



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:39 PM UTC

PDB ID : 1YK0 / pdb_00001yk0
Title : structure of natriuretic peptide receptor-C complexed with atrial natriuretic peptide
Authors : He, X.; Garcia, K.C.
Deposited on : 2005-01-16
Resolution : 2.40 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)
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

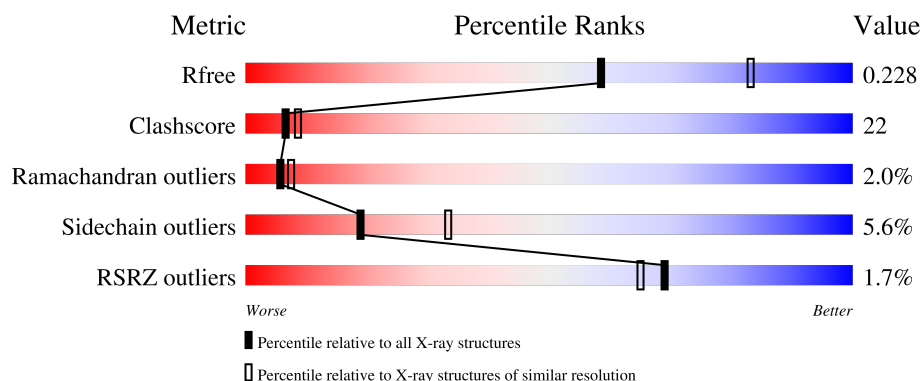
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



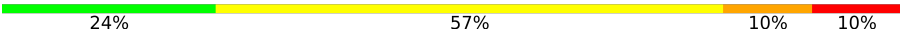
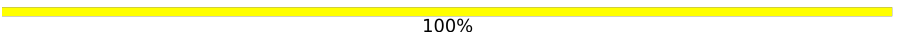
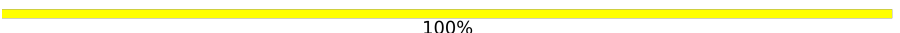
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	1-A	480	
1	1-B	480	
1	2-A	480	
1	2-B	480	
2	1-E	21	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2-E	21	
3	1-C	2	
3	2-C	2	

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	1-A	511	X	-	-	-
4	NAG	1-A	512	X	-	-	-
4	NAG	2-A	511	X	-	-	-
4	NAG	2-A	512	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13526 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.

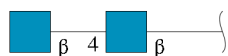
- Molecule 1 is a protein called Atrial natriuretic peptide clearance receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			
1	2-A	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			
1	1-B	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			
1	2-B	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			

- Molecule 2 is a protein called Atrial natriuretic factor.

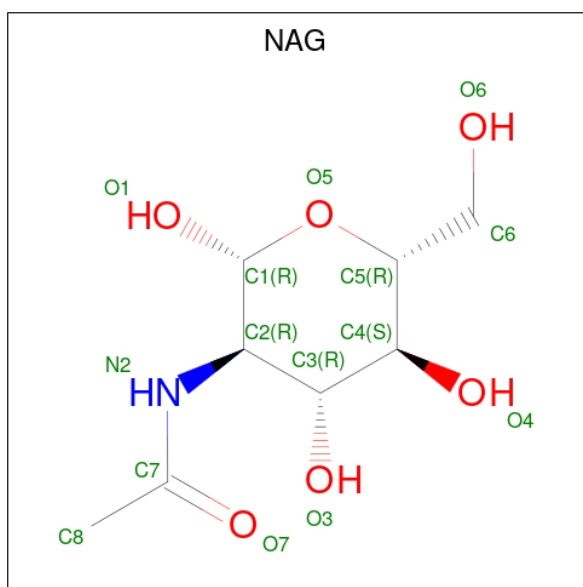
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-E	21	Total	C	N	O	S	0	0	0
			149	88	29	29	3			
2	2-E	21	Total	C	N	O	S	0	0	0
			149	88	29	29	3			

- Molecule 3 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
3	1-C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	2-C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	1-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	2-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	1-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	2-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	1-B	1	Total	C	N	O	0	0
			14	8	1	5		
4	2-B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	1	Total	Cl	0	0
			1	1		
5	2-A	1	Total	Cl	0	0
			1	1		
5	1-B	1	Total	Cl	0	0
			1	1		
5	2-B	1	Total	Cl	0	0
			1	1		

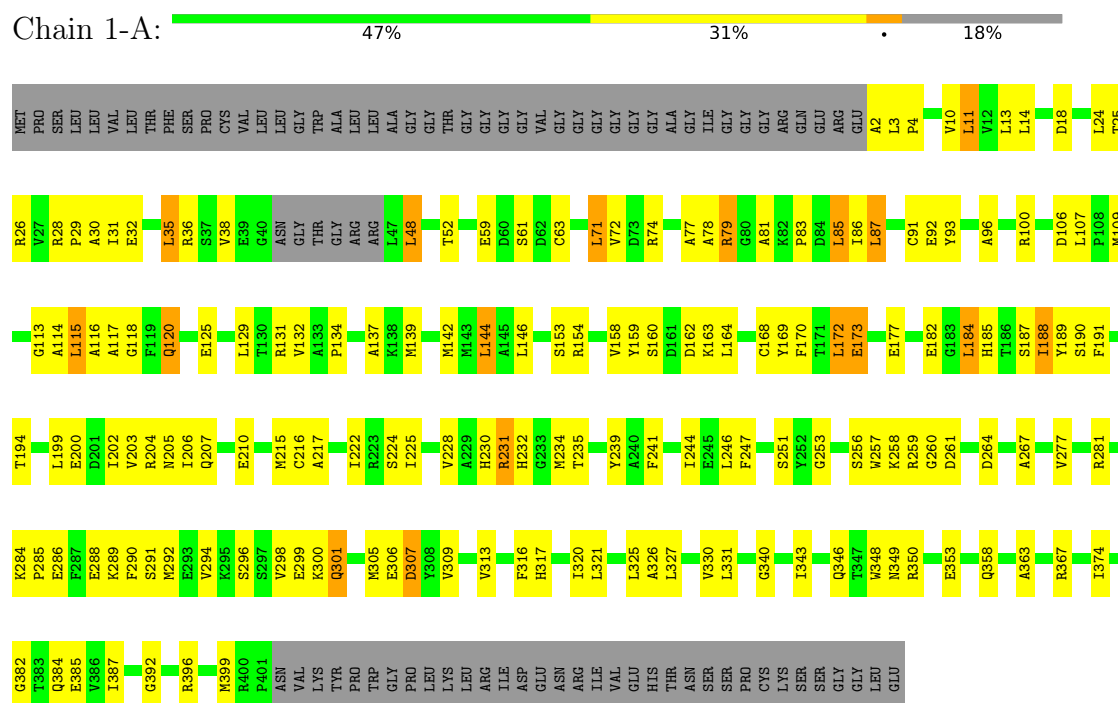
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	167	Total 167	O 167	0	0
6	2-A	168	Total 168	O 168	0	0
6	1-B	152	Total 152	O 152	0	0
6	2-B	151	Total 151	O 151	0	0
6	1-E	1	Total 1	O 1	0	0
6	2-E	1	Total 1	O 1	0	0

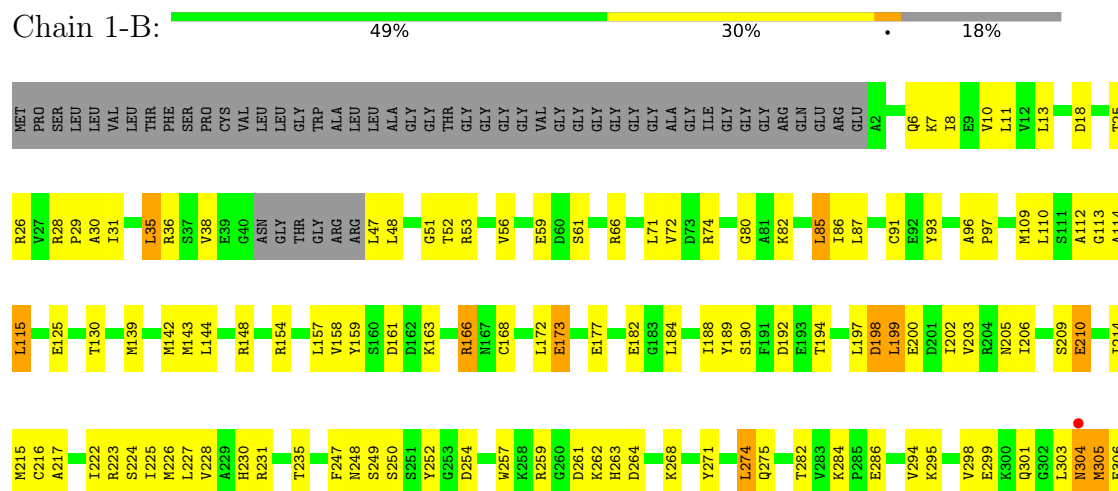
3 Residue-property plots

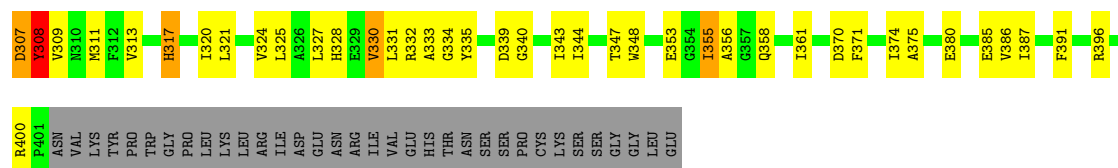
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

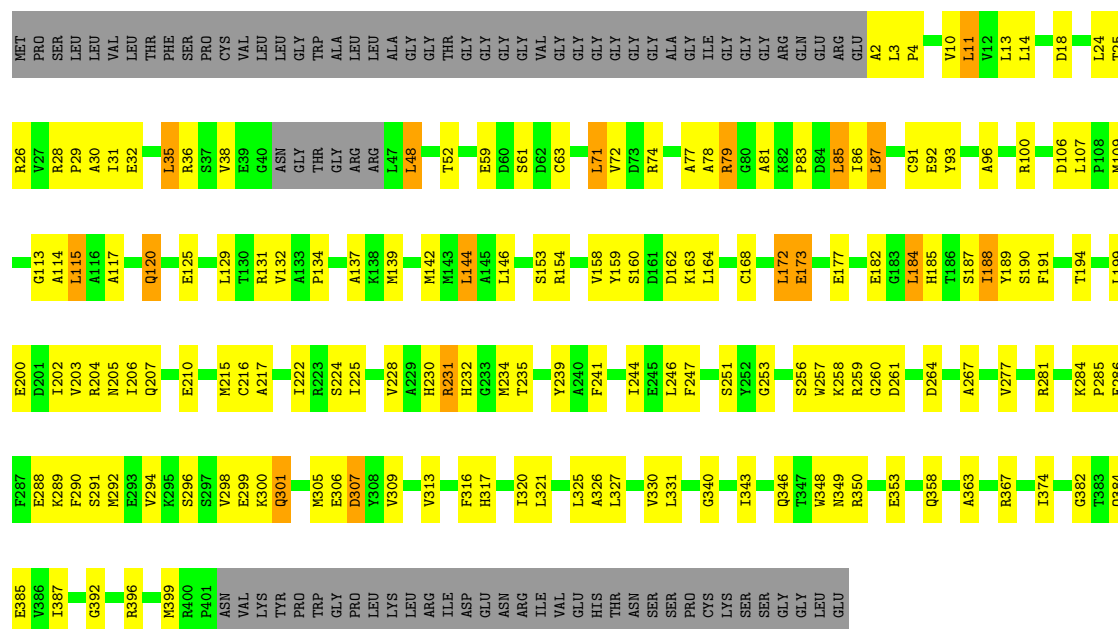


- Molecule 1: Atrial natriuretic peptide clearance receptor

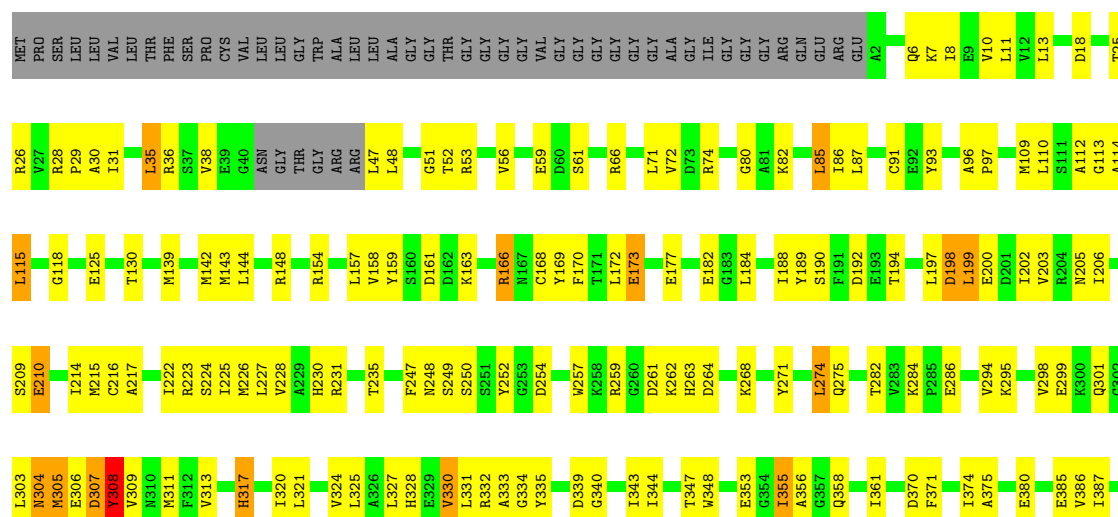


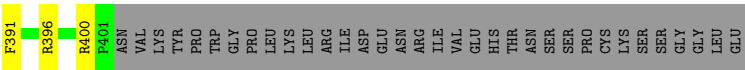


• Molecule 1: Atrial natriuretic peptide clearance receptor

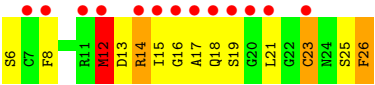


• Molecule 1: Atrial natriuretic peptide clearance receptor

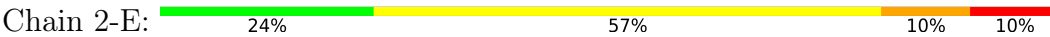




• Molecule 2: Atrial natriuretic factor



• Molecule 2: Atrial natriuretic factor



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



• Molecule 3: 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	56.87Å 135.47Å 137.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.40) 93.0 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.284 0.224 , 0.228	Depositor DCC
R_{free} test set	2321 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.51 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13526	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, CL

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	1-A	0.45	0/3180	0.96	7/4297 (0.2%)
1	1-B	0.44	0/3180	0.93	9/4297 (0.2%)
1	2-A	0.45	0/3180	0.96	7/4297 (0.2%)
1	2-B	0.44	0/3180	0.93	9/4297 (0.2%)
2	1-E	0.60	0/150	1.03	0/195
2	2-E	0.60	0/150	1.03	0/195
All	All	0.45	0/13020	0.95	32/17578 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	253	GLY	N-CA-C	-9.17	103.76	113.58
1	2-A	253	GLY	N-CA-C	-9.17	103.76	113.58
1	1-B	247	PHE	N-CA-C	7.38	122.73	113.43
1	2-B	247	PHE	N-CA-C	7.38	122.73	113.43
1	1-B	112	ALA	N-CA-C	-6.88	104.46	112.92
1	2-B	112	ALA	N-CA-C	-6.88	104.46	112.92
1	1-A	260	GLY	N-CA-C	-6.67	104.67	114.61
1	2-A	260	GLY	N-CA-C	-6.67	104.67	114.61
1	1-B	125	GLU	N-CA-C	6.34	118.19	111.28
1	2-B	125	GLU	N-CA-C	6.34	118.19	111.28
1	1-A	173	GLU	N-CA-C	-6.17	104.67	111.82
1	2-A	173	GLU	N-CA-C	-6.17	104.67	111.82
1	1-B	210	GLU	N-CA-C	5.91	118.83	110.14
1	2-B	210	GLU	N-CA-C	5.91	118.83	110.14
1	1-A	247	PHE	N-CA-C	5.78	121.24	113.72
1	2-A	247	PHE	N-CA-C	5.78	121.24	113.72
1	1-B	56	VAL	N-CA-C	5.78	116.18	107.80
1	2-B	56	VAL	N-CA-C	5.78	116.18	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-B	173	GLU	N-CA-C	-5.78	105.12	111.82
1	2-B	173	GLU	N-CA-C	-5.78	105.12	111.82
1	1-A	92	GLU	N-CA-C	5.51	117.72	111.11
1	2-A	92	GLU	N-CA-C	5.51	117.72	111.11
1	1-B	198	ASP	N-CA-C	-5.28	103.34	110.68
1	2-B	198	ASP	N-CA-C	-5.28	103.34	110.68
1	1-B	205	ASN	N-CA-C	-5.19	105.70	111.36
1	2-B	205	ASN	N-CA-C	-5.19	105.70	111.36
1	1-B	330	VAL	N-CA-C	-5.16	106.11	111.58
1	2-B	330	VAL	N-CA-C	-5.16	106.11	111.58
1	1-A	382	GLY	N-CA-C	-5.13	107.60	116.01
1	2-A	382	GLY	N-CA-C	-5.13	107.60	116.01
1	1-A	301	GLN	N-CA-C	-5.08	108.10	114.56
1	2-A	301	GLN	N-CA-C	-5.08	108.10	114.56

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	1-A	3111	0	3013	142	0
1	1-B	3111	0	3014	132	0
1	2-A	3111	0	3013	140	0
1	2-B	3111	0	3014	137	0
2	1-E	149	0	135	15	0
2	2-E	149	0	135	18	0
3	1-C	28	0	25	0	0
3	2-C	28	0	25	0	0
4	1-A	28	0	26	0	0
4	1-B	14	0	13	0	0
4	2-A	28	0	26	0	0
4	2-B	14	0	13	0	0
5	1-A	1	0	0	0	0
5	1-B	1	0	0	0	0
5	2-A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2-B	1	0	0	0	0
6	1-A	167	0	0	11	0
6	1-B	152	0	0	6	0
6	1-E	1	0	0	0	0
6	2-A	168	0	0	11	0
6	2-B	151	0	0	6	0
6	2-E	1	0	0	0	0
All	All	13526	0	12452	549	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 22.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG22	1:B:348:TRP:HE1	1.13	1.11
1:B:130:THR:HG22	1:B:348:TRP:HE1	1.13	1.11
1:A:215:MET:HE1	1:A:225:ILE:HG21	1.35	1.06
1:A:215:MET:HE1	1:A:225:ILE:HG21	1.35	1.06
1:B:295:LYS:HG3	1:B:305:MET:HG3	1.49	0.94
1:B:295:LYS:HG3	1:B:305:MET:HG3	1.49	0.94
1:A:118:GLY:H	2:E:15:ILE:HD12	1.33	0.94
1:B:31:ILE:HG23	1:B:320:ILE:HD11	1.50	0.93
1:B:31:ILE:HG23	1:B:320:ILE:HD11	1.50	0.93
1:B:215:MET:HE1	1:B:225:ILE:HG21	1.51	0.91
1:B:215:MET:HE1	1:B:225:ILE:HG21	1.51	0.91
1:B:284:LYS:HE3	1:B:286:GLU:HB3	1.54	0.89
1:B:284:LYS:HE3	1:B:286:GLU:HB3	1.54	0.89
1:B:327:LEU:O	1:B:330:VAL:HG12	1.78	0.83
1:B:327:LEU:O	1:B:330:VAL:HG12	1.78	0.83
1:B:74:ARG:HD3	6:B:606:HOH:O	1.78	0.82
1:B:74:ARG:HD3	6:B:605:HOH:O	1.78	0.82
1:A:159:TYR:HB3	1:A:172:LEU:HD22	1.61	0.82
1:A:159:TYR:HB3	1:A:172:LEU:HD22	1.61	0.82
1:A:91:CYS:HB3	6:A:566:HOH:O	1.79	0.82
1:A:91:CYS:HB3	6:A:567:HOH:O	1.79	0.82
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.45	0.82
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.45	0.82
1:A:109:MET:HE2	1:A:129:LEU:HD13	1.62	0.81
1:B:38:VAL:HG21	1:B:324:VAL:HG21	1.62	0.81
1:A:109:MET:HE2	1:A:129:LEU:HD13	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG21	1:B:324:VAL:HG21	1.62	0.81
1:A:387:ILE:HD12	1:A:399:MET:HE1	1.62	0.81
1:A:387:ILE:HD12	1:A:399:MET:HE1	1.62	0.81
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.65	0.79
1:B:130:THR:HG22	1:B:348:TRP:NE1	1.95	0.79
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.65	0.79
1:B:130:THR:HG22	1:B:348:TRP:NE1	1.95	0.79
1:B:118:GLY:H	2:E:15:ILE:HD12	1.49	0.78
1:B:202:ILE:O	1:B:206:ILE:HG12	1.86	0.75
1:B:202:ILE:O	1:B:206:ILE:HG12	1.86	0.75
1:B:93:TYR:CD1	2:E:16:GLY:HA2	2.23	0.74
1:A:93:TYR:CD1	2:E:16:GLY:HA2	2.22	0.74
1:B:143:MET:HE2	1:B:214:ILE:HD12	1.70	0.73
1:B:143:MET:HE2	1:B:214:ILE:HD12	1.70	0.73
1:A:78:ALA:HB1	1:A:81:ALA:HB3	1.70	0.72
1:A:78:ALA:HB1	1:A:81:ALA:HB3	1.70	0.72
1:A:100:ARG:HD3	1:A:125:GLU:OE2	1.90	0.71
1:A:100:ARG:HD3	1:A:125:GLU:OE2	1.90	0.71
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.73	0.71
1:B:330:VAL:HG22	1:B:335:TYR:HB2	1.71	0.71
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.73	0.71
1:B:330:VAL:HG22	1:B:335:TYR:HB2	1.71	0.71
1:A:93:TYR:HD1	2:E:16:GLY:HA2	1.55	0.71
1:B:374:ILE:HG23	6:B:652:HOH:O	1.91	0.70
1:B:374:ILE:HG23	6:B:652:HOH:O	1.91	0.70
1:B:374:ILE:HG12	6:B:652:HOH:O	1.92	0.69
1:B:374:ILE:HG12	6:B:652:HOH:O	1.92	0.69
1:B:386:VAL:HB	1:B:400:ARG:NH1	2.07	0.69
1:B:386:VAL:HB	1:B:400:ARG:NH1	2.07	0.69
1:A:153:SER:HA	1:A:184:LEU:HD13	1.73	0.69
1:A:153:SER:HA	1:A:184:LEU:HD13	1.73	0.69
1:B:93:TYR:HD1	2:E:16:GLY:HA2	1.57	0.69
1:B:31:ILE:HG23	1:B:320:ILE:CD1	2.23	0.68
1:B:130:THR:HG23	1:B:344:ILE:HD12	1.74	0.68
1:B:31:ILE:HG23	1:B:320:ILE:CD1	2.23	0.68
1:B:130:THR:HG23	1:B:344:ILE:HD12	1.74	0.68
1:A:353:GLU:OE2	1:A:358:GLN:HG2	1.95	0.67
1:A:353:GLU:OE2	1:A:358:GLN:HG2	1.95	0.67
1:A:204:ARG:HG3	1:A:204:ARG:HH11	1.60	0.67
1:A:204:ARG:HG3	1:A:204:ARG:HH11	1.60	0.67
1:A:11:LEU:HD22	1:A:13:LEU:HG	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:THR:O	1:B:53:ARG:HD3	1.94	0.66
1:B:249:SER:HA	1:B:252:TYR:CE2	2.31	0.66
1:A:11:LEU:HD22	1:A:13:LEU:HG	1.77	0.66
1:B:52:THR:O	1:B:53:ARG:HD3	1.94	0.66
1:B:249:SER:HA	1:B:252:TYR:CE2	2.31	0.66
1:A:93:TYR:CD1	2:E:17:ALA:HB1	2.32	0.65
1:A:188:ILE:HD12	1:A:188:ILE:N	2.11	0.65
1:A:188:ILE:HD12	1:A:188:ILE:N	2.11	0.65
1:A:326:ALA:O	1:A:330:VAL:HG23	1.97	0.65
1:A:326:ALA:O	1:A:330:VAL:HG23	1.97	0.65
1:A:215:MET:CE	1:A:225:ILE:HG21	2.22	0.64
1:A:215:MET:CE	1:A:225:ILE:HG21	2.22	0.64
1:A:189:TYR:HE2	1:A:202:ILE:HD13	1.63	0.64
1:A:207:GLN:HB3	1:A:234:MET:HE3	1.79	0.64
1:B:217:ALA:HB3	1:B:222:ILE:CD1	2.27	0.64
1:A:189:TYR:HE2	1:A:202:ILE:HD13	1.63	0.64
1:A:207:GLN:HB3	1:A:234:MET:HE3	1.79	0.64
1:B:169:TYR:OH	2:E:12:MET:HE2	1.98	0.64
1:B:217:ALA:HB3	1:B:222:ILE:CD1	2.27	0.64
1:B:173:GLU:OE2	2:E:21:LEU:HB2	1.97	0.64
1:B:192:ASP:OD1	1:B:194:THR:HB	1.97	0.64
1:B:192:ASP:OD1	1:B:194:THR:HB	1.97	0.64
1:A:169:TYR:CE1	2:E:12:MET:HE2	2.32	0.64
1:A:144:LEU:HD11	1:A:182:GLU:HG3	1.80	0.63
1:A:144:LEU:HD11	1:A:182:GLU:HG3	1.80	0.63
1:A:142:MET:HE3	1:A:277:VAL:HG13	1.80	0.63
1:A:142:MET:HE3	1:A:277:VAL:HG13	1.80	0.63
1:A:169:TYR:HE1	2:E:12:MET:HE2	1.63	0.63
1:B:130:THR:HG21	1:B:347:THR:OG1	1.99	0.63
1:B:130:THR:HG21	1:B:347:THR:OG1	1.99	0.63
1:B:148:ARG:HH21	1:B:148:ARG:HG3	1.62	0.63
1:B:148:ARG:HH21	1:B:148:ARG:HG3	1.62	0.63
1:B:118:GLY:N	2:E:15:ILE:HD12	2.13	0.63
1:A:35:LEU:O	1:A:38:VAL:HG22	1.98	0.62
1:A:35:LEU:O	1:A:38:VAL:HG22	1.98	0.62
1:A:215:MET:HE1	1:A:225:ILE:CG2	2.20	0.62
1:A:284:LYS:HD2	1:A:286:GLU:HB2	1.82	0.62
1:B:189:TYR:HE2	1:B:202:ILE:HG12	1.64	0.62
1:A:215:MET:HE1	1:A:225:ILE:CG2	2.20	0.62
1:A:284:LYS:HD2	1:A:286:GLU:HB2	1.82	0.62
1:B:189:TYR:HE2	1:B:202:ILE:HG12	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:OD2	1:A:25:THR:HB	1.99	0.62
1:A:18:ASP:OD2	1:A:25:THR:HB	1.99	0.62
1:A:2:ALA:O	1:A:3:LEU:HD23	2.00	0.61
1:A:2:ALA:O	1:A:3:LEU:HD23	2.00	0.61
1:B:6:GLN:O	1:B:52:THR:HA	2.00	0.61
1:B:80:GLY:O	1:B:82:LYS:HE3	2.00	0.61
1:B:93:TYR:CD1	2:E:17:ALA:HB1	2.35	0.61
1:B:6:GLN:O	1:B:52:THR:HA	2.00	0.61
1:B:80:GLY:O	1:B:82:LYS:HE3	2.00	0.61
1:A:173:GLU:OE1	2:E:21:LEU:HB2	2.01	0.61
1:A:298:VAL:O	1:A:301:GLN:HB3	2.00	0.61
1:A:298:VAL:O	1:A:301:GLN:HB3	2.00	0.61
1:A:187:SER:C	1:A:188:ILE:HD12	2.25	0.60
1:A:187:SER:C	1:A:188:ILE:HD12	2.25	0.60
1:B:170:PHE:CE1	2:E:15:ILE:HG23	2.36	0.60
1:A:217:ALA:HB3	1:A:222:ILE:HD12	1.82	0.60
1:A:217:ALA:HB3	1:A:222:ILE:HD12	1.82	0.60
1:A:203:VAL:O	1:A:207:GLN:HG2	2.01	0.60
1:B:198:ASP:C	1:B:200:GLU:H	2.09	0.60
1:A:203:VAL:O	1:A:207:GLN:HG2	2.01	0.60
1:B:198:ASP:C	1:B:200:GLU:H	2.09	0.60
1:A:85:LEU:HD22	1:A:86:ILE:N	2.16	0.59
1:A:85:LEU:HD22	1:A:86:ILE:N	2.16	0.59
1:B:13:LEU:HD23	1:B:59:GLU:HB3	1.85	0.59
1:B:51:GLY:O	1:B:53:ARG:HG2	2.02	0.59
1:B:13:LEU:HD23	1:B:59:GLU:HB3	1.85	0.59
1:B:51:GLY:O	1:B:53:ARG:HG2	2.02	0.59
1:A:117:ALA:O	1:A:120:GLN:HB2	2.02	0.59
1:A:117:ALA:O	1:A:120:GLN:HB2	2.02	0.59
1:A:31:ILE:HG23	1:A:320:ILE:HD11	1.85	0.58
1:B:148:ARG:HH11	1:B:182:GLU:CG	2.16	0.58
1:A:31:ILE:HG23	1:A:320:ILE:HD11	1.85	0.58
1:B:148:ARG:HH11	1:B:182:GLU:CG	2.16	0.58
1:A:170:PHE:CE1	2:E:15:ILE:HG23	2.38	0.58
1:A:106:ASP:O	1:A:340:GLY:HA3	2.04	0.57
1:A:106:ASP:O	1:A:340:GLY:HA3	2.04	0.57
1:A:158:VAL:HG21	1:A:206:ILE:CD1	2.34	0.57
1:A:173:GLU:O	1:A:177:GLU:HG2	2.03	0.57
1:A:158:VAL:HG21	1:A:206:ILE:CD1	2.34	0.57
1:A:173:GLU:O	1:A:177:GLU:HG2	2.03	0.57
1:B:303:LEU:HD23	1:B:303:LEU:C	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:HD23	1:B:303:LEU:C	2.29	0.57
1:A:325:LEU:HD13	6:A:621:HOH:O	2.03	0.57
1:A:325:LEU:HD13	6:A:623:HOH:O	2.03	0.57
1:B:30:ALA:HB2	1:B:313:VAL:HG13	1.87	0.57
1:B:30:ALA:HB2	1:B:313:VAL:HG13	1.87	0.57
1:A:132:VAL:O	1:A:132:VAL:HG12	2.04	0.56
1:A:132:VAL:O	1:A:132:VAL:HG12	2.04	0.56
1:B:321:LEU:O	1:B:325:LEU:HD13	2.05	0.56
1:B:321:LEU:O	1:B:325:LEU:HD13	2.05	0.56
1:A:159:TYR:HB3	1:A:172:LEU:CD2	2.33	0.56
1:B:385:GLU:C	6:B:652:HOH:O	2.48	0.56
1:A:159:TYR:HB3	1:A:172:LEU:CD2	2.33	0.56
1:B:385:GLU:C	6:B:652:HOH:O	2.48	0.56
1:B:294:VAL:O	1:B:298:VAL:HG23	2.06	0.56
1:B:294:VAL:O	1:B:298:VAL:HG23	2.06	0.56
1:B:148:ARG:HG3	1:B:148:ARG:NH2	2.21	0.56
1:B:148:ARG:HG3	1:B:148:ARG:NH2	2.21	0.56
1:B:161:ASP:OD2	1:B:166:ARG:HD2	2.06	0.56
1:B:161:ASP:OD2	1:B:166:ARG:HD2	2.06	0.56
1:A:158:VAL:HG21	1:A:206:ILE:HD11	1.88	0.56
1:B:110:LEU:HG	1:B:130:THR:OG1	2.06	0.56
1:A:158:VAL:HG21	1:A:206:ILE:HD11	1.88	0.56
1:A:163:LYS:NZ	2:E:9:GLY:HA3	2.21	0.56
1:B:110:LEU:HG	1:B:130:THR:OG1	2.06	0.56
1:A:217:ALA:HB3	1:A:222:ILE:CD1	2.35	0.56
1:A:217:ALA:HB3	1:A:222:ILE:CD1	2.35	0.56
1:A:251:SER:HB3	1:A:256:SER:HA	1.87	0.55
1:A:309:VAL:HG22	6:A:647:HOH:O	2.05	0.55
1:B:189:TYR:HE1	2:E:26:PHE:O	1.90	0.55
1:A:251:SER:HB3	1:A:256:SER:HA	1.87	0.55
1:A:309:VAL:HG22	6:A:649:HOH:O	2.05	0.55
1:A:330:VAL:HG21	1:A:343:ILE:HG12	1.88	0.55
1:A:330:VAL:HG21	1:A:343:ILE:HG12	1.88	0.55
1:A:199:LEU:HD11	1:A:224:SER:HB3	1.88	0.55
1:B:203:VAL:HG21	1:B:228:VAL:CG1	2.36	0.55
1:B:227:LEU:O	1:B:230:HIS:HB3	2.07	0.55
1:A:199:LEU:HD11	1:A:224:SER:HB3	1.88	0.55
1:B:203:VAL:HG21	1:B:228:VAL:CG1	2.36	0.55
1:B:227:LEU:O	1:B:230:HIS:HB3	2.07	0.55
1:B:159:TYR:HB3	1:B:172:LEU:HD12	1.87	0.55
1:B:159:TYR:HB3	1:B:172:LEU:HD12	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HB3	1:A:4:PRO:HD2	1.88	0.55
1:B:173:GLU:O	1:B:177:GLU:HG2	2.07	0.55
1:A:3:LEU:HB3	1:A:4:PRO:HD2	1.88	0.55
1:B:173:GLU:O	1:B:177:GLU:HG2	2.07	0.55
1:B:215:MET:CE	1:B:225:ILE:HG21	2.31	0.55
1:B:215:MET:CE	1:B:225:ILE:HG21	2.31	0.55
1:A:291:SER:HB2	6:A:647:HOH:O	2.06	0.54
1:A:291:SER:HB2	6:A:649:HOH:O	2.06	0.54
1:A:194:THR:HG21	6:A:537:HOH:O	2.07	0.54
1:A:228:VAL:O	1:A:232:HIS:HD2	1.90	0.54
1:A:194:THR:HG21	6:A:538:HOH:O	2.07	0.54
1:A:228:VAL:O	1:A:232:HIS:HD2	1.90	0.54
1:B:157:LEU:HD12	1:B:188:ILE:CD1	2.38	0.54
1:B:157:LEU:HD12	1:B:188:ILE:CD1	2.38	0.54
1:A:305:MET:CE	1:A:309:VAL:HG12	2.37	0.54
1:A:305:MET:CE	1:A:309:VAL:HG12	2.37	0.54
1:B:223:ARG:HA	1:B:271:TYR:OH	2.08	0.53
1:B:223:ARG:HA	1:B:271:TYR:OH	2.08	0.53
1:B:7:LYS:HE2	1:B:53:ARG:HG2	1.91	0.53
1:B:7:LYS:HE2	1:B:53:ARG:HG2	1.91	0.53
1:B:35:LEU:C	1:B:38:VAL:HG12	2.34	0.53
1:A:93:TYR:CE2	2:E:14:ARG:HG3	2.42	0.53
1:B:35:LEU:C	1:B:38:VAL:HG12	2.34	0.53
1:B:91:CYS:HB3	6:B:631:HOH:O	2.09	0.53
1:B:282:THR:O	1:B:356:ALA:HB1	2.08	0.53
1:B:91:CYS:HB3	6:B:629:HOH:O	2.09	0.53
1:B:282:THR:O	1:B:356:ALA:HB1	2.08	0.53
1:A:306:GLU:O	1:A:307:ASP:C	2.51	0.53
1:B:35:LEU:HA	1:B:38:VAL:HG12	1.90	0.53
1:A:306:GLU:O	1:A:307:ASP:C	2.51	0.53
1:B:35:LEU:HA	1:B:38:VAL:HG12	1.90	0.53
1:A:327:LEU:O	1:A:331:LEU:HD13	2.07	0.53
1:A:327:LEU:O	1:A:331:LEU:HD13	2.07	0.53
1:B:200:GLU:OE1	1:B:231:ARG:NH2	2.42	0.53
1:B:200:GLU:OE1	1:B:231:ARG:NH2	2.42	0.53
1:B:257:TRP:CE3	1:B:268:LYS:HB2	2.44	0.52
1:B:257:TRP:CE3	1:B:268:LYS:HB2	2.44	0.52
1:A:160:SER:HA	1:A:191:PHE:O	2.09	0.52
1:A:160:SER:HA	1:A:191:PHE:O	2.09	0.52
1:B:226:MET:HE2	1:B:274:LEU:HB2	1.92	0.52
1:B:311:MET:HE3	1:B:311:MET:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:MET:HE2	1:B:274:LEU:HB2	1.92	0.52
1:B:311:MET:HE3	1:B:311:MET:O	2.10	0.52
1:A:284:LYS:HG2	1:A:285:PRO:HD2	1.90	0.52
1:B:7:LYS:HD3	1:B:53:ARG:H	1.74	0.52
1:A:284:LYS:HG2	1:A:285:PRO:HD2	1.90	0.52
1:B:7:LYS:HD3	1:B:53:ARG:H	1.74	0.52
1:A:48:LEU:HD23	1:A:52:THR:HG21	1.91	0.52
1:B:261:ASP:CG	1:B:262:LYS:H	2.16	0.52
1:B:317:HIS:CE1	1:B:355:ILE:HG23	2.45	0.52
1:A:48:LEU:HD23	1:A:52:THR:HG21	1.91	0.52
1:B:261:ASP:CG	1:B:262:LYS:H	2.16	0.52
1:B:317:HIS:CE1	1:B:355:ILE:HG23	2.45	0.52
1:B:192:ASP:C	1:B:194:THR:H	2.17	0.52
1:A:163:LYS:HZ1	2:E:9:GLY:HA3	1.74	0.52
1:B:192:ASP:C	1:B:194:THR:H	2.17	0.52
1:B:197:LEU:HB3	1:B:199:LEU:HG	1.91	0.51
1:B:197:LEU:HB3	1:B:199:LEU:HG	1.91	0.51
1:A:162:ASP:O	1:A:163:LYS:HB2	2.10	0.51
1:A:162:ASP:O	1:A:163:LYS:HB2	2.10	0.51
1:A:158:VAL:O	1:A:215:MET:HA	2.10	0.51
1:A:158:VAL:O	1:A:215:MET:HA	2.10	0.51
1:B:48:LEU:HD13	1:B:52:THR:HG21	1.92	0.51
1:B:48:LEU:HD13	1:B:52:THR:HG21	1.92	0.51
1:A:118:GLY:N	2:E:15:ILE:HD12	2.14	0.51
1:A:299:GLU:C	1:A:301:GLN:H	2.17	0.51
1:A:299:GLU:C	1:A:301:GLN:H	2.17	0.51
1:A:168:CYS:SG	1:A:216:CYS:C	2.93	0.51
1:A:168:CYS:SG	1:A:216:CYS:C	2.93	0.51
1:A:93:TYR:HD1	2:E:17:ALA:HB1	1.75	0.51
1:A:392:GLY:HA3	6:A:605:HOH:O	2.11	0.50
1:A:392:GLY:HA3	6:A:607:HOH:O	2.11	0.50
1:B:309:VAL:HG23	1:B:309:VAL:O	2.11	0.50
1:B:309:VAL:HG23	1:B:309:VAL:O	2.11	0.50
1:A:146:LEU:HG	6:A:666:HOH:O	2.11	0.50
1:B:303:LEU:HD23	1:B:304:ASN:C	2.36	0.50
1:A:146:LEU:HG	6:A:666:HOH:O	2.11	0.50
1:B:303:LEU:HD23	1:B:304:ASN:C	2.36	0.50
1:B:157:LEU:HD12	1:B:188:ILE:HD11	1.93	0.50
1:B:157:LEU:HD12	1:B:188:ILE:HD11	1.93	0.50
1:B:35:LEU:HA	1:B:38:VAL:CG1	2.42	0.50
1:B:35:LEU:HA	1:B:38:VAL:CG1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:CD2	2:E:14:ARG:HG3	2.47	0.49
1:A:83:PRO:HD3	6:A:675:HOH:O	2.11	0.49
1:A:83:PRO:HD3	6:A:676:HOH:O	2.11	0.49
1:B:142:MET:HG3	1:B:371:PHE:HB2	1.94	0.49
1:B:217:ALA:HB3	1:B:222:ILE:HD12	1.93	0.49
1:B:334:GLY:HA2	6:B:571:HOH:O	2.11	0.49
1:B:142:MET:HG3	1:B:371:PHE:HB2	1.94	0.49
1:B:217:ALA:HB3	1:B:222:ILE:HD12	1.93	0.49
1:B:334:GLY:HA2	6:B:571:HOH:O	2.11	0.49
1:A:85:LEU:HD11	1:A:87:LEU:HD13	1.95	0.49
1:A:85:LEU:HD11	1:A:87:LEU:HD13	1.95	0.49
1:A:31:ILE:HD11	1:A:316:PHE:HB3	1.94	0.49
1:A:199:LEU:CD1	1:A:224:SER:HB3	2.43	0.49
1:A:31:ILE:HD11	1:A:316:PHE:HB3	1.94	0.49
1:A:199:LEU:CD1	1:A:224:SER:HB3	2.43	0.49
1:A:25:THR:HG23	1:A:301:GLN:HG2	1.94	0.49
1:A:25:THR:HG23	1:A:301:GLN:HG2	1.94	0.49
1:A:28:ARG:HB3	1:A:29:PRO:HD3	1.94	0.49
1:B:370:ASP:OD1	1:B:391:PHE:HA	2.13	0.49
1:A:28:ARG:HB3	1:A:29:PRO:HD3	1.94	0.49
1:B:370:ASP:OD1	1:B:391:PHE:HA	2.13	0.49
1:B:307:ASP:O	1:B:308:TYR:HB3	2.12	0.48
1:B:307:ASP:O	1:B:308:TYR:HB3	2.12	0.48
1:A:203:VAL:HG21	1:A:228:VAL:CG1	2.43	0.48
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.27	0.48
1:A:374:ILE:HD13	6:A:660:HOH:O	2.12	0.48
1:A:203:VAL:HG21	1:A:228:VAL:CG1	2.43	0.48
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.27	0.48
1:A:374:ILE:HD13	6:A:660:HOH:O	2.12	0.48
1:A:85:LEU:CD1	1:A:87:LEU:HD13	2.43	0.48
1:A:85:LEU:CD1	1:A:87:LEU:HD13	2.43	0.48
1:A:96:ALA:O	1:A:100:ARG:HG3	2.14	0.48
1:A:96:ALA:O	1:A:100:ARG:HG3	2.14	0.48
1:A:32:GLU:O	1:A:36:ARG:HG3	2.13	0.48
1:A:32:GLU:O	1:A:36:ARG:HG3	2.13	0.48
1:A:203:VAL:CG1	1:A:234:MET:SD	3.01	0.48
1:A:203:VAL:CG1	1:A:234:MET:SD	3.01	0.48
1:B:215:MET:HE1	1:B:225:ILE:CG2	2.32	0.48
1:B:215:MET:HE1	1:B:225:ILE:CG2	2.32	0.48
1:A:113:GLY:C	1:A:115:LEU:HD13	2.39	0.48
1:A:113:GLY:C	1:A:115:LEU:HD13	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TYR:CE1	2:E:12:MET:HE2	2.48	0.48
1:B:188:ILE:HD12	2:E:8:PHE:HE2	1.78	0.48
1:B:158:VAL:HG21	1:B:206:ILE:HD11	1.96	0.48
1:B:158:VAL:HG21	1:B:206:ILE:HD11	1.96	0.48
1:A:203:VAL:HG21	1:A:228:VAL:HG12	1.96	0.47
1:A:203:VAL:HG21	1:A:228:VAL:HG12	1.96	0.47
1:A:77:ALA:C	1:A:79:ARG:H	2.22	0.47
1:B:317:HIS:ND1	1:B:317:HIS:C	2.73	0.47
1:A:77:ALA:C	1:A:79:ARG:H	2.22	0.47
1:B:317:HIS:ND1	1:B:317:HIS:C	2.73	0.47
1:A:116:ALA:HB1	2:E:15:ILE:HD13	1.95	0.47
1:A:284:LYS:HG2	1:A:285:PRO:CD	2.45	0.47
1:A:346:GLN:O	1:A:350:ARG:HD2	2.14	0.47
1:B:330:VAL:HG11	1:B:343:ILE:HD13	1.96	0.47
1:A:284:LYS:HG2	1:A:285:PRO:CD	2.45	0.47
1:A:346:GLN:O	1:A:350:ARG:HD2	2.14	0.47
1:B:330:VAL:HG11	1:B:343:ILE:HD13	1.96	0.47
1:A:18:ASP:HB3	1:A:26:ARG:HH22	1.80	0.47
1:A:231:ARG:NH2	1:A:232:HIS:CE1	2.82	0.47
1:A:257:TRP:HB2	1:A:267:ALA:HB1	1.97	0.47
1:B:93:TYR:HD1	2:E:17:ALA:HB1	1.79	0.47
1:A:18:ASP:HB3	1:A:26:ARG:HH22	1.80	0.47
1:A:231:ARG:NH2	1:A:232:HIS:CE1	2.82	0.47
1:A:257:TRP:HB2	1:A:267:ALA:HB1	1.97	0.47
1:B:8:ILE:HG22	1:B:10:VAL:HG23	1.97	0.47
1:B:168:CYS:SG	1:B:216:CYS:C	2.97	0.47
1:B:8:ILE:HG22	1:B:10:VAL:HG23	1.97	0.47
1:B:168:CYS:SG	1:B:216:CYS:C	2.97	0.47
1:A:114:ALA:O	1:A:131:ARG:HD3	2.15	0.47
1:A:259:ARG:C	1:A:261:ASP:N	2.71	0.47
1:A:114:ALA:O	1:A:131:ARG:HD3	2.15	0.47
1:A:259:ARG:C	1:A:261:ASP:N	2.71	0.47
1:A:159:TYR:CZ	1:A:190:SER:HB3	2.51	0.46
1:A:159:TYR:CZ	1:A:190:SER:HB3	2.51	0.46
1:B:299:GLU:HG2	1:B:305:MET:HB2	1.96	0.46
1:B:299:GLU:HG2	1:B:305:MET:HB2	1.96	0.46
1:A:163:LYS:O	1:A:164:LEU:HD12	2.15	0.46
1:A:163:LYS:O	1:A:164:LEU:HD12	2.15	0.46
1:B:158:VAL:HG21	1:B:206:ILE:CD1	2.46	0.46
1:B:274:LEU:HD23	1:B:275:GLN:N	2.29	0.46
1:B:158:VAL:HG21	1:B:206:ILE:CD1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:HD23	1:B:275:GLN:N	2.29	0.46
1:A:189:TYR:CE1	1:A:205:ASN:ND2	2.83	0.46
1:B:249:SER:HA	1:B:252:TYR:CZ	2.51	0.46
1:A:189:TYR:CE1	1:A:205:ASN:ND2	2.83	0.46
1:B:249:SER:HA	1:B:252:TYR:CZ	2.51	0.46
1:A:285:PRO:O	1:A:288:GLU:HB2	2.16	0.46
1:A:285:PRO:O	1:A:288:GLU:HB2	2.16	0.46
1:A:173:GLU:OE2	2:E:15:ILE:HD11	2.16	0.46
1:B:189:TYR:CE1	2:E:26:PHE:O	2.69	0.46
1:B:387:ILE:O	1:B:400:ARG:N	2.49	0.46
1:B:387:ILE:O	1:B:400:ARG:N	2.49	0.46
1:A:109:MET:HE2	1:A:129:LEU:CD1	2.39	0.46
1:B:199:LEU:O	1:B:203:VAL:HG23	2.16	0.46
1:A:109:MET:HE2	1:A:129:LEU:CD1	2.39	0.46
1:B:199:LEU:O	1:B:203:VAL:HG23	2.16	0.46
1:B:177:GLU:OE1	2:E:11:ARG:NH1	2.49	0.46
1:B:194:THR:HG22	1:B:194:THR:O	2.15	0.45
1:B:194:THR:HG22	1:B:194:THR:O	2.15	0.45
1:A:11:LEU:C	1:A:11:LEU:CD2	2.89	0.45
1:B:332:ARG:C	1:B:334:GLY:H	2.24	0.45
1:A:11:LEU:C	1:A:11:LEU:CD2	2.89	0.45
1:B:332:ARG:C	1:B:334:GLY:H	2.24	0.45
1:B:61:SER:O	1:B:66:ARG:HB3	2.16	0.45
1:B:61:SER:O	1:B:66:ARG:HB3	2.16	0.45
1:A:120:GLN:HE22	1:A:137:ALA:CB	2.30	0.45
1:A:294:VAL:O	1:A:298:VAL:HG23	2.16	0.45
1:A:120:GLN:HE22	1:A:137:ALA:CB	2.30	0.45
1:A:294:VAL:O	1:A:298:VAL:HG23	2.16	0.45
1:A:188:ILE:N	1:A:188:ILE:CD1	2.80	0.45
1:B:159:TYR:CZ	1:B:190:SER:HB3	2.51	0.45
1:A:188:ILE:N	1:A:188:ILE:CD1	2.80	0.45
1:B:159:TYR:CZ	1:B:190:SER:HB3	2.51	0.45
1:B:274:LEU:HD23	1:B:275:GLN:H	1.81	0.45
1:B:274:LEU:HD23	1:B:275:GLN:H	1.81	0.45
1:B:192:ASP:C	1:B:194:THR:N	2.75	0.44
1:B:192:ASP:C	1:B:194:THR:N	2.75	0.44
1:B:330:VAL:HG11	1:B:343:ILE:CD1	2.47	0.44
1:B:330:VAL:HG11	1:B:343:ILE:CD1	2.47	0.44
1:B:198:ASP:C	1:B:200:GLU:N	2.72	0.44
1:B:198:ASP:C	1:B:200:GLU:N	2.72	0.44
1:B:148:ARG:HH11	1:B:182:GLU:HG2	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:HH11	1:B:182:GLU:HG2	1.80	0.44
1:B:198:ASP:O	1:B:200:GLU:N	2.50	0.44
1:B:298:VAL:CG1	1:B:303:LEU:HD22	2.48	0.44
1:B:198:ASP:O	1:B:200:GLU:N	2.50	0.44
1:B:298:VAL:CG1	1:B:303:LEU:HD22	2.48	0.44
1:B:223:ARG:NE	1:B:259:ARG:HG3	2.33	0.44
1:B:223:ARG:NE	1:B:259:ARG:HG3	2.33	0.44
1:A:349:ASN:HB2	1:A:363:ALA:HA	2.00	0.44
1:B:36:ARG:C	1:B:38:VAL:H	2.26	0.44
1:A:349:ASN:HB2	1:A:363:ALA:HA	2.00	0.44
1:B:36:ARG:C	1:B:38:VAL:H	2.26	0.44
1:A:13:LEU:HD23	1:A:59:GLU:HB3	2.00	0.43
1:B:47:LEU:O	1:B:328:HIS:ND1	2.51	0.43
1:A:13:LEU:HD23	1:A:59:GLU:HB3	2.00	0.43
1:B:47:LEU:O	1:B:328:HIS:ND1	2.51	0.43
1:A:72:VAL:HG13	1:B:72:VAL:HG13	2.00	0.43
1:B:361:ILE:N	1:B:361:ILE:HD12	2.33	0.43
1:A:72:VAL:HG13	1:B:72:VAL:HG13	2.00	0.43
1:B:361:ILE:N	1:B:361:ILE:HD12	2.33	0.43
1:B:261:ASP:CG	1:B:262:LYS:N	2.76	0.43
1:B:330:VAL:HG22	1:B:335:TYR:CB	2.46	0.43
1:B:261:ASP:CG	1:B:262:LYS:N	2.76	0.43
1:B:330:VAL:HG22	1:B:335:TYR:CB	2.46	0.43
1:B:113:GLY:C	1:B:115:LEU:HD13	2.43	0.43
1:B:113:GLY:C	1:B:115:LEU:HD13	2.43	0.43
1:B:25:THR:HG23	1:B:301:GLN:HG2	2.01	0.43
1:B:85:LEU:HD22	1:B:86:ILE:N	2.34	0.43
1:B:25:THR:HG23	1:B:301:GLN:HG2	2.01	0.43
1:B:85:LEU:HD22	1:B:86:ILE:N	2.34	0.43
1:A:107:LEU:HD22	6:A:646:HOH:O	2.19	0.43
1:A:200:GLU:OE1	1:A:200:GLU:HA	2.19	0.43
1:A:107:LEU:HD22	6:A:648:HOH:O	2.19	0.43
1:A:200:GLU:OE1	1:A:200:GLU:HA	2.19	0.43
1:B:28:ARG:HB3	1:B:29:PRO:HD3	2.00	0.43
1:B:28:ARG:HB3	1:B:29:PRO:HD3	2.00	0.43
1:B:375:ALA:HB3	1:B:387:ILE:HG13	2.01	0.43
1:B:375:ALA:HB3	1:B:387:ILE:HG13	2.01	0.43
1:A:31:ILE:HG22	1:A:35:LEU:HD22	2.00	0.43
1:A:74:ARG:HH11	1:A:74:ARG:HB3	1.84	0.43
1:A:396:ARG:O	1:A:396:ARG:HG3	2.19	0.43
1:A:31:ILE:HG22	1:A:35:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:HH11	1:A:74:ARG:HB3	1.84	0.43
1:A:396:ARG:O	1:A:396:ARG:HG3	2.19	0.43
1:A:203:VAL:HG13	1:A:234:MET:SD	2.59	0.42
1:A:203:VAL:HG13	1:A:234:MET:SD	2.59	0.42
1:A:79:ARG:HH11	1:A:79:ARG:CB	2.22	0.42
1:A:202:ILE:O	1:A:206:ILE:HG12	2.19	0.42
1:A:244:ILE:CG2	1:A:246:LEU:HG	2.48	0.42
1:B:113:GLY:O	1:B:114:ALA:C	2.62	0.42
1:B:224:SER:HA	1:B:227:LEU:HD12	2.01	0.42
1:A:79:ARG:HH11	1:A:79:ARG:CB	2.22	0.42
1:A:202:ILE:O	1:A:206:ILE:HG12	2.19	0.42
1:A:244:ILE:CG2	1:A:246:LEU:HG	2.48	0.42
1:B:113:GLY:O	1:B:114:ALA:C	2.62	0.42
1:B:224:SER:HA	1:B:227:LEU:HD12	2.01	0.42
1:A:61:SER:C	1:A:63:CYS:N	2.77	0.42
1:A:132:VAL:O	1:A:367:ARG:HD3	2.18	0.42
1:A:281:ARG:NH1	1:A:309:VAL:O	2.51	0.42
1:B:259:ARG:HH21	1:B:259:ARG:HG2	1.84	0.42
1:A:61:SER:C	1:A:63:CYS:N	2.77	0.42
1:A:132:VAL:O	1:A:367:ARG:HD3	2.18	0.42
1:A:281:ARG:NH1	1:A:309:VAL:O	2.51	0.42
1:B:259:ARG:HH21	1:B:259:ARG:HG2	1.84	0.42
1:A:14:LEU:HB2	1:A:24:LEU:CD2	2.50	0.42
1:A:134:PRO:HD2	6:A:603:HOH:O	2.19	0.42
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.90	0.42
1:A:14:LEU:HB2	1:A:24:LEU:CD2	2.50	0.42
1:A:134:PRO:HD2	6:A:605:HOH:O	2.19	0.42
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.90	0.42
1:A:71:LEU:C	1:A:71:LEU:CD2	2.92	0.42
1:A:258:LYS:HG3	1:A:264:ASP:OD2	2.18	0.42
1:A:317:HIS:HE1	1:A:321:LEU:HD11	1.83	0.42
1:A:71:LEU:C	1:A:71:LEU:CD2	2.92	0.42
1:A:258:LYS:HG3	1:A:264:ASP:OD2	2.18	0.42
1:A:317:HIS:HE1	1:A:321:LEU:HD11	1.83	0.42
1:A:239:TYR:HB2	1:A:241:PHE:CE1	2.54	0.42
1:A:239:TYR:HB2	1:A:241:PHE:CE1	2.54	0.42
1:A:162:ASP:HB3	1:A:164:LEU:HB2	2.00	0.42
1:A:162:ASP:HB3	1:A:164:LEU:HB2	2.00	0.42
1:A:139:MET:HE3	1:A:139:MET:HB3	1.97	0.42
1:A:188:ILE:CD1	2:E:6:SER:HB2	2.50	0.42
1:A:139:MET:HE3	1:A:139:MET:HB3	1.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HG2	1:A:185:HIS:HB3	2.01	0.42
1:A:228:VAL:O	1:A:232:HIS:CD2	2.72	0.42
1:A:93:TYR:CD1	2:E:14:ARG:HD2	2.54	0.42
1:A:154:ARG:HG2	1:A:185:HIS:HB3	2.01	0.42
1:A:228:VAL:O	1:A:232:HIS:CD2	2.72	0.42
1:A:290:PHE:O	1:A:294:VAL:HG23	2.19	0.42
1:A:290:PHE:O	1:A:294:VAL:HG23	2.19	0.42
1:A:18:ASP:O	1:A:26:ARG:NH2	2.54	0.41
1:A:289:LYS:HA	1:A:292:MET:HE3	2.02	0.41
1:B:284:LYS:HE3	1:B:286:GLU:CB	2.37	0.41
1:A:18:ASP:O	1:A:26:ARG:NH2	2.54	0.41
1:A:289:LYS:HA	1:A:292:MET:HE3	2.02	0.41
1:B:284:LYS:HE3	1:B:286:GLU:CB	2.37	0.41
1:A:30:ALA:HB2	1:A:313:VAL:HG13	2.02	0.41
1:A:30:ALA:HB2	1:A:313:VAL:HG13	2.02	0.41
1:A:384:GLN:C	1:A:385:GLU:HG3	2.45	0.41
1:B:8:ILE:HD12	1:B:8:ILE:N	2.35	0.41
1:B:139:MET:O	1:B:142:MET:HB3	2.20	0.41
1:B:154:ARG:HD3	1:B:210:GLU:OE2	2.21	0.41
1:B:304:ASN:O	1:B:305:MET:C	2.63	0.41
1:A:384:GLN:C	1:A:385:GLU:HG3	2.45	0.41
1:B:8:ILE:HD12	1:B:8:ILE:N	2.35	0.41
1:B:139:MET:O	1:B:142:MET:HB3	2.20	0.41
1:B:154:ARG:HD3	1:B:210:GLU:OE2	2.21	0.41
1:B:304:ASN:O	1:B:305:MET:C	2.63	0.41
1:B:35:LEU:CA	1:B:38:VAL:HG12	2.51	0.41
1:B:109:MET:C	1:B:110:LEU:HD12	2.45	0.41
1:B:263:HIS:O	1:B:264:ASP:C	2.63	0.41
1:B:35:LEU:CA	1:B:38:VAL:HG12	2.51	0.41
1:B:109:MET:C	1:B:110:LEU:HD12	2.45	0.41
1:B:163:LYS:HD2	2:E:20:GLY:O	2.21	0.41
1:B:263:HIS:O	1:B:264:ASP:C	2.63	0.41
1:A:346:GLN:O	1:A:350:ARG:NH1	2.51	0.41
1:A:346:GLN:O	1:A:350:ARG:NH1	2.51	0.41
1:B:223:ARG:NH1	1:B:259:ARG:HB2	2.36	0.41
1:B:223:ARG:NH1	1:B:259:ARG:HB2	2.36	0.41
1:A:85:LEU:HD11	1:A:87:LEU:CD1	2.50	0.41
1:A:348:TRP:O	1:A:349:ASN:C	2.63	0.41
1:B:18:ASP:O	1:B:26:ARG:NH2	2.34	0.41
1:B:157:LEU:HB2	1:B:188:ILE:HD13	2.03	0.41
1:B:203:VAL:HG21	1:B:228:VAL:HB	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD11	1:A:87:LEU:CD1	2.50	0.41
1:A:348:TRP:O	1:A:349:ASN:C	2.63	0.41
1:B:18:ASP:O	1:B:26:ARG:NH2	2.34	0.41
1:B:157:LEU:HB2	1:B:188:ILE:HD13	2.03	0.41
1:B:203:VAL:HG21	1:B:228:VAL:HB	2.01	0.41
1:A:11:LEU:C	1:A:11:LEU:HD23	2.46	0.41
1:A:207:GLN:HA	1:A:239:TYR:OH	2.20	0.41
1:B:396:ARG:CB	1:B:396:ARG:NH1	2.84	0.41
1:A:11:LEU:C	1:A:11:LEU:HD23	2.46	0.41
1:A:207:GLN:HA	1:A:239:TYR:OH	2.20	0.41
1:B:396:ARG:CB	1:B:396:ARG:NH1	2.84	0.41
1:A:230:HIS:HA	1:A:235:THR:HG23	2.02	0.41
1:A:296:SER:O	1:A:300:LYS:HG2	2.21	0.41
1:A:301:GLN:OE1	1:A:301:GLN:HA	2.20	0.41
1:A:230:HIS:HA	1:A:235:THR:HG23	2.02	0.41
1:A:296:SER:O	1:A:300:LYS:HG2	2.21	0.41
1:A:301:GLN:OE1	1:A:301:GLN:HA	2.20	0.41
1:B:396:ARG:HB3	1:B:396:ARG:HH11	1.86	0.41
1:B:396:ARG:HB3	1:B:396:ARG:HH11	1.86	0.41
1:A:284:LYS:HG2	1:A:285:PRO:N	2.36	0.40
1:B:339:ASP:O	1:B:340:GLY:C	2.64	0.40
1:A:284:LYS:HG2	1:A:285:PRO:N	2.36	0.40
1:B:339:ASP:O	1:B:340:GLY:C	2.64	0.40
1:A:244:ILE:HD12	1:A:244:ILE:N	2.36	0.40
1:B:248:ASN:OD1	1:B:250:SER:HB2	2.21	0.40
1:B:353:GLU:OE2	1:B:358:GLN:NE2	2.54	0.40
1:A:244:ILE:HD12	1:A:244:ILE:N	2.36	0.40
1:B:248:ASN:OD1	1:B:250:SER:HB2	2.21	0.40
1:B:353:GLU:OE2	1:B:358:GLN:NE2	2.54	0.40
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.91	0.40
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.91	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	1-A	390/480 (81%)	363 (93%)	26 (7%)	1 (0%)	36	50
1	1-B	390/480 (81%)	359 (92%)	24 (6%)	7 (2%)	6	9
1	2-A	390/480 (81%)	363 (93%)	26 (7%)	1 (0%)	36	50
1	2-B	390/480 (81%)	359 (92%)	24 (6%)	7 (2%)	6	9
2	1-E	19/21 (90%)	8 (42%)	3 (16%)	8 (42%)	0	0
2	2-E	19/21 (90%)	8 (42%)	3 (16%)	8 (42%)	0	0
All	All	1598/1962 (81%)	1460 (91%)	106 (7%)	32 (2%)	6	7

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	209	SER
2	1-E	13	ASP
2	1-E	18	GLN
2	1-E	19	SER
1	2-B	209	SER
2	2-E	13	ASP
2	2-E	18	GLN
2	2-E	19	SER
1	1-B	199	LEU
1	1-B	306	GLU
2	1-E	12	MET
2	1-E	23	CYS
2	1-E	25	SER
1	2-B	199	LEU
1	2-B	306	GLU
2	2-E	12	MET
2	2-E	23	CYS
2	2-E	25	SER
1	1-A	307	ASP
1	1-B	308	TYR
1	1-B	333	ALA
2	1-E	14	ARG
1	2-A	307	ASP
1	2-B	308	TYR
1	2-B	333	ALA
2	2-E	14	ARG
1	1-B	304	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1-E	8	PHE
1	2-B	304	ASN
2	2-E	8	PHE
1	1-B	254	ASP
1	2-B	254	ASP

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	1-A	329/390 (84%)	313 (95%)	16 (5%)	22	39
1	1-B	329/390 (84%)	311 (94%)	18 (6%)	19	34
1	2-A	329/390 (84%)	313 (95%)	16 (5%)	22	39
1	2-B	329/390 (84%)	311 (94%)	18 (6%)	19	34
2	1-E	15/15 (100%)	11 (73%)	4 (27%)	0	0
2	2-E	15/15 (100%)	11 (73%)	4 (27%)	0	0
All	All	1346/1590 (85%)	1270 (94%)	76 (6%)	19	33

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	10	VAL
1	1-A	11	LEU
1	1-A	35	LEU
1	1-A	48	LEU
1	1-A	71	LEU
1	1-A	79	ARG
1	1-A	85	LEU
1	1-A	87	LEU
1	1-A	115	LEU
1	1-A	120	GLN
1	1-A	144	LEU
1	1-A	172	LEU
1	1-A	184	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	188	ILE
1	1-A	210	GLU
1	1-A	231	ARG
1	1-B	11	LEU
1	1-B	35	LEU
1	1-B	71	LEU
1	1-B	85	LEU
1	1-B	87	LEU
1	1-B	115	LEU
1	1-B	144	LEU
1	1-B	166	ARG
1	1-B	184	LEU
1	1-B	235	THR
1	1-B	274	LEU
1	1-B	305	MET
1	1-B	307	ASP
1	1-B	308	TYR
1	1-B	317	HIS
1	1-B	331	LEU
1	1-B	355	ILE
1	1-B	380	GLU
2	1-E	12	MET
2	1-E	14	ARG
2	1-E	23	CYS
2	1-E	26	PHE
1	2-A	10	VAL
1	2-A	11	LEU
1	2-A	35	LEU
1	2-A	48	LEU
1	2-A	71	LEU
1	2-A	79	ARG
1	2-A	85	LEU
1	2-A	87	LEU
1	2-A	115	LEU
1	2-A	120	GLN
1	2-A	144	LEU
1	2-A	172	LEU
1	2-A	184	LEU
1	2-A	188	ILE
1	2-A	210	GLU
1	2-A	231	ARG
1	2-B	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	35	LEU
1	2-B	71	LEU
1	2-B	85	LEU
1	2-B	87	LEU
1	2-B	115	LEU
1	2-B	144	LEU
1	2-B	166	ARG
1	2-B	184	LEU
1	2-B	235	THR
1	2-B	274	LEU
1	2-B	305	MET
1	2-B	307	ASP
1	2-B	308	TYR
1	2-B	317	HIS
1	2-B	331	LEU
1	2-B	355	ILE
1	2-B	380	GLU
2	2-E	12	MET
2	2-E	14	ARG
2	2-E	23	CYS
2	2-E	26	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	205	ASN
1	1-A	207	GLN
1	1-A	232	HIS
1	1-B	120	GLN
1	1-B	205	ASN
1	1-B	230	HIS
1	1-B	345	GLN
1	1-B	358	GLN
1	2-A	205	ASN
1	2-A	207	GLN
1	2-A	232	HIS
1	2-B	120	GLN
1	2-B	205	ASN
1	2-B	230	HIS
1	2-B	345	GLN
1	2-B	358	GLN

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	$\# Z > 2$
3	NAG	1-C	1	3,1	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
3	NAG	1-C	2	3	14,14,15	0.46	0	17,19,21	0.88	1 (5%)
3	NAG	2-C	1	3,1	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
3	NAG	2-C	2	3	14,14,15	0.46	0	17,19,21	0.88	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
3	NAG	1-C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	1-C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	2-C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	2-C	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-C	2	NAG	C2-N2-C7	-2.93	118.98	122.90
3	2-C	2	NAG	C2-N2-C7	-2.93	118.98	122.90
3	1-C	1	NAG	C2-N2-C7	-2.40	119.68	122.90
3	2-C	1	NAG	C2-N2-C7	-2.40	119.68	122.90

There are no chirality outliers.

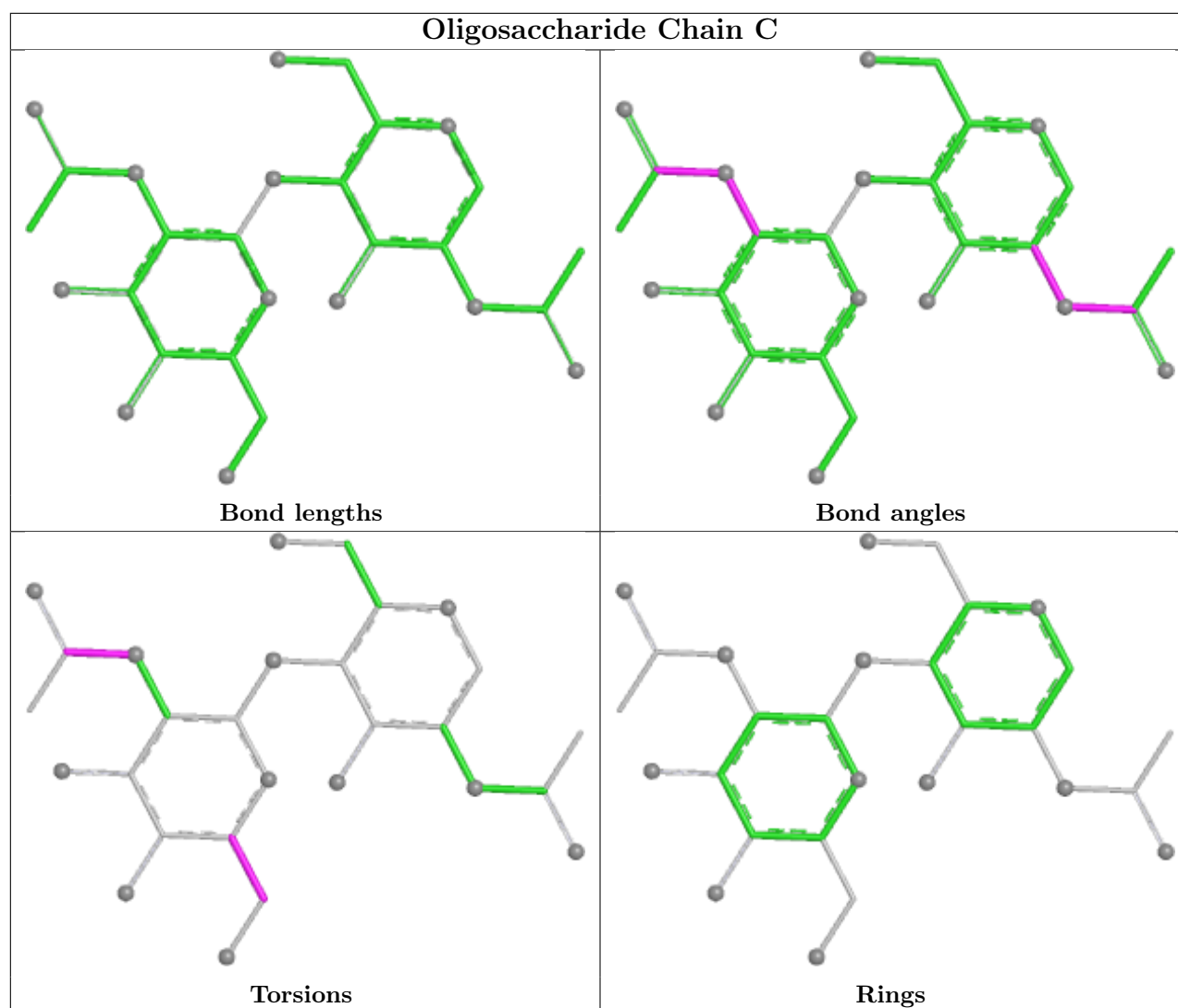
All (8) torsion outliers are listed below:

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

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
4	NAG	1-B	511	1	14,14,15	0.55	0	17,19,21	0.74	1 (5%)
4	NAG	2-A	511	1	14,14,15	0.69	0	17,19,21	0.68	1 (5%)
4	NAG	1-A	511	1	14,14,15	0.69	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	2-A	512	1	14,14,15	0.55	0	17,19,21	0.68	0
4	NAG	1-A	512	1	14,14,15	0.55	0	17,19,21	0.68	0
4	NAG	2-B	511	1	14,14,15	0.55	0	17,19,21	0.74	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
4	NAG	1-B	511	1	-	2/6/23/26	0/1/1/1
4	NAG	2-A	511	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	1-A	511	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	2-A	512	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	1-A	512	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	2-B	511	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-B	511	NAG	C2-N2-C7	-2.38	119.71	122.90
4	2-B	511	NAG	C2-N2-C7	-2.38	119.71	122.90
4	1-A	511	NAG	C2-N2-C7	-2.03	120.18	122.90
4	2-A	511	NAG	C2-N2-C7	-2.03	120.18	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	1-A	511	NAG	C1
4	2-A	511	NAG	C1
4	1-A	512	NAG	C1
4	2-A	512	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1-A	511	NAG	C8-C7-N2-C2
4	1-A	511	NAG	O7-C7-N2-C2
4	2-A	511	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	2-A	511	NAG	O7-C7-N2-C2
4	1-A	512	NAG	C8-C7-N2-C2
4	1-A	512	NAG	O7-C7-N2-C2
4	2-A	512	NAG	C8-C7-N2-C2
4	2-A	512	NAG	O7-C7-N2-C2
4	1-B	511	NAG	C8-C7-N2-C2
4	1-B	511	NAG	O7-C7-N2-C2
4	2-B	511	NAG	C8-C7-N2-C2
4	2-B	511	NAG	O7-C7-N2-C2
4	1-A	512	NAG	C4-C5-C6-O6
4	2-A	512	NAG	C4-C5-C6-O6
4	1-A	512	NAG	O5-C5-C6-O6
4	2-A	512	NAG	O5-C5-C6-O6
4	1-A	512	NAG	C3-C2-N2-C7
4	2-A	512	NAG	C3-C2-N2-C7

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	1-A	394/480 (82%)	-0.63	0 100 100	26, 47, 83, 96	0
1	1-B	394/480 (82%)	-0.56	1 (0%) 90 88	28, 51, 87, 98	0
1	2-A	0/480	-	-	-	-
1	2-B	0/480	-	-	-	-
2	1-E	21/21 (100%)	3.06	13 (61%) 0 0	28, 45, 49, 49	21 (100%)
2	2-E	0/21	-	-	-	-
All	All	809/1962 (41%)	-0.50	14 (1%) 69 65	26, 49, 85, 98	21 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-E	16	GLY	6.1
2	1-E	12	MET	5.6
2	1-E	23	CYS	5.1
2	1-E	20	GLY	4.6
2	1-E	19	SER	4.6
2	1-E	17	ALA	4.5
2	1-E	7	CYS	4.3
2	1-E	15	ILE	3.9
2	1-E	21	LEU	3.8
2	1-E	8	PHE	3.0
2	1-E	18	GLN	2.8
2	1-E	14	ARG	2.7
2	1-E	11	ARG	2.5
1	1-B	304	ASN	2.1

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

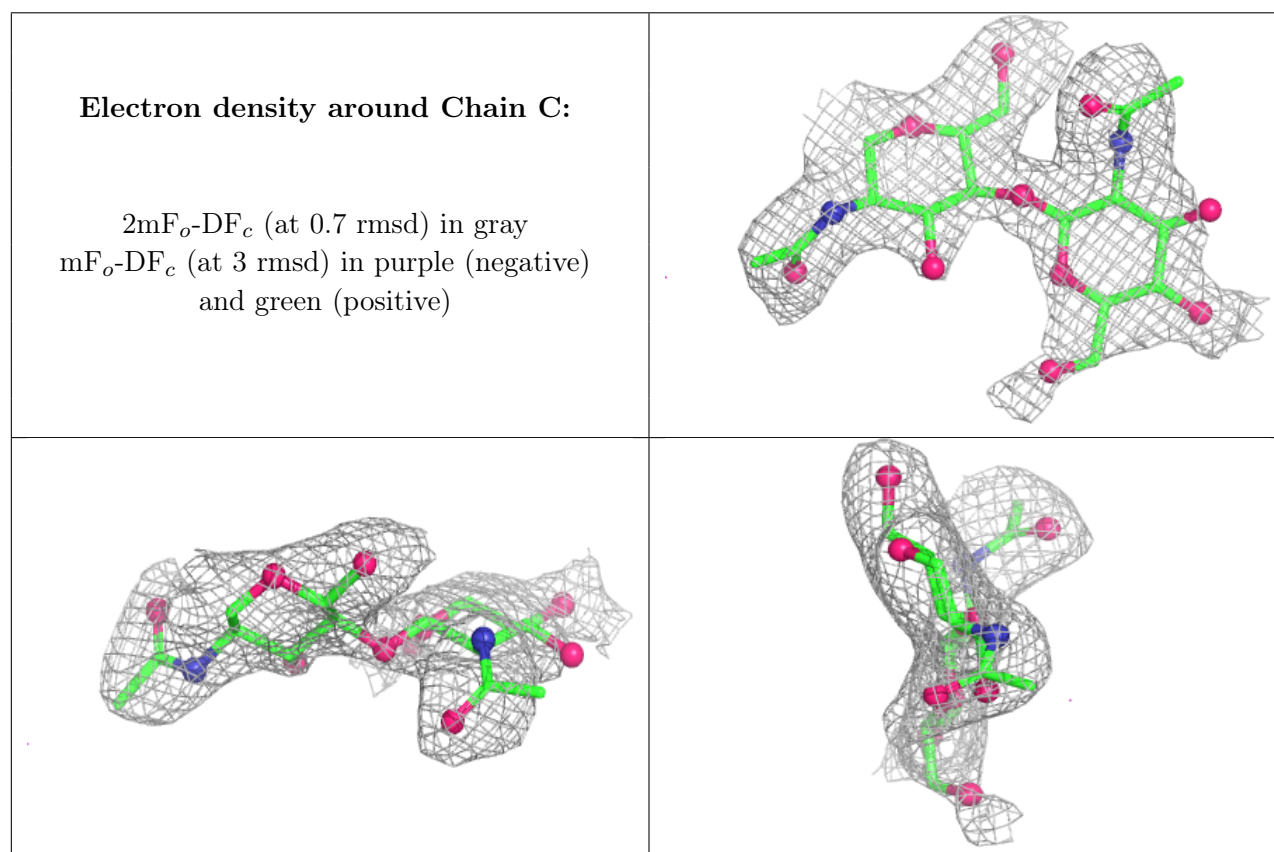
There are no non-standard protein/DNA/RNA residues in this entry.

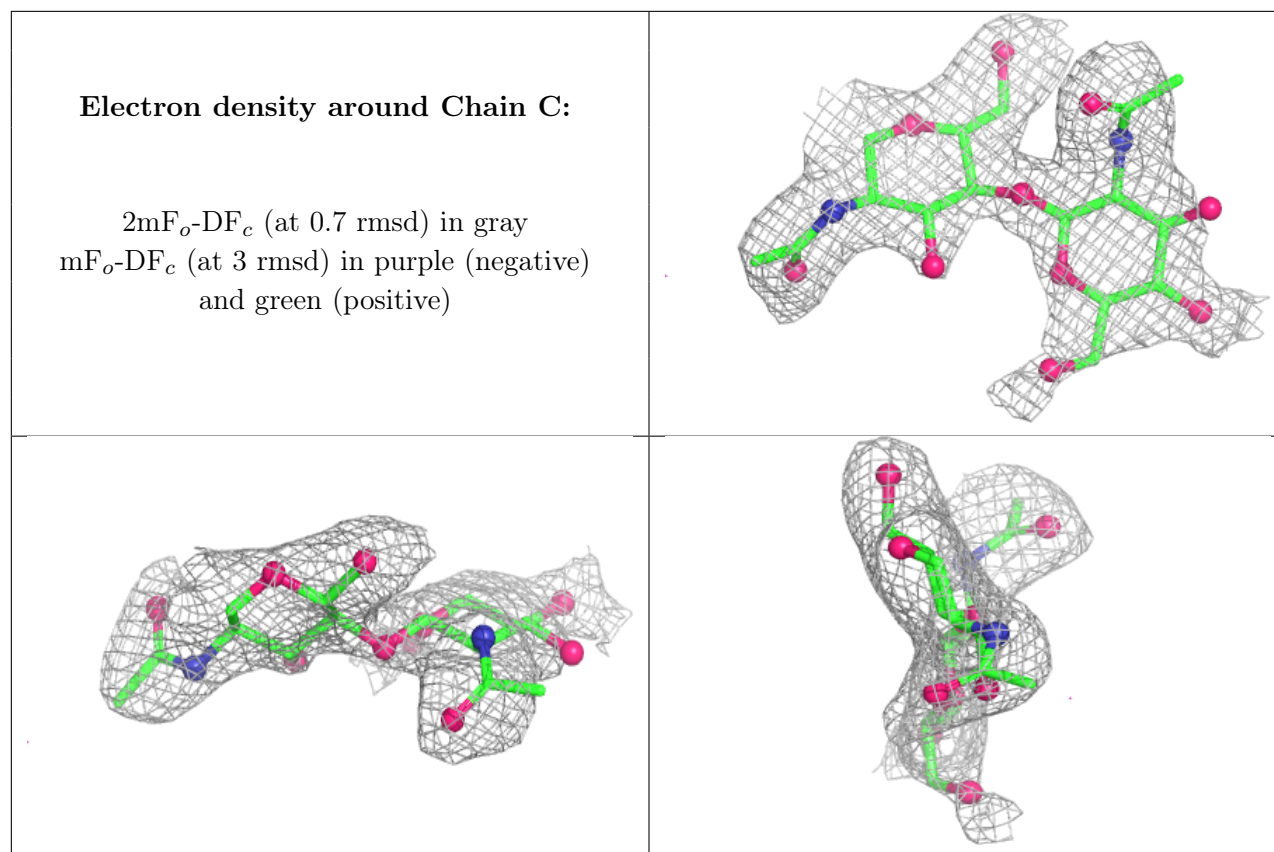
6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
3	NAG	1-C	1	14/15	-	-	57,61,65,71	0
3	NAG	2-C	1	14/15	-	-	57,61,65,71	0
3	NAG	1-C	2	14/15	-	-	76,79,81,81	0
3	NAG	2-C	2	14/15	-	-	76,79,81,81	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($\text{\AA}^2$)	Q<0.9
4	NAG	1-A	512	14/15	0.57	0.12	89,96,97,97	0
4	NAG	2-A	511	14/15	-	-	91,96,98,98	0
4	NAG	1-B	511	14/15	0.71	0.10	94,98,98,98	0
4	NAG	2-A	512	14/15	-	-	89,96,97,97	0
4	NAG	1-A	511	14/15	0.75	0.09	91,96,98,98	0
4	NAG	2-B	511	14/15	-	-	94,98,98,98	0
5	CL	1-A	513	1/1	0.94	0.04	36,36,36,36	0
5	CL	2-A	513	1/1	-	-	36,36,36,36	0
5	CL	1-B	512	1/1	0.98	0.02	35,35,35,35	0
5	CL	2-B	512	1/1	-	-	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.