LYS
1	A	277	GLU
1	A	280	LEU
1	A	285	LEU
1	A	289	VAL
1	A	295	GLU
1	A	301	SER
1	A	317	VAL
1	A	322	SER
1	A	328	THR
1	A	336	THR
1	A	338	THR
1	A	350	LEU
1	A	354	VAL
1	A	365	VAL
1	A	377	SER
1	A	379	THR
1	A	389	ILE

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Mol	Chain	Res	Type
1	A	399	SER
1	A	404	THR
1	A	409	LEU
1	A	416	THR
1	A	426	THR
1	A	438	VAL
1	A	443	LEU
1	A	448	THR
1	A	452	ASN
1	A	454	LEU
1	A	462	GLU
1	A	464	LYS
1	A	471	LEU
1	A	474	ASN
1	A	494	VAL
1	A	498	SER
1	A	500	THR
1	A	509	LEU
1	A	514	THR
1	A	515	LEU
1	A	521	GLN
1	A	528	SER
1	A	537	CYS
1	A	538	VAL
1	A	540	SER
1	A	542	VAL
1	A	551	ARG
1	A	554	VAL
1	A	585	LYS
1	A	587	ASN
1	A	611	LYS
1	A	618	SER
1	A	625	THR
1	A	639	GLN
2	B	733	ILE
2	B	748	SER
2	B	752	ASN
2	B	758	GLU
2	B	766	THR
2	B	771	ILE
2	B	789	ASP
2	B	802	THR

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Mol	Chain	Res	Type
2	B	809	ILE
2	B	818	VAL
2	B	825	ILE
2	B	835	ASN
2	B	836	GLN
2	B	841	ARG
2	B	863	THR
2	B	869	LYS
2	B	890	VAL
2	B	910	VAL
2	B	917	ASN
2	B	922	VAL
2	B	953	GLU
2	B	957	ARG
2	B	959	LEU
2	B	963	THR
2	B	968	MET
2	B	974	ASP
2	B	984	THR
2	B	994	ILE
2	B	1018	GLU
2	B	1024	LEU
2	B	1066	LEU
2	B	1076	GLN
2	B	1136	CYS
2	B	1137	GLU
2	B	1138	GLU
2	B	1141	ASN
2	B	1204	GLN
2	B	1255	GLN
2	B	1259	GLN
2	B	1263	ASP
2	B	1266	ASP
2	B	1288	ARG
2	B	1295	SER
2	B	1302	THR
2	B	1305	ASN
2	B	1311	THR
2	B	1320	LEU
2	B	1337	ASN
2	B	1344	THR
2	B	1361	THR

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Mol	Chain	Res	Type
2	B	1369	ARG
2	B	1374	GLN
2	B	1387	THR
2	B	1393	THR
2	B	1403	VAL
2	B	1408	SER
2	B	1418	ASP
2	B	1422	LEU
2	B	1429	VAL
2	B	1432	SER
2	B	1445	PHE
2	B	1457	VAL
2	B	1462	ASN
2	B	1487	GLU
2	B	1504	LYS
2	B	1505	VAL
2	B	1506	THR
2	B	1507	LEU
2	B	1529	LYS
2	B	1541	MET
2	B	1543	ILE
2	B	1546	THR
2	B	1561	THR
2	B	1564	SER
2	B	1566	ILE
2	B	1578	LYS
2	B	1593	LYS
2	B	1597	SER
2	B	1604	THR
2	B	1606	VAL
2	B	1624	CYS
2	B	1631	THR
2	B	1639	CYS
3	S	1	ARG
3	S	3	ILE
3	S	10	VAL
3	S	17	ASP
3	S	23	THR
3	S	31	THR
3	S	50	LEU
3	S	81	LEU
3	S	85	GLU

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Mol	Chain	Res	Type
3	S	87	ASP
3	S	90	SER
3	S	95	GLU

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	10	ASN
1	A	38	HIS
1	A	59	ASN
1	A	81	ASN
1	A	93	GLN
1	A	144	ASN
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	193	GLN
1	A	376	GLN
1	A	420	GLN
1	A	432	ASN
1	A	490	GLN
1	A	521	GLN
1	A	557	GLN
1	A	567	HIS
1	A	631	GLN
2	B	835	ASN
2	B	836	GLN
2	B	846	HIS
2	B	861	GLN
2	B	897	HIS
2	B	961	GLN
2	B	1004	HIS
2	B	1033	GLN
2	B	1105	GLN
2	B	1141	ASN
2	B	1160	ASN
2	B	1204	GLN
2	B	1207	ASN
2	B	1235	ASN
2	B	1267	HIS
2	B	1271	ASN
2	B	1277	GLN

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Mol	Chain	Res	Type
2	B	1360	ASN
2	B	1401	ASN
2	B	1462	ASN
2	B	1481	ASN
3	S	40	GLN

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](#)

4 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	$\# Z > 2$
4	NAG	C	1	4,1	14,14,15	0.81	0	17,19,21	1.62	3 (17%)
4	NAG	C	2	4	14,14,15	0.46	0	17,19,21	2.01	3 (17%)
4	BMA	C	3	4	11,11,12	0.68	0	15,15,17	1.34	1 (6%)
4	BMA	C	4	4	11,11,12	0.58	0	15,15,17	0.59	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	C	1	4,1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2	4	-	4/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	BMA	C	4	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	C1-O5-C5	6.39	120.74	112.19
4	C	3	BMA	C1-O5-C5	4.37	118.04	112.19
4	C	1	NAG	C4-C3-C2	3.88	116.71	111.02
4	C	1	NAG	C1-O5-C5	-3.34	107.70	112.19
4	C	2	NAG	O4-C4-C5	3.02	116.75	109.32
4	C	2	NAG	C4-C3-C2	-2.51	107.34	111.02
4	C	1	NAG	O5-C5-C4	-2.23	105.41	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1	NAG	C1

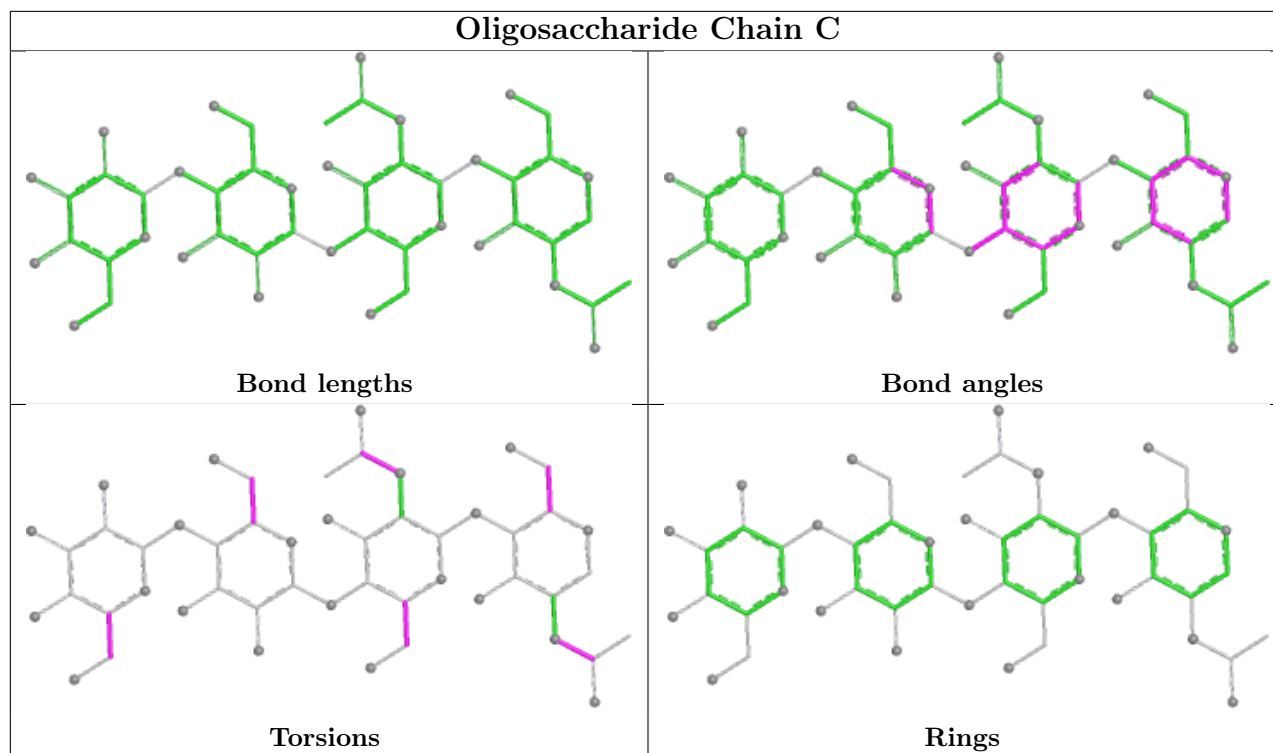
All (11) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	5	2	14,14,15	0.62	0	17,19,21	1.28	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	5	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5	NAG	C1-O5-C5	3.22	116.50	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	5	NAG	O7-C7-N2-C2
6	B	5	NAG	C8-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	642/642 (100%)	-0.44	0 100 100	147, 191, 237, 314	0
2	B	761/915 (83%)	-0.44	4 (0%) 87 74	135, 206, 258, 294	0
3	S	119/119 (100%)	-0.53	0 100 100	167, 203, 249, 289	0
All	All	1522/1676 (90%)	-0.45	4 (0%) 90 79	135, 199, 249, 314	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1294	ALA	3.4
2	B	1002	ALA	2.6
2	B	1136	CYS	2.1
2	B	1082	VAL	2.0

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

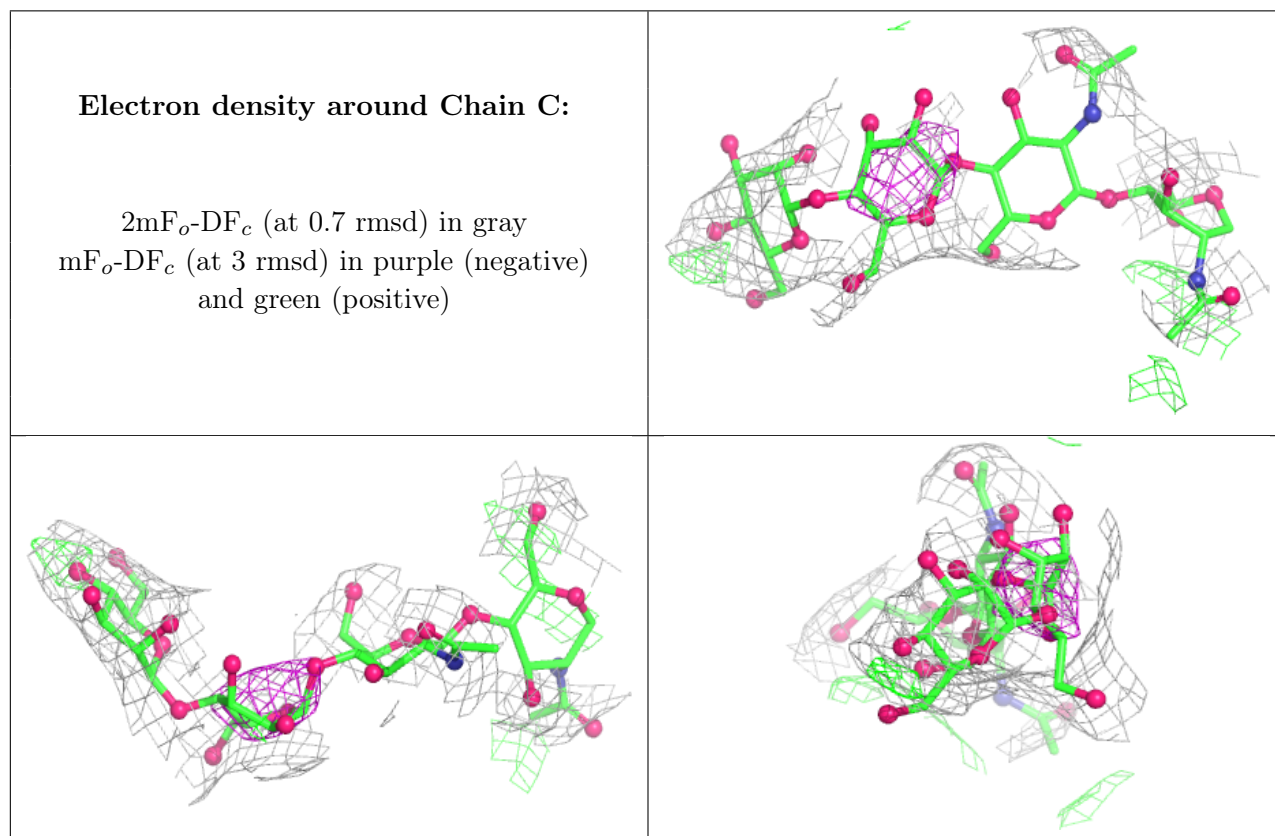
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	1	14/15	-	-	207,210,212,214	0
4	NAG	C	2	14/15	-	-	215,220,226,233	0
4	BMA	C	3	11/12	-	-	233,236,238,238	0
4	BMA	C	4	11/12	-	-	222,223,226,228	11

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



6.4 Ligands [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
6	NAG	B	5	14/15	0.85	0.07	232,236,237,238	0
5	CA	A	647	1/1	0.99	0.04	123,123,123,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.