



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:30 AM UTC

PDB ID : 3O4O / pdb_00003o4o
Title : Crystal structure of an Interleukin-1 receptor complex
Authors : Wang, X.Q.; Wang, D.L.; Zhang, S.Y.; Li, L.; Liu, X.; Mei, K.R.
Deposited on : 2010-07-27
Resolution : 3.30 Å(reported)

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

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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)
Xtriage (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

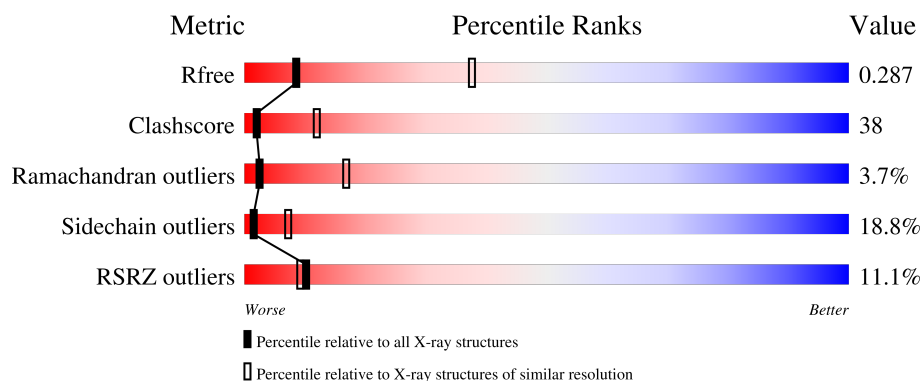
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	158	
2	C	339	
3	B	339	
4	D	2	
4	E	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6506 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 Interleukin-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1212	770	200	234	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01584
A	-3	PRO	-	expression tag	UNP P01584
A	-2	LEU	-	expression tag	UNP P01584
A	-1	GLY	-	expression tag	UNP P01584
A	0	SER	-	expression tag	UNP P01584

- Molecule 2 is a protein called Interleukin-1 receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	316	2562	1631	439	480	12	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P27930
C	-1	ASP	-	expression tag	UNP P27930
C	0	PRO	-	expression tag	UNP P27930
C	331	HIS	-	expression tag	UNP P27930
C	332	HIS	-	expression tag	UNP P27930
C	333	HIS	-	expression tag	UNP P27930
C	334	HIS	-	expression tag	UNP P27930
C	335	HIS	-	expression tag	UNP P27930
C	336	HIS	-	expression tag	UNP P27930

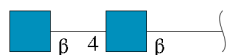
- Molecule 3 is a protein called Interleukin-1 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	323	Total	C	N	O	S	0	0	0
			2620	1673	442	489	16			

There are 9 discrepancies between the modelled and reference sequences:

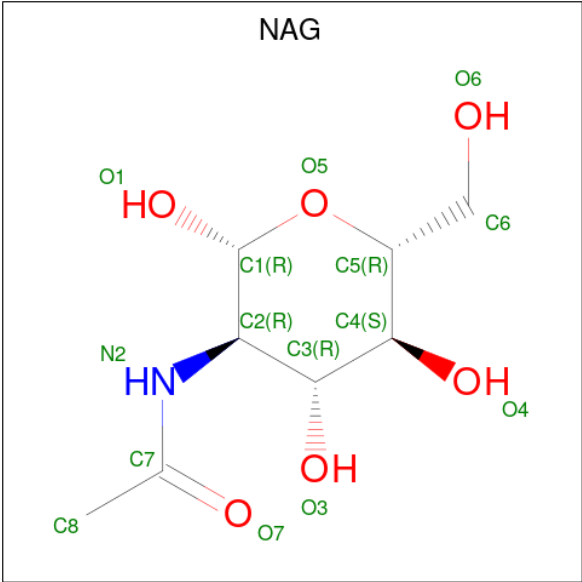
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP Q9NPH3
B	-1	ASP	-	expression tag	UNP Q9NPH3
B	0	PRO	-	expression tag	UNP Q9NPH3
B	331	HIS	-	expression tag	UNP Q9NPH3
B	332	HIS	-	expression tag	UNP Q9NPH3
B	333	HIS	-	expression tag	UNP Q9NPH3
B	334	HIS	-	expression tag	UNP Q9NPH3
B	335	HIS	-	expression tag	UNP Q9NPH3
B	336	HIS	-	expression tag	UNP Q9NPH3

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O		0	0	0
			28	16	2	10				
4	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

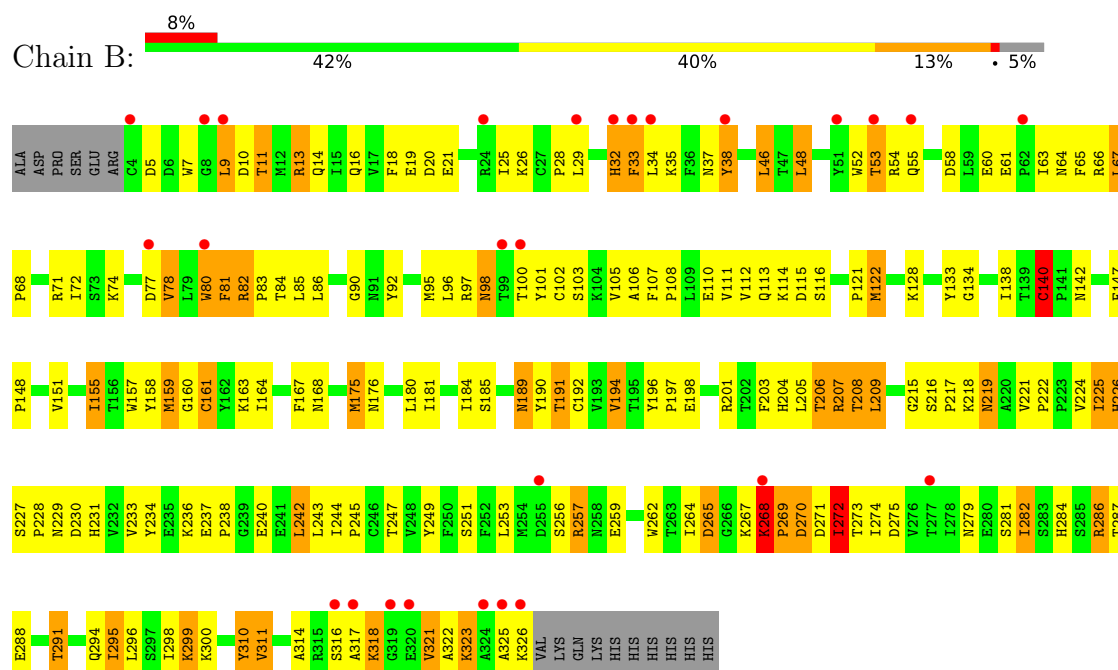


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

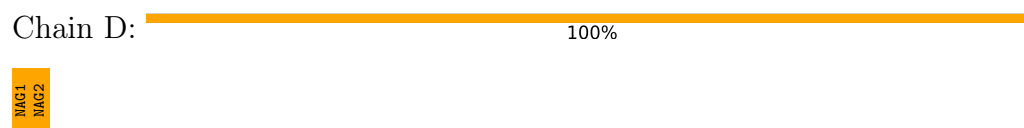
- Molecule 1: Interleukin-1 beta



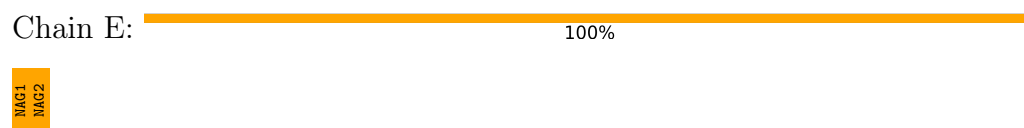
- Molecule 3: Interleukin-1 receptor accessory protein



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.83Å 177.47Å 180.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.59 – 3.30 36.59 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (36.59-3.30) 94.7 (36.59-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.252 , 0.289 0.248 , 0.287	Depositor DCC
R_{free} test set	1101 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	4/1235 (0.3%)	0.81	1/1662 (0.1%)
2	C	0.42	3/2626 (0.1%)	0.83	9/3573 (0.3%)
3	B	0.45	3/2689 (0.1%)	0.88	14/3659 (0.4%)
All	All	0.45	10/6550 (0.2%)	0.84	24/8894 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	HIS	ND1-CE1	5.25	1.37	1.32
3	B	32	HIS	ND1-CE1	5.24	1.37	1.32
1	A	38	GLN	CD-OE1	5.18	1.33	1.23
1	A	48	GLN	CD-OE1	5.16	1.33	1.23
1	A	129	ASN	CG-OD1	5.13	1.33	1.23
2	C	267	HIS	ND1-CE1	5.13	1.37	1.32
3	B	226	HIS	ND1-CE1	5.12	1.37	1.32
3	B	113	GLN	CD-OE1	5.07	1.33	1.23
2	C	178	HIS	ND1-CE1	5.05	1.37	1.32
1	A	149	GLN	CD-OE1	5.01	1.33	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	226	HIS	CB-CG-CD2	-6.80	122.36	131.20
2	C	178	HIS	CB-CG-CD2	-6.77	122.40	131.20
2	C	57	HIS	CB-CG-CD2	-6.65	122.56	131.20
3	B	32	HIS	CB-CG-CD2	-6.52	122.73	131.20
2	C	267	HIS	CB-CG-CD2	-6.34	122.96	131.20
3	B	98	ASN	N-CA-C	-6.31	99.53	109.50
2	C	274	GLY	N-CA-C	-6.29	104.67	115.61
3	B	268	LYS	CA-C-N	6.22	127.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	268	LYS	C-N-CA	6.22	127.61	119.84
3	B	140	CYS	CA-C-N	6.21	127.60	119.84
3	B	140	CYS	C-N-CA	6.21	127.60	119.84
3	B	286	ARG	N-CA-C	-6.17	104.61	111.71
3	B	226	HIS	CB-CG-ND1	5.85	131.47	122.70
2	C	57	HIS	CB-CG-ND1	5.76	131.34	122.70
2	C	178	HIS	CB-CG-ND1	5.73	131.30	122.70
3	B	147	PHE	CA-C-N	5.68	126.00	119.92
3	B	147	PHE	C-N-CA	5.68	126.00	119.92
3	B	161	CYS	N-CA-C	-5.53	106.51	113.20
3	B	32	HIS	CB-CG-ND1	5.49	130.93	122.70
2	C	267	HIS	CB-CG-ND1	5.43	130.84	122.70
3	B	217	PRO	N-CA-C	-5.29	107.53	114.03
1	A	108	ASN	N-CA-C	5.21	121.91	110.80
2	C	228	SER	CA-C-N	5.12	124.81	119.64
2	C	228	SER	C-N-CA	5.12	124.81	119.64

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	1212	0	1213	82	0
2	C	2562	0	2520	258	0
3	B	2620	0	2564	163	0
4	D	28	0	25	5	0
4	E	28	0	25	1	0
5	B	28	0	26	0	0
5	C	28	0	26	0	0
All	All	6506	0	6399	493	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 38.

All (493) 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)
3:B:234:TYR:O	3:B:326:LYS:HA	1.52	1.06
2:C:214:ARG:HH11	2:C:214:ARG:HG3	1.19	1.05
2:C:74:TRP:HZ3	2:C:83:LEU:HD11	1.24	1.01
3:B:55:GLN:HA	4:D:1:NAG:O7	1.59	1.01
2:C:127:GLN:HG3	2:C:211:ILE:HG23	1.44	0.99
2:C:38:PRO:HG3	2:C:108:ILE:HD13	1.49	0.94
2:C:99:ASN:O	2:C:102:TYR:N	1.99	0.93
3:B:191:THR:HB	3:B:208:THR:HB	1.49	0.93
2:C:243:ILE:HG21	2:C:298:ILE:CG2	2.02	0.90
1:A:105:GLU:HG3	1:A:110:LEU:HB3	1.53	0.88
2:C:243:ILE:HG21	2:C:298:ILE:HG22	1.53	0.88
3:B:236:LYS:HG3	3:B:242:LEU:HB2	1.53	0.88
2:C:147:ARG:HG2	2:C:147:ARG:HH11	1.35	0.88
2:C:312:LYS:HA	2:C:324:LEU:O	1.74	0.87
1:A:5:SER:HB3	1:A:45:SER:HB3	1.57	0.87
1:A:69:LEU:H	1:A:69:LEU:HD23	1.38	0.86
2:C:16:ARG:HG2	2:C:104:ASP:HB3	1.57	0.86
2:C:274:GLY:N	2:C:276:ARG:HH11	1.75	0.84
2:C:285:TYR:HB3	2:C:287:GLU:HG2	1.61	0.83
2:C:274:GLY:H	2:C:276:ARG:HD3	1.43	0.82
2:C:193:ARG:HH21	2:C:208:THR:HG21	1.43	0.82
3:B:311:VAL:HG22	3:B:323:LYS:HA	1.61	0.82
1:A:31:LEU:HB2	1:A:36:MET:HE3	1.61	0.81
2:C:131:LEU:HA	2:C:184:VAL:HG13	1.61	0.81
2:C:152:VAL:HG12	2:C:154:ILE:HG13	1.63	0.81
2:C:231:LYS:HB3	2:C:327:THR:HB	1.63	0.81
3:B:67:LEU:N	3:B:68:PRO:HA	1.97	0.80
3:B:98:ASN:HB3	3:B:101:TYR:H	1.48	0.79
2:C:231:LYS:HE3	2:C:233:ILE:HD12	1.66	0.78
2:C:193:ARG:NH2	2:C:208:THR:HG21	1.99	0.77
2:C:64:THR:HB	2:C:66:PRO:HA	1.64	0.77
3:B:279:ASN:HB3	3:B:295:ILE:HG13	1.65	0.77
3:B:46:LEU:HA	3:B:97:ARG:O	1.83	0.77
2:C:176:THR:HG22	2:C:177:THR:H	1.50	0.76
2:C:133:THR:O	2:C:184:VAL:HG12	1.86	0.76
3:B:5:ASP:O	3:B:103:SER:HA	1.86	0.76
3:B:26:LYS:HA	3:B:78:VAL:HG22	1.69	0.75
1:A:7:ASN:HA	1:A:42:PHE:O	1.88	0.74
2:C:49:SER:HB3	2:C:50:PRO:HD2	1.69	0.74
2:C:139:CYS:HB3	2:C:177:THR:HG22	1.70	0.73
2:C:24:ARG:HG2	2:C:109:GLU:HB3	1.68	0.73
2:C:219:LYS:HE3	2:C:219:LYS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:64:ASN:HA	3:B:67:LEU:HD23	1.70	0.73
1:A:3:VAL:HG12	1:A:93:LYS:HG2	1.70	0.72
2:C:93:TYR:O	2:C:107:SER:HA	1.89	0.72
2:C:238:GLY:HA3	2:C:240:ARG:NH1	2.04	0.72
3:B:221:VAL:HG22	3:B:222:PRO:HD2	1.72	0.72
3:B:10:ASP:HB3	3:B:13:ARG:HB3	1.71	0.71
1:A:94:LYS:HD3	1:A:94:LYS:N	2.05	0.71
2:C:48:VAL:O	2:C:51:ARG:HG2	1.90	0.71
3:B:259:GLU:O	3:B:314:ALA:HA	1.91	0.70
2:C:214:ARG:HG3	2:C:214:ARG:NH1	1.97	0.70
2:C:237:LEU:HD13	2:C:237:LEU:O	1.89	0.70
1:A:120:TRP:HB3	1:A:134:LEU:CD1	2.22	0.70
2:C:74:TRP:CZ3	2:C:83:LEU:HD11	2.16	0.70
2:C:26:PHE:HB3	2:C:113:PHE:HE1	1.56	0.70
2:C:145:PHE:HB3	2:C:198:PHE:CE2	2.26	0.70
2:C:263:ALA:HB1	2:C:310:ASP:O	1.91	0.70
2:C:131:LEU:HB3	2:C:215:ILE:CG2	2.22	0.69
2:C:109:GLU:HG3	2:C:110:LEU:N	2.08	0.69
3:B:274:ILE:O	3:B:274:ILE:HG23	1.93	0.69
1:A:4:ARG:HG3	2:C:282:ARG:HE	1.58	0.69
3:B:224:VAL:HG12	3:B:249:TYR:HB3	1.73	0.69
2:C:231:LYS:CB	2:C:327:THR:HB	2.22	0.68
2:C:140:PRO:HD3	2:C:211:ILE:HD11	1.75	0.68
3:B:159:MET:HE2	3:B:190:TYR:CZ	2.28	0.68
2:C:87:GLN:O	2:C:88:GLU:HB3	1.92	0.68
2:C:255:LEU:HG	2:C:256:THR:H	1.59	0.68
2:C:52:ILE:CG2	2:C:98:ARG:H	2.06	0.68
1:A:41:VAL:HG21	1:A:151:VAL:HG11	1.75	0.68
3:B:55:GLN:CA	4:D:1:NAG:O7	2.38	0.68
3:B:95:MET:HA	3:B:103:SER:O	1.93	0.68
3:B:77:ASP:O	3:B:78:VAL:HG23	1.94	0.67
2:C:127:GLN:HG3	2:C:211:ILE:CG2	2.22	0.67
2:C:227:ILE:HG22	2:C:227:ILE:O	1.92	0.67
2:C:273:PRO:HA	2:C:276:ARG:HG2	1.75	0.67
2:C:38:PRO:HB2	2:C:106:MET:HE2	1.75	0.67
1:A:46:PHE:HD1	1:A:58:VAL:HG12	1.58	0.67
3:B:9:LEU:HD13	3:B:11:THR:HG23	1.76	0.67
1:A:126:GLN:OE1	3:B:168:ASN:HA	1.94	0.67
3:B:46:LEU:HD22	3:B:98:ASN:HB2	1.77	0.67
3:B:237:GLU:HB3	3:B:238:PRO:HD2	1.76	0.66
1:A:120:TRP:HB3	1:A:134:LEU:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:312:LYS:HG3	2:C:325:ARG:HG3	1.77	0.66
1:A:92:LYS:HG2	1:A:95:MET:HE2	1.76	0.66
2:C:274:GLY:H	2:C:276:ARG:HH11	1.44	0.66
3:B:21:GLU:O	3:B:84:THR:HG22	1.96	0.66
2:C:40:VAL:HB	2:C:41:PRO:HD3	1.77	0.66
2:C:102:TYR:C	2:C:102:TYR:CD2	2.73	0.66
1:A:3:VAL:CG1	1:A:93:LYS:HG2	2.26	0.66
2:C:223:ILE:HD13	2:C:223:ILE:H	1.61	0.66
2:C:208:THR:O	2:C:209:ARG:HD2	1.96	0.66
3:B:14:GLN:HG2	3:B:108:PRO:HG2	1.78	0.66
2:C:110:LEU:HD23	2:C:111:ARG:N	2.12	0.65
3:B:225:ILE:HG22	3:B:228:PRO:HD2	1.79	0.65
2:C:215:ILE:O	2:C:216:LYS:HD3	1.95	0.65
2:C:243:ILE:HG21	2:C:298:ILE:HG23	1.79	0.65
2:C:214:ARG:HH11	2:C:214:ARG:CG	2.04	0.64
2:C:219:LYS:HE3	2:C:220:GLU:H	1.62	0.64
3:B:299:LYS:HB2	3:B:299:LYS:NZ	2.13	0.64
2:C:299:PHE:O	2:C:301:PRO:HD3	1.97	0.64
2:C:235:ALA:HB3	2:C:330:GLU:HB3	1.79	0.64
2:C:256:THR:HG21	2:C:318:THR:HG22	1.80	0.64
2:C:263:ALA:HA	2:C:311:PHE:HA	1.78	0.64
2:C:61:SER:C	2:C:63:ARG:HH12	2.06	0.64
3:B:11:THR:O	3:B:14:GLN:HG3	1.97	0.64
4:D:1:NAG:H61	4:D:2:NAG:N2	2.12	0.64
2:C:136:VAL:CG2	2:C:178:HIS:HB3	2.28	0.64
2:C:327:THR:HG22	2:C:328:VAL:N	2.13	0.64
2:C:253:THR:N	2:C:254:PRO:HD3	2.13	0.63
1:A:58:VAL:N	1:A:101:PHE:O	2.24	0.63
3:B:92:TYR:O	3:B:106:ALA:HA	1.98	0.63
2:C:82:LEU:O	2:C:85:ALA:N	2.32	0.63
1:A:6:LEU:HD11	1:A:150:PHE:CD2	2.34	0.63
2:C:147:ARG:HG2	2:C:147:ARG:NH1	2.10	0.63
2:C:125:TYR:CD2	2:C:140:PRO:HG2	2.33	0.63
2:C:327:THR:CG2	2:C:328:VAL:H	2.11	0.63
3:B:234:TYR:O	3:B:325:ALA:O	2.17	0.62
2:C:240:ARG:H	2:C:240:ARG:HD3	1.63	0.62
1:A:22:GLY:HA3	1:A:24:TYR:N	2.15	0.62
2:C:37:CYS:O	2:C:41:PRO:HD2	1.99	0.62
2:C:102:TYR:C	2:C:102:TYR:HD2	2.07	0.62
3:B:229:ASN:O	3:B:230:ASP:HB2	1.99	0.62
3:B:267:LYS:O	3:B:268:LYS:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:52:TRP:CZ3	3:B:54:ARG:HB2	2.35	0.62
2:C:45:TRP:CG	2:C:48:VAL:HG21	2.35	0.61
3:B:287:THR:O	3:B:288:GLU:HB2	1.99	0.61
3:B:19:GLU:HG2	3:B:20:ASP:N	2.15	0.61
3:B:299:LYS:HG2	3:B:300:LYS:H	1.64	0.61
3:B:21:GLU:HB2	3:B:204:HIS:O	1.99	0.61
3:B:221:VAL:CG2	3:B:222:PRO:HD2	2.31	0.61
2:C:58:LYS:HB3	2:C:61:SER:HB2	1.83	0.60
3:B:234:TYR:HB2	3:B:325:ALA:O	2.01	0.60
1:A:73:LEU:HD12	1:A:73:LEU:H	1.66	0.60
3:B:155:ILE:HD12	3:B:175:MET:HE2	1.84	0.60
2:C:237:LEU:H	2:C:304:ARG:HH22	1.48	0.60
3:B:316:SER:C	3:B:318:LYS:H	2.08	0.60
2:C:255:LEU:CG	2:C:256:THR:H	2.13	0.60
3:B:67:LEU:N	3:B:68:PRO:CA	2.64	0.60
3:B:85:LEU:HD12	3:B:86:LEU:H	1.67	0.59
3:B:37:ASN:O	3:B:38:TYR:HB2	2.00	0.59
2:C:228:SER:N	2:C:229:PRO:HD3	2.17	0.59
2:C:128:ILE:O	2:C:129:LEU:HD12	2.03	0.59
2:C:263:ALA:O	2:C:264:ASN:HB2	2.03	0.59
2:C:109:GLU:HG3	2:C:110:LEU:H	1.66	0.59
3:B:74:LYS:HG3	3:B:74:LYS:O	2.03	0.59
2:C:128:ILE:C	2:C:129:LEU:HD12	2.28	0.59
2:C:327:THR:CG2	2:C:328:VAL:N	2.66	0.59
3:B:9:LEU:HA	3:B:106:ALA:O	2.03	0.59
1:A:20:MET:HE2	1:A:62:LEU:HD13	1.85	0.59
3:B:221:VAL:HG12	3:B:251:SER:OG	2.03	0.59
3:B:310:TYR:OH	3:B:326:LYS:HE3	2.02	0.58
2:C:271:ALA:H	2:C:273:PRO:HD2	1.67	0.58
3:B:81:PHE:CD1	3:B:81:PHE:N	2.71	0.58
2:C:247:VAL:O	2:C:293:ILE:HG23	2.04	0.58
2:C:223:ILE:HG13	3:B:226:HIS:CD2	2.38	0.58
3:B:55:GLN:HB2	4:D:1:NAG:H81	1.86	0.58
1:A:30:HIS:CG	2:C:140:PRO:HB3	2.39	0.58
2:C:86:LEU:O	2:C:89:ASP:HB2	2.04	0.58
1:A:6:LEU:HD22	1:A:7:ASN:N	2.18	0.58
1:A:69:LEU:HD23	1:A:69:LEU:N	2.16	0.58
1:A:18:LEU:HD11	1:A:132:VAL:HG21	1.86	0.58
2:C:76:GLN:CB	2:C:81:TRP:HE1	2.17	0.58
2:C:139:CYS:CB	2:C:177:THR:HG22	2.33	0.58
2:C:239:SER:HB3	2:C:302:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HE3	3:B:185:SER:HA	1.85	0.57
1:A:22:GLY:HA3	1:A:24:TYR:H	1.69	0.57
2:C:20:ARG:HD3	2:C:21:HIS:O	2.03	0.57
1:A:86:ASP:O	1:A:90:TYR:HD1	1.88	0.57
2:C:98:ARG:HB3	2:C:98:ARG:NH1	2.20	0.57
3:B:264:ILE:O	3:B:265:ASP:HB2	2.03	0.57
2:C:65:VAL:N	2:C:66:PRO:CA	2.68	0.57
2:C:180:LEU:HD11	3:B:134:GLY:O	2.05	0.56
2:C:234:SER:O	2:C:235:ALA:HB2	2.06	0.56
3:B:54:ARG:HA	3:B:90:GLY:HA3	1.86	0.56
2:C:229:PRO:HA	2:C:324:LEU:HD21	1.87	0.56
2:C:129:LEU:CD2	2:C:135:GLY:HA3	2.36	0.56
2:C:238:GLY:HA3	2:C:240:ARG:HH11	1.71	0.56
3:B:224:VAL:CG1	3:B:249:TYR:HB3	2.34	0.56
1:A:28:ALA:O	1:A:128:GLU:O	2.24	0.56
3:B:164:ILE:HA	3:B:167:PHE:CE1	2.41	0.56
2:C:64:THR:CB	2:C:66:PRO:HA	2.35	0.56
2:C:227:ILE:C	2:C:229:PRO:HD3	2.31	0.56
2:C:74:TRP:CD1	2:C:75:ALA:N	2.74	0.55
3:B:227:SER:HB2	3:B:247:THR:H	1.71	0.55
2:C:131:LEU:HA	2:C:184:VAL:CG1	2.35	0.55
2:C:64:THR:HB	2:C:66:PRO:CA	2.35	0.55
2:C:72:ARG:NH1	2:C:84:PRO:HD2	2.21	0.55
2:C:42:TYR:HB2	2:C:44:LEU:HD13	1.88	0.55
3:B:80:TRP:CE3	3:B:82:ARG:HD2	2.42	0.55
3:B:197:PRO:HA	3:B:201:ARG:O	2.06	0.55
2:C:98:ARG:HB3	2:C:98:ARG:HH11	1.71	0.55
3:B:298:ILE:HG22	3:B:299:LYS:O	2.07	0.55
2:C:58:LYS:HG3	2:C:59:ASN:N	2.19	0.55
2:C:49:SER:O	2:C:50:PRO:C	2.50	0.55
2:C:214:ARG:NH1	2:C:214:ARG:CG	2.68	0.55
2:C:260:TRP:HE3	2:C:314:VAL:HG11	1.71	0.55
2:C:236:SER:O	2:C:237:LEU:HB3	2.07	0.54
3:B:155:ILE:CD1	3:B:175:MET:HE2	2.37	0.54
1:A:36:MET:HA	1:A:36:MET:HE2	1.90	0.54
1:A:99:PHE:N	1:A:99:PHE:HD2	2.06	0.54
2:C:87:GLN:O	2:C:88:GLU:CB	2.56	0.54
2:C:302:VAL:O	2:C:303:THR:HG23	2.08	0.54
2:C:327:THR:HG22	2:C:328:VAL:H	1.72	0.54
1:A:56:ILE:HG12	2:C:316:HIS:NE2	2.23	0.54
2:C:129:LEU:HD23	2:C:135:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:268:LYS:O	3:B:269:PRO:O	2.25	0.54
3:B:316:SER:O	3:B:318:LYS:HD2	2.08	0.54
2:C:219:LYS:HA	2:C:219:LYS:CE	2.37	0.54
2:C:123:ILE:HD12	2:C:123:ILE:N	2.23	0.53
3:B:86:LEU:HA	3:B:111:VAL:HG11	1.89	0.53
3:B:311:VAL:HG13	3:B:322:ALA:O	2.08	0.53
3:B:96:LEU:O	3:B:102:CYS:HA	2.08	0.53
2:C:16:ARG:CG	2:C:104:ASP:HB3	2.33	0.53
2:C:65:VAL:N	2:C:66:PRO:HA	2.23	0.53
2:C:225:VAL:HG11	3:B:229:ASN:ND2	2.24	0.53
1:A:20:MET:HG2	1:A:21:SER:N	2.23	0.52
1:A:99:PHE:N	1:A:99:PHE:CD2	2.77	0.52
2:C:76:GLN:HB2	2:C:81:TRP:NE1	2.23	0.52
2:C:253:THR:O	2:C:255:LEU:HD22	2.09	0.52
2:C:99:ASN:O	2:C:100:ALA:C	2.53	0.52
2:C:196:LEU:HD12	2:C:197:THR:N	2.23	0.52
2:C:283:GLN:O	2:C:294:GLU:HA	2.09	0.52
1:A:36:MET:HA	1:A:36:MET:CE	2.39	0.52
1:A:63:LYS:HD2	1:A:64:GLU:HB3	1.92	0.52
3:B:66:ARG:C	3:B:68:PRO:HA	2.34	0.52
3:B:114:LYS:NZ	3:B:206:THR:HG21	2.25	0.52
2:C:308:HIS:O	2:C:309:MET:HG2	2.10	0.51
1:A:6:LEU:C	1:A:6:LEU:HD13	2.35	0.51
3:B:317:ALA:O	3:B:318:LYS:HG3	2.11	0.51
3:B:219:ASN:N	3:B:219:ASN:OD1	2.44	0.51
3:B:299:LYS:HB2	3:B:299:LYS:HZ2	1.76	0.51
2:C:268:ILE:HG23	2:C:268:ILE:O	2.11	0.51
3:B:194:VAL:HG13	3:B:205:LEU:HB2	1.91	0.51
3:B:295:ILE:O	3:B:296:LEU:HD23	2.11	0.51
3:B:63:ILE:HG22	3:B:67:LEU:HD22	1.93	0.51
1:A:41:VAL:CG2	1:A:151:VAL:HG11	2.41	0.51
2:C:176:THR:HG22	2:C:177:THR:N	2.21	0.51
2:C:123:ILE:O	2:C:123:ILE:HG22	2.11	0.51
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.25	0.50
2:C:99:ASN:O	2:C:102:TYR:O	2.28	0.50
3:B:29:LEU:O	3:B:33:PHE:HA	2.11	0.50
1:A:6:LEU:HD22	1:A:7:ASN:H	1.75	0.50
1:A:10:LEU:HD23	1:A:148:MET:HB2	1.93	0.50
1:A:85:VAL:HB	1:A:90:TYR:CE1	2.46	0.50
2:C:266:THR:O	2:C:267:HIS:CB	2.60	0.50
1:A:12:ASP:OD2	1:A:16:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:281:SER:O	3:B:282:ILE:HG13	2.11	0.50
2:C:81:TRP:CD1	2:C:81:TRP:N	2.79	0.50
3:B:9:LEU:CD1	3:B:11:THR:HG23	2.41	0.50
3:B:16:GLN:HG2	3:B:112:VAL:HG21	1.92	0.50
3:B:53:THR:O	3:B:54:ARG:HB3	2.10	0.50
2:C:64:THR:C	2:C:66:PRO:HA	2.36	0.50
3:B:18:PHE:CD1	3:B:114:LYS:HB2	2.47	0.50
3:B:64:ASN:C	3:B:64:ASN:OD1	2.55	0.50
2:C:61:SER:CA	2:C:63:ARG:HH12	2.25	0.49
3:B:204:HIS:O	3:B:205:LEU:HD12	2.12	0.49
1:A:50:GLU:H	1:A:57:PRO:HG2	1.77	0.49
3:B:316:SER:C	3:B:318:LYS:N	2.70	0.49
2:C:38:PRO:O	2:C:40:VAL:N	2.45	0.49
2:C:147:ARG:NH1	2:C:147:ARG:CG	2.74	0.49
2:C:254:PRO:HB3	2:C:284:GLU:OE2	2.12	0.49
2:C:328:VAL:O	2:C:329:LYS:HD3	2.12	0.49
2:C:36:ARG:HH12	2:C:43:TRP:H	1.60	0.49
2:C:120:LEU:HD21	2:C:193:ARG:NH1	2.28	0.49
2:C:223:ILE:H	2:C:223:ILE:CD1	2.25	0.49
2:C:272:TYR:CE2	2:C:277:VAL:HG21	2.48	0.49
2:C:42:TYR:HB2	2:C:44:LEU:CD1	2.43	0.49
2:C:212:GLU:O	2:C:212:GLU:HG3	2.10	0.49
3:B:209:LEU:N	3:B:209:LEU:HD13	2.28	0.49
2:C:328:VAL:O	2:C:329:LYS:CB	2.60	0.49
3:B:114:LYS:HZ2	3:B:206:THR:HG21	1.78	0.49
2:C:23:LYS:NZ	2:C:23:LYS:HB2	2.28	0.49
3:B:46:LEU:N	3:B:46:LEU:HD23	2.27	0.49
3:B:142:ASN:HB3	3:B:207:ARG:NH1	2.28	0.49
2:C:256:THR:HG23	2:C:317:ASN:HB2	1.94	0.48
3:B:245:PRO:HA	3:B:295:ILE:HG23	1.94	0.48
1:A:127:ALA:HB3	1:A:130:MET:HG2	1.95	0.48
2:C:45:TRP:CD2	2:C:48:VAL:HG21	2.47	0.48
2:C:223:ILE:HD13	2:C:223:ILE:N	2.27	0.48
3:B:71:ARG:HH12	3:B:85:LEU:HB3	1.79	0.48
3:B:216:SER:HB3	3:B:218:LYS:HB3	1.96	0.48
2:C:42:TYR:C	2:C:44:LEU:H	2.21	0.48
2:C:76:GLN:HB3	2:C:81:TRP:HE1	1.76	0.48
2:C:298:ILE:O	2:C:299:PHE:HD1	1.97	0.48
1:A:22:GLY:CA	1:A:24:TYR:H	2.26	0.48
2:C:129:LEU:HD13	2:C:213:LEU:HD13	1.95	0.48
1:A:66:ASN:O	1:A:85:VAL:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:LEU:C	2:C:80:LEU:HD12	2.39	0.48
2:C:99:ASN:C	2:C:101:SER:N	2.69	0.48
3:B:54:ARG:HG2	3:B:55:GLN:N	2.29	0.48
1:A:29:LEU:HD11	2:C:22:TYR:CE1	2.49	0.48
2:C:22:TYR:HD1	2:C:23:LYS:N	2.12	0.48
2:C:48:VAL:HG13	2:C:51:ARG:HG2	1.95	0.48
3:B:112:VAL:CG1	3:B:121:PRO:HD2	2.44	0.48
2:C:33:VAL:O	2:C:81:TRP:HA	2.13	0.48
2:C:40:VAL:CB	2:C:41:PRO:HD3	2.44	0.48
2:C:86:LEU:HB2	2:C:89:ASP:OD2	2.14	0.48
2:C:312:LYS:HE2	2:C:323:THR:OG1	2.14	0.48
2:C:223:ILE:HG12	2:C:223:ILE:O	2.13	0.48
2:C:131:LEU:HB3	2:C:215:ILE:HG21	1.95	0.47
3:B:215:GLY:N	3:B:287:THR:HG23	2.29	0.47
2:C:22:TYR:CD1	2:C:23:LYS:N	2.82	0.47
2:C:125:TYR:CG	2:C:140:PRO:HG2	2.49	0.47
2:C:328:VAL:O	2:C:329:LYS:HB3	2.13	0.47
1:A:20:MET:CE	1:A:62:LEU:HD13	2.43	0.47
2:C:108:ILE:H	2:C:108:ILE:HG12	1.62	0.47
3:B:28:PRO:O	3:B:29:LEU:HD23	2.15	0.47
3:B:271:ASP:O	3:B:272:ILE:HG12	2.13	0.47
2:C:245:CYS:H	2:C:296:PRO:HD2	1.79	0.47
2:C:188:ASP:O	2:C:213:LEU:HD23	2.14	0.47
2:C:237:LEU:N	2:C:304:ARG:HH22	2.11	0.47
2:C:154:ILE:HG23	2:C:195:VAL:H	1.79	0.47
3:B:112:VAL:HG13	3:B:121:PRO:HD2	1.96	0.47
1:A:151:VAL:HG22	1:A:152:SER:H	1.79	0.47
2:C:38:PRO:C	2:C:40:VAL:H	2.22	0.47
2:C:99:ASN:O	2:C:101:SER:N	2.47	0.47
3:B:198:GLU:HB3	3:B:203:PHE:HE2	1.79	0.47
3:B:270:ASP:HA	3:B:274:ILE:CG2	2.45	0.47
1:A:18:LEU:HD11	1:A:132:VAL:CG2	2.45	0.47
2:C:56:TRP:CH2	2:C:79:ALA:HA	2.50	0.47
3:B:196:TYR:HE2	3:B:205:LEU:HD13	1.77	0.47
3:B:97:ARG:HD3	3:B:98:ASN:N	2.30	0.47
1:A:78:PRO:HG2	1:A:120:TRP:CD2	2.50	0.47
2:C:241:LEU:HD23	2:C:300:ASP:OD2	2.15	0.47
3:B:26:LYS:HA	3:B:78:VAL:CG2	2.43	0.47
3:B:115:ASP:OD1	3:B:116:SER:N	2.48	0.47
3:B:159:MET:HE2	3:B:190:TYR:OH	2.15	0.47
2:C:161:LEU:O	2:C:163:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:279:GLU:O	2:C:279:GLU:HG2	2.15	0.46
3:B:138:ILE:O	3:B:176:ASN:HA	2.16	0.46
3:B:262:TRP:CD1	3:B:296:LEU:HD21	2.50	0.46
1:A:90:TYR:HB3	1:A:91:PRO:HA	1.96	0.46
2:C:23:LYS:HG3	2:C:23:LYS:O	2.15	0.46
3:B:242:LEU:HD23	3:B:298:ILE:HG13	1.97	0.46
1:A:3:VAL:CG2	1:A:91:PRO:HB2	2.46	0.46
1:A:16:LYS:HZ3	1:A:126:GLN:HA	1.81	0.46
2:C:272:TYR:N	2:C:273:PRO:CD	2.79	0.46
3:B:291:THR:O	3:B:291:THR:OG1	2.34	0.46
3:B:311:VAL:HG11	3:B:321:VAL:HG23	1.98	0.46
2:C:36:ARG:NH1	2:C:41:PRO:HG2	2.30	0.46
2:C:76:GLN:HB2	2:C:81:TRP:HE1	1.81	0.46
3:B:209:LEU:O	3:B:209:LEU:HD22	2.15	0.46
2:C:21:HIS:ND1	2:C:38:PRO:HB3	2.31	0.45
2:C:76:GLN:HG3	2:C:77:ASP:H	1.81	0.45
2:C:237:LEU:H	2:C:304:ARG:NH2	2.14	0.45
1:A:94:LYS:N	1:A:94:LYS:CD	2.75	0.45
1:A:110:LEU:HD12	1:A:110:LEU:O	2.16	0.45
3:B:228:PRO:HB2	3:B:322:ALA:HB1	1.99	0.45
1:A:78:PRO:HG2	1:A:120:TRP:CE2	2.51	0.45
2:C:146:THR:HG22	2:C:146:THR:O	2.17	0.45
2:C:263:ALA:HA	2:C:311:PHE:CD1	2.51	0.45
3:B:25:ILE:O	3:B:78:VAL:HG13	2.16	0.45
2:C:42:TYR:N	2:C:42:TYR:CD2	2.84	0.45
2:C:94:VAL:HA	2:C:106:MET:O	2.15	0.45
3:B:142:ASN:HB3	3:B:207:ARG:HH11	1.82	0.45
1:A:29:LEU:H	1:A:29:LEU:HD23	1.81	0.45
2:C:104:ASP:C	2:C:105:LYS:HG3	2.41	0.45
3:B:310:TYR:N	3:B:310:TYR:CD2	2.84	0.45
3:B:189:ASN:N	3:B:189:ASN:ND2	2.64	0.45
3:B:236:LYS:NZ	3:B:242:LEU:HA	2.32	0.45
2:C:225:VAL:HG11	3:B:229:ASN:HD21	1.82	0.44
3:B:37:ASN:O	3:B:38:TYR:CB	2.64	0.44
2:C:136:VAL:HG21	2:C:178:HIS:HB3	1.99	0.44
3:B:32:HIS:O	3:B:33:PHE:C	2.60	0.44
3:B:140:CYS:HB2	3:B:175:MET:HG3	1.99	0.44
2:C:129:LEU:O	2:C:215:ILE:HA	2.17	0.44
3:B:122:MET:HE2	3:B:122:MET:HB3	1.63	0.44
2:C:58:LYS:HG2	2:C:61:SER:H	1.82	0.44
2:C:93:TYR:N	2:C:93:TYR:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:LEU:HD11	2:C:110:LEU:HD12	1.99	0.44
2:C:194:CYS:HB2	2:C:209:ARG:HB2	1.99	0.44
2:C:231:LYS:HE3	2:C:233:ILE:CD1	2.44	0.44
2:C:231:LYS:O	2:C:232:THR:C	2.60	0.44
3:B:157:TRP:HZ2	3:B:175:MET:O	2.01	0.44
3:B:243:LEU:HD12	3:B:243:LEU:O	2.18	0.44
3:B:107:PHE:HA	3:B:108:PRO:HD2	1.85	0.44
1:A:31:LEU:CB	1:A:36:MET:HE3	2.39	0.44
2:C:92:THR:C	2:C:93:TYR:CD1	2.96	0.44
3:B:224:VAL:HG13	3:B:224:VAL:O	2.17	0.44
1:A:29:LEU:N	1:A:29:LEU:CD2	2.81	0.44
2:C:99:ASN:ND2	2:C:101:SER:HB2	2.33	0.44
3:B:253:LEU:HB2	3:B:256:SER:HB2	2.00	0.44
2:C:236:SER:O	2:C:237:LEU:CB	2.66	0.44
3:B:7:TRP:HZ2	3:B:32:HIS:CD2	2.36	0.44
3:B:54:ARG:CG	3:B:55:GLN:N	2.81	0.44
1:A:74:LYS:HB2	1:A:79:THR:OG1	2.18	0.43
2:C:124:SER:HA	2:C:210:SER:O	2.18	0.43
2:C:139:CYS:HA	2:C:140:PRO:HD3	1.78	0.43
3:B:198:GLU:HB3	3:B:203:PHE:CE2	2.53	0.43
2:C:268:ILE:O	2:C:268:ILE:CG2	2.65	0.43
3:B:274:ILE:O	3:B:275:ASP:C	2.61	0.43
4:E:1:NAG:H61	4:E:2:NAG:N2	2.34	0.43
2:C:113:PHE:CD2	2:C:119:PHE:CD1	3.07	0.43
3:B:323:LYS:H	3:B:323:LYS:HG2	1.54	0.43
1:A:92:LYS:O	1:A:95:MET:HE3	2.19	0.43
1:A:121:TYR:O	1:A:135:GLY:N	2.50	0.43
2:C:268:ILE:HD11	2:C:298:ILE:CD1	2.48	0.43
3:B:157:TRP:CZ3	3:B:192:CYS:HB3	2.54	0.43
1:A:36:MET:HG3	2:C:126:PRO:HG2	1.99	0.43
2:C:36:ARG:HH12	2:C:41:PRO:C	2.27	0.43
2:C:149:LYS:HD2	2:C:149:LYS:HA	1.71	0.43
2:C:314:VAL:O	2:C:314:VAL:HG12	2.19	0.43
1:A:69:LEU:H	1:A:69:LEU:CD2	2.18	0.43
2:C:123:ILE:O	2:C:123:ILE:CG2	2.67	0.43
2:C:151:ASP:O	2:C:175:GLY:HA2	2.19	0.43
2:C:272:TYR:N	2:C:273:PRO:HD3	2.33	0.43
2:C:31:GLU:HB2	2:C:32:PRO:HD2	2.00	0.43
2:C:240:ARG:O	2:C:240:ARG:HG2	2.18	0.43
1:A:18:LEU:HD13	1:A:18:LEU:HA	1.74	0.42
3:B:48:LEU:HA	3:B:96:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:82:ARG:HA	3:B:83:PRO:HA	1.83	0.42
3:B:222:PRO:HG3	3:B:318:LYS:HG2	2.01	0.42
3:B:229:ASN:ND2	3:B:231:HIS:HB2	2.33	0.42
1:A:63:LYS:O	1:A:64:GLU:HG2	2.19	0.42
2:C:227:ILE:O	2:C:227:ILE:CG2	2.63	0.42
2:C:260:TRP:O	2:C:314:VAL:HB	2.18	0.42
2:C:312:LYS:HG2	2:C:323:THR:OG1	2.20	0.42
1:A:63:LYS:C	1:A:65:LYS:N	2.75	0.42
3:B:225:ILE:HG21	3:B:322:ALA:HB3	2.00	0.42
1:A:63:LYS:C	1:A:65:LYS:H	2.28	0.42
2:C:65:VAL:HG12	2:C:65:VAL:O	2.19	0.42
2:C:252:GLY:HA2	2:C:292:TYR:HB2	2.01	0.42
3:B:7:TRP:CZ2	3:B:32:HIS:CD2	3.07	0.42
3:B:25:ILE:HG21	3:B:107:PHE:CE2	2.55	0.42
3:B:148:PRO:HG2	3:B:151:VAL:HG13	2.00	0.42
3:B:244:ILE:O	3:B:295:ILE:HA	2.19	0.42
1:A:120:TRP:HB3	1:A:134:LEU:HD12	1.99	0.42
2:C:158:LYS:HG2	2:C:192:TYR:CE2	2.54	0.42
2:C:245:CYS:HB2	2:C:261:TRP:CZ3	2.54	0.42
3:B:67:LEU:HG	3:B:72:ILE:HG13	2.00	0.42
1:A:34:GLN:O	2:C:24:ARG:NH2	2.53	0.42
3:B:158:TYR:CD2	3:B:163:LYS:HA	2.54	0.42
1:A:74:LYS:HD2	1:A:74:LYS:HA	1.73	0.42
2:C:139:CYS:HB3	2:C:177:THR:CG2	2.47	0.42
3:B:257:ARG:H	3:B:257:ARG:HD2	1.85	0.42
2:C:54:LEU:O	2:C:55:THR:HG23	2.20	0.42
2:C:266:THR:O	2:C:267:HIS:HB2	2.20	0.42
2:C:109:GLU:CG	2:C:110:LEU:N	2.82	0.41
3:B:97:ARG:HD3	3:B:97:ARG:C	2.45	0.41
1:A:1:ALA:HA	1:A:2:PRO:HD3	1.83	0.41
1:A:47:VAL:HG13	1:A:95:MET:H	1.86	0.41
2:C:62:ALA:N	2:C:63:ARG:HH12	2.17	0.41
2:C:37:CYS:HA	2:C:38:PRO:HD3	1.89	0.41
2:C:64:THR:HB	2:C:66:PRO:O	2.20	0.41
2:C:81:TRP:C	2:C:82:LEU:HD12	2.45	0.41
2:C:83:LEU:HA	2:C:84:PRO:HA	1.77	0.41
2:C:168:GLU:H	2:C:168:GLU:HG2	1.66	0.41
3:B:98:ASN:HB3	3:B:101:TYR:HB2	2.03	0.41
1:A:60:LEU:H	1:A:60:LEU:HD23	1.86	0.41
1:A:73:LEU:HD12	1:A:73:LEU:N	2.33	0.41
3:B:245:PRO:HA	3:B:294:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CD1	1:A:58:VAL:HG12	2.47	0.41
2:C:68:GLU:OE2	2:C:71:THR:HA	2.21	0.41
2:C:156:TRP:HZ2	2:C:177:THR:O	2.04	0.41
2:C:158:LYS:HB2	2:C:163:LEU:HD11	2.03	0.41
2:C:219:LYS:HE3	2:C:219:LYS:CA	2.46	0.41
2:C:231:LYS:O	2:C:233:ILE:N	2.54	0.41
3:B:114:LYS:HB3	3:B:114:LYS:HE2	1.61	0.41
3:B:134:GLY:O	3:B:180:LEU:O	2.38	0.41
3:B:155:ILE:HD13	3:B:175:MET:HA	2.01	0.41
1:A:90:TYR:CD1	1:A:90:TYR:N	2.89	0.41
2:C:16:ARG:O	2:C:104:ASP:HA	2.21	0.41
2:C:300:ASP:OD2	2:C:300:ASP:N	2.54	0.41
3:B:95:MET:CA	3:B:103:SER:O	2.67	0.41
3:B:236:LYS:HD2	3:B:240:GLU:CB	2.51	0.41
2:C:22:TYR:HD1	2:C:23:LYS:H	1.67	0.41
2:C:58:LYS:HB3	2:C:61:SER:O	2.20	0.41
2:C:102:TYR:HD2	2:C:103:CYS:N	2.18	0.41
1:A:61:GLY:HA3	1:A:68:TYR:CD2	2.56	0.41
2:C:38:PRO:C	2:C:40:VAL:N	2.77	0.41
2:C:117:ASP:OD2	2:C:120:LEU:HD22	2.21	0.41
2:C:223:ILE:HA	2:C:224:PRO:HD3	1.89	0.41
2:C:265:ASP:OD2	2:C:265:ASP:N	2.53	0.41
3:B:158:TYR:HB2	3:B:191:THR:HG23	2.01	0.41
3:B:287:THR:O	3:B:287:THR:HG22	2.21	0.41
1:A:30:HIS:CB	2:C:140:PRO:HB3	2.51	0.41
1:A:111:GLU:HG2	1:A:145:ASP:HB3	2.03	0.41
2:C:234:SER:O	2:C:235:ALA:CB	2.69	0.41
2:C:237:LEU:C	2:C:239:SER:H	2.28	0.41
3:B:72:ILE:HG22	3:B:72:ILE:O	2.21	0.41
3:B:98:ASN:C	3:B:100:THR:N	2.76	0.41
2:C:36:ARG:NH1	2:C:43:TRP:H	2.19	0.40
2:C:123:ILE:N	2:C:123:ILE:CD1	2.83	0.40
1:A:93:LYS:HB2	1:A:94:LYS:HD3	2.03	0.40
2:C:198:PHE:O	2:C:204:GLN:HA	2.21	0.40
4:D:1:NAG:H61	4:D:2:NAG:C7	2.51	0.40
3:B:184:ILE:HD13	3:B:286:ARG:HD3	2.03	0.40
3:B:236:LYS:HD2	3:B:240:GLU:HB2	2.04	0.40
2:C:231:LYS:HB3	2:C:327:THR:H	1.87	0.40
2:C:238:GLY:O	2:C:239:SER:HB2	2.22	0.40
3:B:287:THR:O	3:B:288:GLU:CB	2.69	0.40
3:B:105:VAL:HG22	3:B:106:ALA:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/158 (95%)	134 (89%)	14 (9%)	2 (1%)	9	35
2	C	314/339 (93%)	254 (81%)	41 (13%)	19 (6%)	1	9
3	B	321/339 (95%)	271 (84%)	42 (13%)	8 (2%)	4	23
All	All	785/836 (94%)	659 (84%)	97 (12%)	29 (4%)	2	17

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
2	C	50	PRO
2	C	236	SER
2	C	244	PRO
2	C	264	ASN
2	C	268	ILE
2	C	329	LYS
3	B	38	TYR
3	B	265	ASP
3	B	269	PRO
2	C	151	ASP
2	C	152	VAL
2	C	232	THR
2	C	235	ALA
3	B	272	ILE
2	C	39	GLN
2	C	77	ASP
2	C	88	GLU
2	C	150	THR
2	C	255	LEU
2	C	271	ALA

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Mol	Chain	Res	Type
3	B	273	THR
2	C	273	PRO
3	B	159	MET
3	B	268	LYS
2	C	141	ASP
1	A	22	GLY
2	C	41	PRO
3	B	160	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/143 (97%)	117 (84%)	22 (16%)	2	12
2	C	287/304 (94%)	224 (78%)	63 (22%)	1	5
3	B	299/314 (95%)	248 (83%)	51 (17%)	2	10
All	All	725/761 (95%)	589 (81%)	136 (19%)	1	7

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	ARG
1	A	18	LEU
1	A	29	LEU
1	A	36	MET
1	A	48	GLN
1	A	50	GLU
1	A	53	ASN
1	A	63	LYS
1	A	69	LEU
1	A	71	CYS
1	A	73	LEU
1	A	89	ASN
1	A	93	LYS

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Mol	Chain	Res	Type
1	A	97	LYS
1	A	99	PHE
1	A	107	ASN
1	A	110	LEU
1	A	124	THR
1	A	134	LEU
1	A	137	THR
1	A	145	ASP
2	C	20	ARG
2	C	23	LYS
2	C	35	LEU
2	C	42	TYR
2	C	43	TRP
2	C	48	VAL
2	C	55	THR
2	C	57	HIS
2	C	63	ARG
2	C	72	ARG
2	C	77	ASP
2	C	83	LEU
2	C	86	LEU
2	C	88	GLU
2	C	90	SER
2	C	94	VAL
2	C	102	TYR
2	C	108	ILE
2	C	115	ASN
2	C	120	LEU
2	C	130	THR
2	C	138	VAL
2	C	144	GLU
2	C	151	ASP
2	C	161	LEU
2	C	177	THR
2	C	179	LEU
2	C	180	LEU
2	C	201	GLU
2	C	208	THR
2	C	210	SER
2	C	212	GLU
2	C	214	ARG
2	C	219	LYS

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Mol	Chain	Res	Type
2	C	221	GLU
2	C	223	ILE
2	C	225	VAL
2	C	231	LYS
2	C	232	THR
2	C	233	ILE
2	C	237	LEU
2	C	240	ARG
2	C	243	ILE
2	C	255	LEU
2	C	259	LEU
2	C	268	ILE
2	C	269	GLU
2	C	276	ARG
2	C	284	GLU
2	C	290	GLU
2	C	297	LEU
2	C	298	ILE
2	C	300	ASP
2	C	303	THR
2	C	304	ARG
2	C	307	LEU
2	C	308	HIS
2	C	314	VAL
2	C	315	VAL
2	C	318	THR
2	C	326	THR
2	C	328	VAL
2	C	329	LYS
3	B	9	LEU
3	B	11	THR
3	B	13	ARG
3	B	33	PHE
3	B	34	LEU
3	B	35	LYS
3	B	46	LEU
3	B	48	LEU
3	B	53	THR
3	B	58	ASP
3	B	60	GLU
3	B	61	GLU
3	B	65	PHE

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Mol	Chain	Res	Type
3	B	67	LEU
3	B	78	VAL
3	B	80	TRP
3	B	81	PHE
3	B	82	ARG
3	B	110	GLU
3	B	122	MET
3	B	128	LYS
3	B	133	TYR
3	B	140	CYS
3	B	155	ILE
3	B	161	CYS
3	B	175	MET
3	B	181	ILE
3	B	189	ASN
3	B	191	THR
3	B	194	VAL
3	B	206	THR
3	B	207	ARG
3	B	208	THR
3	B	209	LEU
3	B	219	ASN
3	B	225	ILE
3	B	233	VAL
3	B	242	LEU
3	B	257	ARG
3	B	270	ASP
3	B	272	ILE
3	B	282	ILE
3	B	284	HIS
3	B	291	THR
3	B	295	ILE
3	B	299	LYS
3	B	310	TYR
3	B	311	VAL
3	B	318	LYS
3	B	321	VAL
3	B	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
3	B	169	ASN
3	B	186	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	D	1	3,4	14,14,15	0.68	0	17,19,21	1.84	4 (23%)
4	NAG	D	2	4	14,14,15	0.53	0	17,19,21	1.54	3 (17%)
4	NAG	E	1	3,4	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
4	NAG	E	2	4	14,14,15	0.55	0	17,19,21	1.28	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	-4.94	116.29	122.90
4	D	2	NAG	C2-N2-C7	-3.75	117.87	122.90
4	E	2	NAG	C1-O5-C5	3.65	117.08	112.19
4	D	2	NAG	C1-O5-C5	3.52	116.90	112.19
4	D	1	NAG	C4-C3-C2	2.89	115.26	111.02
4	D	1	NAG	O4-C4-C5	2.67	115.90	109.32
4	D	1	NAG	C1-C2-N2	-2.41	106.64	110.43
4	D	2	NAG	O5-C1-C2	2.38	114.97	111.29
4	E	1	NAG	C4-C3-C2	2.26	114.33	111.02
4	E	2	NAG	C2-N2-C7	-2.08	120.11	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

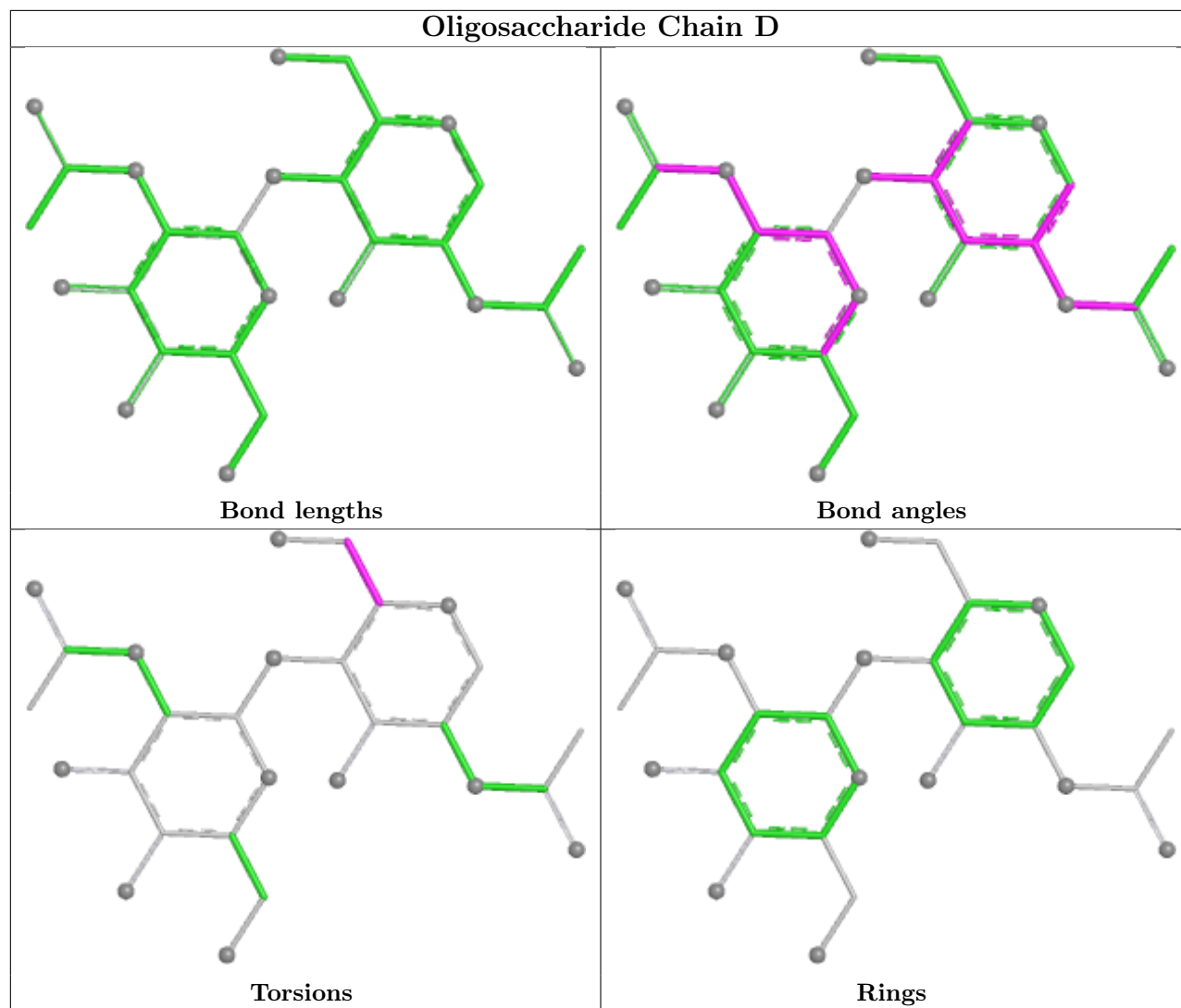
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

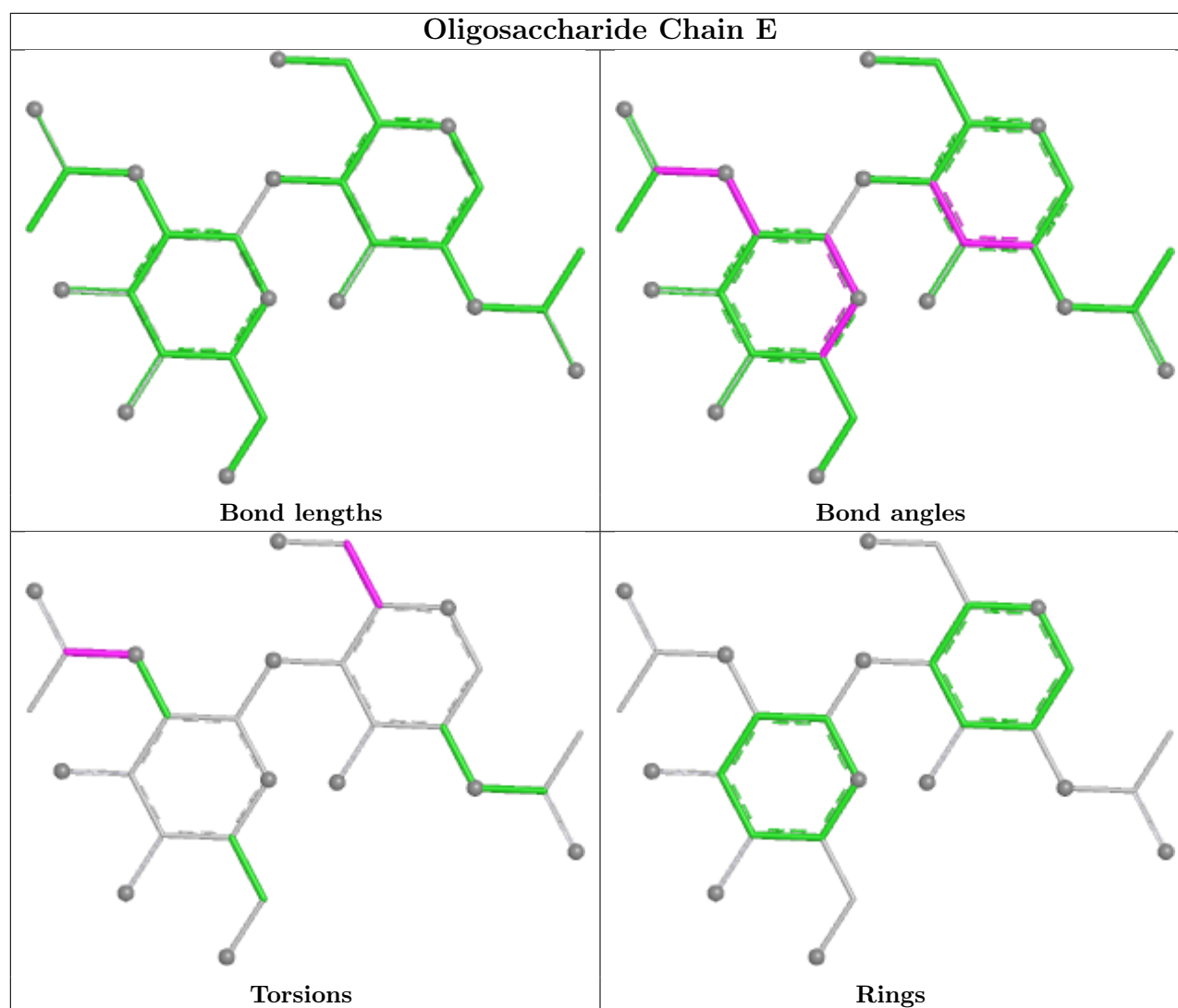
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	5	0
4	E	2	NAG	1	0
4	E	1	NAG	1	0
4	D	2	NAG	2	0

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





5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	NAG	B	337	3	14,14,15	0.53	0	17,19,21	0.77	0
5	NAG	C	337	2	14,14,15	0.58	0	17,19,21	1.13	2 (11%)
5	NAG	B	340	3	14,14,15	0.57	0	17,19,21	1.48	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	338	2	14,14,15	0.50	0	17,19,21	1.16	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
5	NAG	B	337	3	-	0/6/23/26	0/1/1/1
5	NAG	C	337	2	-	1/6/23/26	0/1/1/1
5	NAG	B	340	3	-	4/6/23/26	0/1/1/1
5	NAG	C	338	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	340	NAG	C1-O5-C5	3.73	117.19	112.19
5	B	340	NAG	C2-N2-C7	-3.70	117.94	122.90
5	C	338	NAG	C1-O5-C5	3.28	116.58	112.19
5	C	337	NAG	C1-O5-C5	2.62	115.69	112.19
5	C	337	NAG	C2-N2-C7	-2.57	119.45	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	340	NAG	C8-C7-N2-C2
5	B	340	NAG	O7-C7-N2-C2
5	B	340	NAG	C4-C5-C6-O6
5	B	340	NAG	O5-C5-C6-O6
5	C	337	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	152/158 (96%)	0.50	10 (6%) 24 16	53, 99, 166, 210	0
2	C	316/339 (93%)	0.99	51 (16%) 4 4	54, 139, 207, 253	0
3	B	323/339 (95%)	0.72	27 (8%) 17 13	46, 118, 199, 231	0
All	All	791/836 (94%)	0.78	88 (11%) 10 9	46, 122, 202, 253	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	40	VAL	6.4
3	B	8	GLY	5.1
2	C	50	PRO	4.6
3	B	4	CYS	4.4
2	C	256	THR	4.2
2	C	39	GLN	4.1
2	C	47	SER	4.0
2	C	302	VAL	3.8
3	B	32	HIS	3.8
3	B	34	LEU	3.6
2	C	160	SER	3.6
3	B	99	THR	3.5
2	C	152	VAL	3.5
3	B	29	LEU	3.5
2	C	71	THR	3.4
2	C	243	ILE	3.4
2	C	304	ARG	3.2
2	C	307	LEU	3.2
1	A	54	ASP	3.2
1	A	24	TYR	3.2
2	C	41	PRO	3.2
1	A	152	SER	3.1
3	B	80	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	15	CYS	3.1
3	B	33	PHE	3.1
2	C	319	LEU	3.0
1	A	66	ASN	3.0
2	C	234	SER	2.9
2	C	49	SER	2.9
3	B	100	THR	2.9
1	A	37	GLU	2.8
2	C	77	ASP	2.7
2	C	265	ASP	2.7
2	C	294	GLU	2.7
2	C	328	VAL	2.7
1	A	94	LYS	2.7
2	C	306	ASP	2.7
2	C	241	LEU	2.7
3	B	38	TYR	2.7
2	C	53	ASN	2.6
3	B	319	GLY	2.6
2	C	278	THR	2.6
3	B	77	ASP	2.6
3	B	325	ALA	2.6
3	B	316	SER	2.5
3	B	55	GLN	2.5
2	C	233	ILE	2.5
2	C	54	LEU	2.5
2	C	260	TRP	2.5
3	B	62	PRO	2.5
3	B	268	LYS	2.5
2	C	45	TRP	2.5
2	C	42	TYR	2.5
1	A	34	GLN	2.5
2	C	245	CYS	2.4
2	C	282	ARG	2.4
3	B	53	THR	2.4
2	C	296	PRO	2.4
1	A	21	SER	2.4
2	C	266	THR	2.4
2	C	201	GLU	2.4
2	C	244	PRO	2.4
3	B	317	ALA	2.3
2	C	151	ASP	2.3
2	C	257	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	303	THR	2.3
3	B	51	TYR	2.3
2	C	159	ASP	2.3
2	C	297	LEU	2.3
1	A	129	ASN	2.3
2	C	242	THR	2.3
2	C	308	HIS	2.2
2	C	272	TYR	2.2
3	B	24	ARG	2.2
3	B	9	LEU	2.2
2	C	109	GLU	2.2
1	A	48	GLN	2.1
3	B	324	ALA	2.1
3	B	277	THR	2.1
2	C	279	GLU	2.1
3	B	320	GLU	2.1
3	B	255	ASP	2.1
2	C	263	ALA	2.0
2	C	300	ASP	2.0
2	C	70	GLU	2.0
2	C	56	TRP	2.0
3	B	326	LYS	2.0
2	C	237	LEU	2.0

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

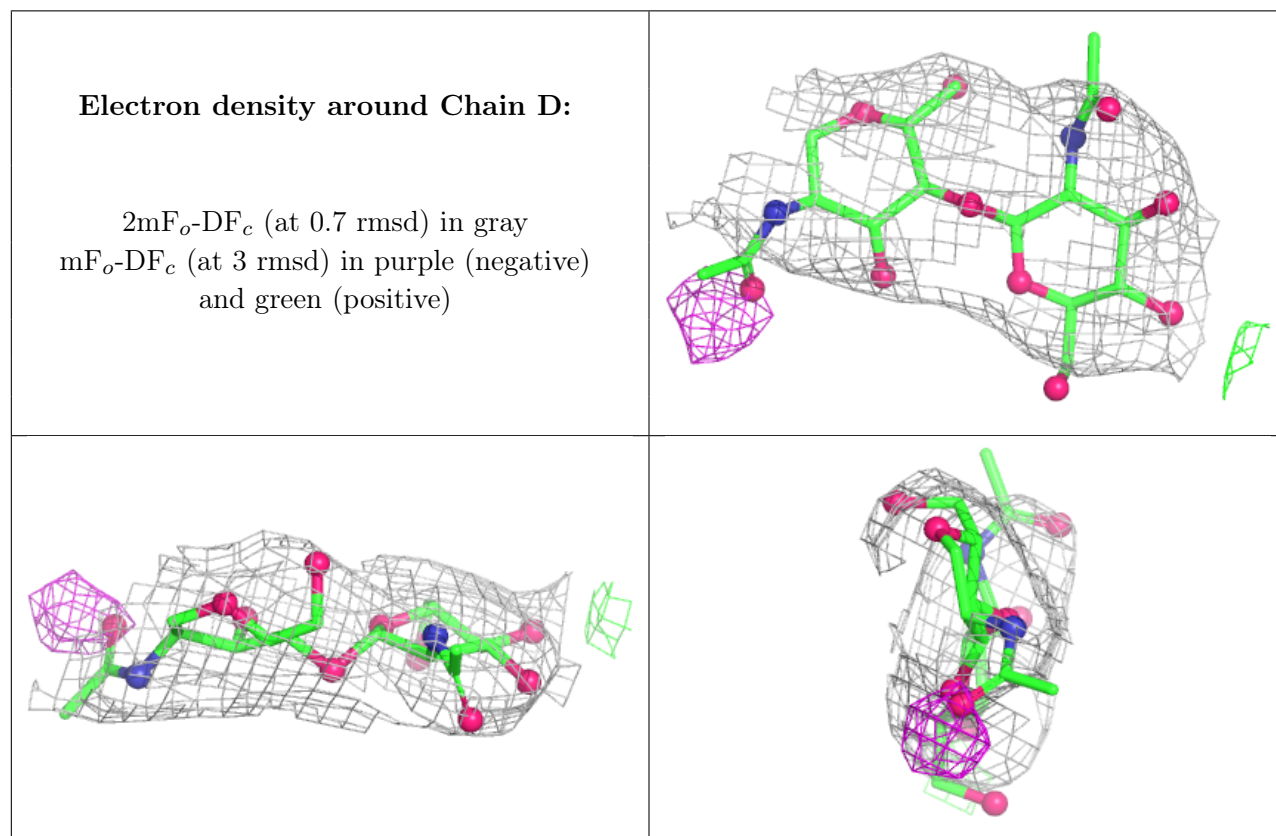
There are no non-standard protein/DNA/RNA residues in this entry.

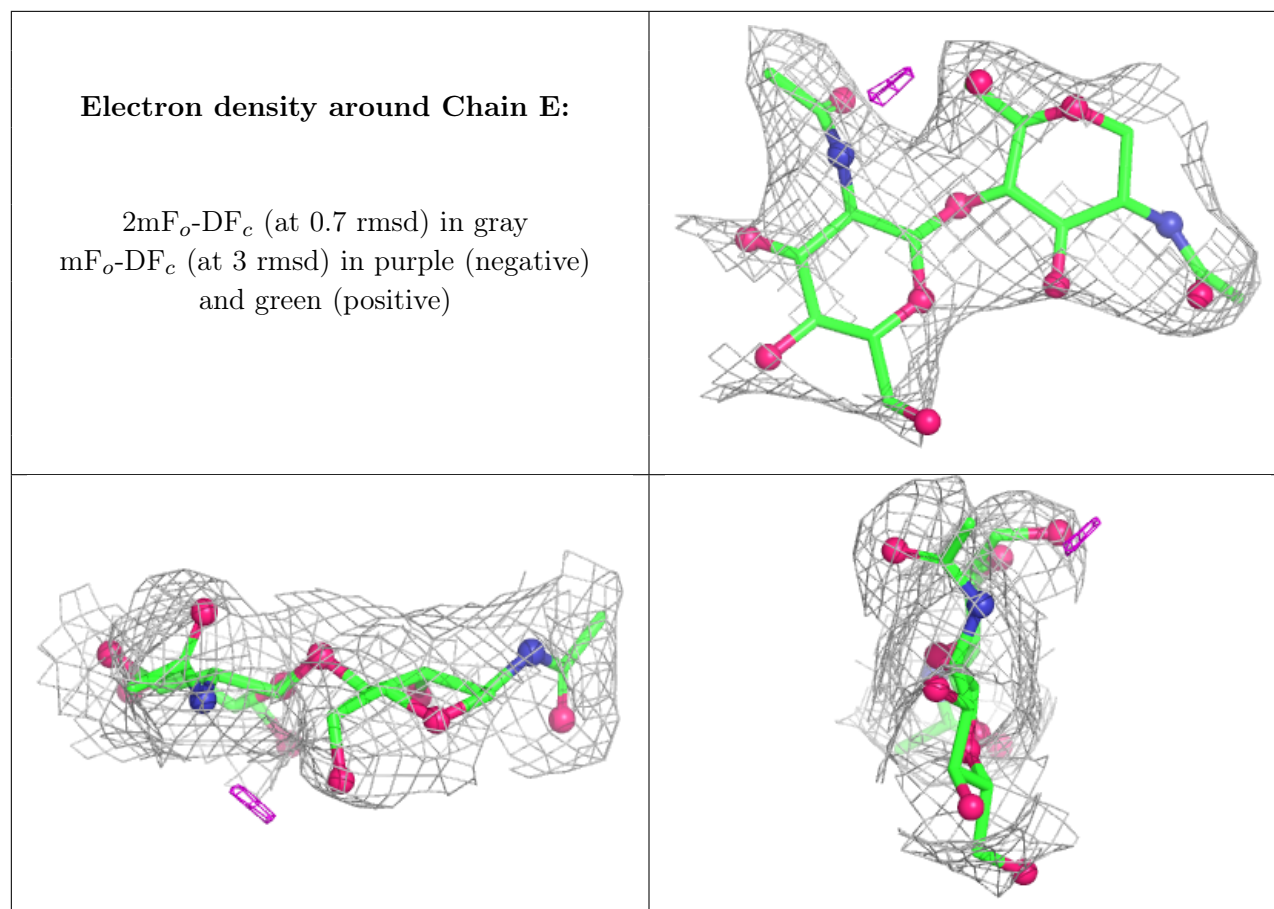
6.3 Carbohydrates [i](#)

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	E	2	14/15	0.68	0.12	114,118,119,121	0
4	NAG	D	2	14/15	0.78	0.11	142,148,154,155	0
4	NAG	E	1	14/15	0.83	0.13	116,118,120,122	0
4	NAG	D	1	14/15	0.87	0.14	148,154,159,161	0

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





6.4 Ligands [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
5	NAG	C	337	14/15	0.54	0.18	151,160,169,169	0
5	NAG	B	337	14/15	0.61	0.17	182,187,191,192	0
5	NAG	C	338	14/15	0.81	0.12	127,136,142,145	0
5	NAG	B	340	14/15	0.84	0.14	154,162,170,173	0

6.5 Other polymers [i](#)

There are no such residues in this entry.