



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:58 AM BST

PDB ID : 3LII  
Title : Recombinant human acetylcholinesterase  
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Deposited on : 2010-01-25  
Resolution : 3.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

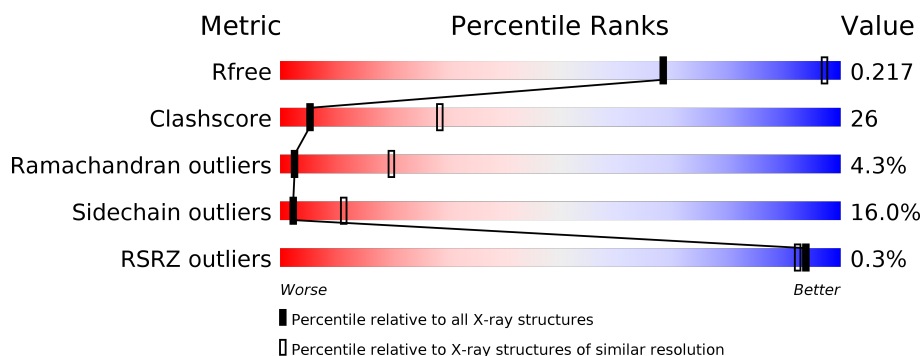
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	540	
1	B	540	
2	C	2	
2	D	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	1	X	-	-	-
2	NAG	D	1	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8448 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4154	2666	726	749	13			
1	B	532	Total	C	N	O	S	0	0	0
			4139	2658	721	747	13			

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

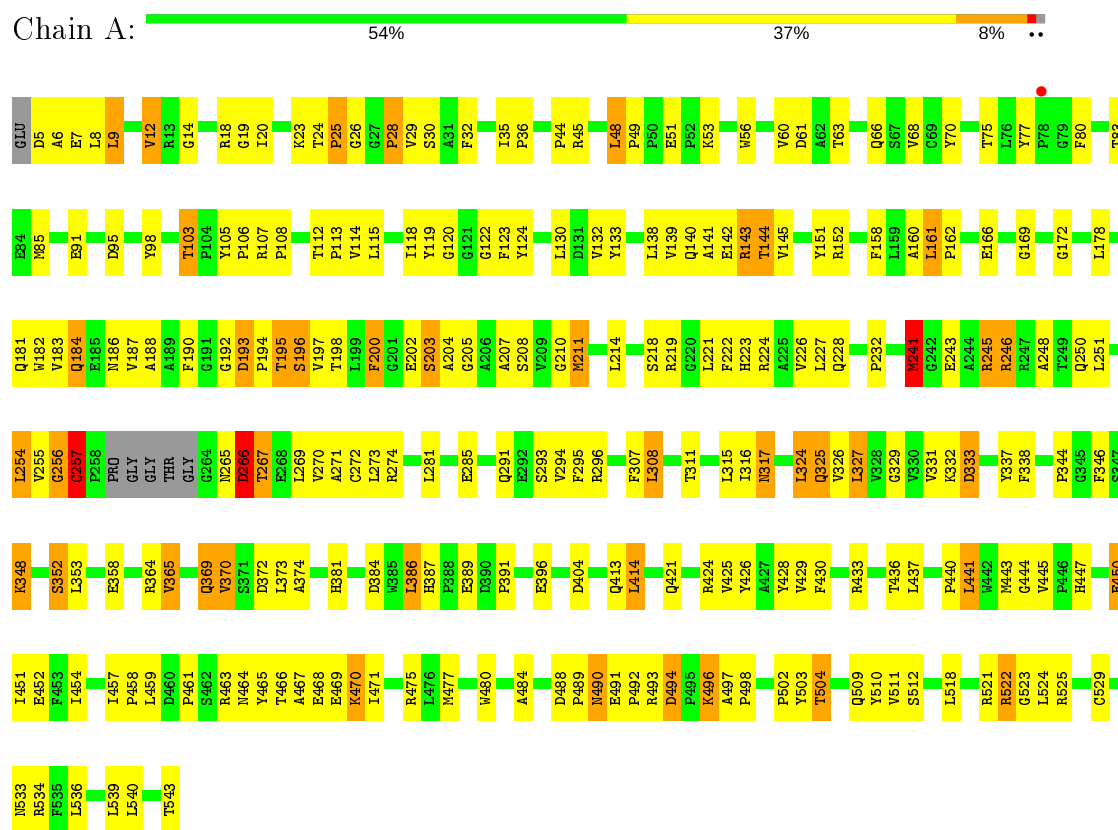
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	20	Total	O	0	0
			20	20		

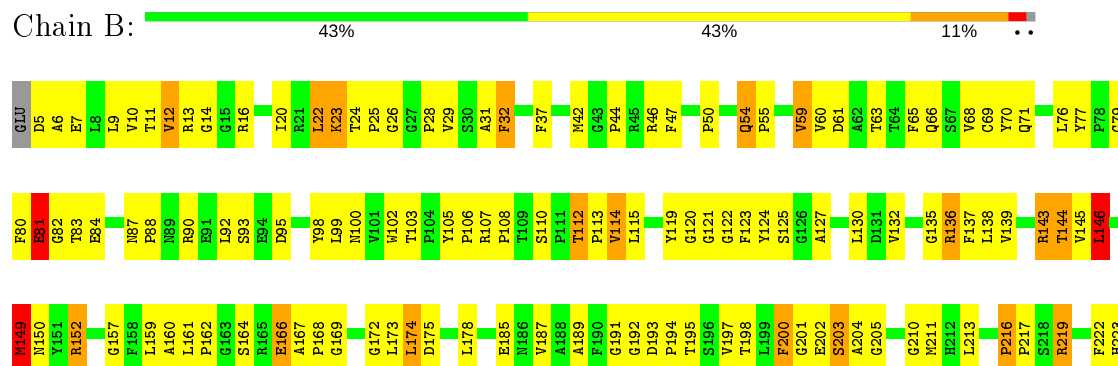
### 3 Residue-property plots

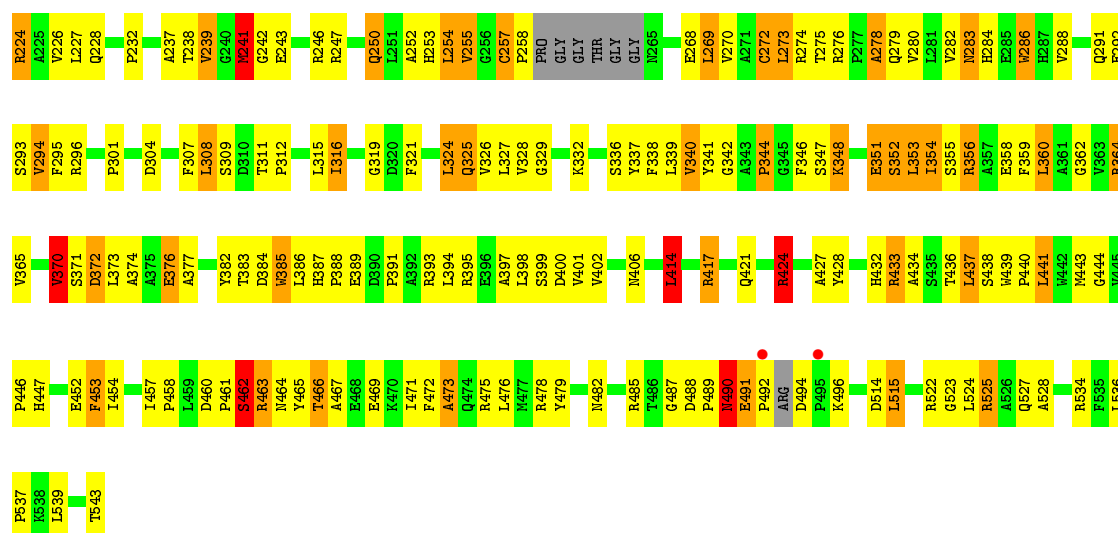
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



#### • Molecule 1: Acetylcholinesterase





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

Chain C: 100%

MAG1  
MAG2

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

Chain D: 100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.90Å 210.90Å 115.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.05 – 3.20 31.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.05-3.20) 99.7 (31.05-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.176 , 0.220 0.176 , 0.217	Depositor DCC
$R_{free}$ test set	2470 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, SO4

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	1.17	4/4281 (0.1%)	1.12	11/5851 (0.2%)
1	B	1.15	8/4265 (0.2%)	1.16	19/5829 (0.3%)
All	All	1.16	12/8546 (0.1%)	1.14	30/11680 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	GLU	CG-CD	11.26	1.68	1.51
1	A	529	CYS	CB-SG	10.33	1.99	1.82
1	B	376	GLU	CB-CG	10.09	1.71	1.52
1	A	51	GLU	CG-CD	6.38	1.61	1.51
1	B	81	GLU	CG-CD	6.16	1.61	1.51
1	B	286	TRP	CB-CG	-6.04	1.39	1.50
1	B	385	TRP	CB-CG	-5.80	1.39	1.50
1	B	166	GLU	CG-CD	5.59	1.60	1.51
1	B	364	ARG	CB-CG	5.42	1.67	1.52
1	B	424	ARG	CB-CG	5.25	1.66	1.52
1	A	68	VAL	CB-CG2	-5.12	1.42	1.52
1	A	331	VAL	CB-CG2	-5.00	1.42	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	A	152	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	B	417	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	152	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	B	130	LEU	CB-CG-CD1	-6.95	99.19	111.00
1	A	386	LEU	CA-CB-CG	-6.78	99.71	115.30
1	A	193	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	92	LEU	CB-CG-CD1	-6.54	99.88	111.00
1	B	149	MET	CG-SD-CE	6.36	110.37	100.20
1	B	370	VAL	N-CA-C	-6.36	93.83	111.00
1	A	470	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	A	95	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	360	LEU	CA-CB-CG	5.88	128.83	115.30
1	B	376	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	B	174	LEU	CA-CB-CG	-5.73	102.11	115.30
1	A	327	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	B	224	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	273	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	376	GLU	CB-CA-C	5.46	121.32	110.40
1	B	304	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	360	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	B	417	ARG	CG-CD-NE	5.18	122.67	111.80
1	B	120	GLY	N-CA-C	5.13	125.92	113.10
1	A	257	CYS	CA-CB-SG	5.10	123.19	114.00
1	B	273	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	146	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	296	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	9	LEU	CB-CG-CD2	5.03	119.55	111.00
1	B	414	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	B	174	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	TYR	Peptide
1	B	22	LEU	Peptide
1	B	490	ASN	Peptide
1	B	491	GLU	Peptide

## 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	4154	0	4039	183	0
1	B	4139	0	4022	257	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
3	A	30	0	0	1	0
3	B	15	0	0	1	0
4	A	34	0	0	1	0
4	B	20	0	0	4	0
All	All	8448	0	8111	435	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 26.

All (435) 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:351:GLU:HA	1:B:351:GLU:OE1	1.43	1.17
1:B:50:PRO:HG3	1:B:175:ASP:OD1	1.53	1.09
1:B:54:GLN:HA	1:B:54:GLN:HE21	1.08	1.08
1:A:426:TYR:CE1	1:A:489:PRO:HD2	1.95	1.00
1:B:417:ARG:NH2	4:B:649:HOH:O	1.91	0.96
1:B:354:ILE:O	1:B:391:PRO:HB3	1.66	0.96
1:B:54:GLN:HA	1:B:54:GLN:NE2	1.80	0.95
1:B:54:GLN:CA	1:B:54:GLN:HE21	1.82	0.93
1:A:24:THR:HG22	1:A:26:GLY:H	1.33	0.92
1:B:54:GLN:NE2	1:B:55:PRO:HD3	1.83	0.92
1:B:69:CYS:O	1:B:71:GLN:HG2	1.68	0.92
1:B:417:ARG:NH1	4:B:649:HOH:O	2.02	0.90
1:B:76:LEU:HD23	1:B:77:TYR:CE2	2.08	0.89
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.09	0.87
1:A:184:GLN:HA	1:A:184:GLN:HE21	1.40	0.86
1:A:224:ARG:NH1	1:A:484:ALA:O	2.09	0.86
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.40	0.86
1:B:433:ARG:CG	1:B:433:ARG:HH11	1.90	0.85
1:A:5:ASP:OD1	1:A:7:GLU:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:HD11	1:B:523:GLY:HA3	1.59	0.84
1:A:373:LEU:HD23	1:A:539:LEU:HD21	1.61	0.82
1:B:54:GLN:HE21	1:B:55:PRO:HD3	1.43	0.82
1:A:426:TYR:CD1	1:A:489:PRO:HD2	2.18	0.79
1:A:114:VAL:HG12	1:A:197:VAL:HG22	1.62	0.79
1:A:490:ASN:HD22	1:A:490:ASN:H	1.28	0.79
1:B:46:ARG:O	1:B:274:ARG:NH1	2.17	0.78
1:B:203:SER:HB2	1:B:447:HIS:NE2	2.00	0.77
1:B:433:ARG:HH21	1:B:441:LEU:HA	1.48	0.77
1:B:362:GLY:O	1:B:365:VAL:HG12	1.84	0.77
1:A:19:GLY:HA3	1:A:32:PHE:CE1	2.21	0.75
1:B:76:LEU:HD23	1:B:77:TYR:HE2	1.49	0.75
1:A:7:GLU:O	1:A:107:ARG:NH2	2.20	0.74
1:B:114:VAL:HG13	1:B:145:VAL:HB	1.69	0.74
1:A:324:LEU:HD22	1:A:326:VAL:HG12	1.70	0.74
1:A:195:THR:HA	1:A:223:HIS:NE2	2.02	0.73
1:B:108:PRO:HG2	1:B:112:THR:HG21	1.71	0.73
1:B:463:ARG:HG3	1:B:463:ARG:NH1	2.03	0.72
1:A:426:TYR:CD1	1:A:489:PRO:CD	2.73	0.72
1:B:293:SER:HA	1:B:365:VAL:HG22	1.73	0.71
1:A:108:PRO:HG3	1:A:112:THR:HG21	1.72	0.71
1:A:214:LEU:HB3	1:A:315:LEU:HD23	1.70	0.71
1:A:257:CYS:HB2	1:A:272:CYS:SG	2.29	0.71
1:B:340:VAL:O	1:B:340:VAL:HG23	1.91	0.70
1:B:348:LYS:O	1:B:440:PRO:HG3	1.91	0.70
1:A:490:ASN:H	1:A:490:ASN:ND2	1.88	0.70
1:A:270:VAL:HG12	1:A:274:ARG:HE	1.56	0.70
1:A:26:GLY:O	1:A:140:GLN:NE2	2.25	0.70
1:B:458:PRO:HG2	1:B:473:ALA:HB2	1.74	0.70
1:A:218:SER:HA	1:A:221:LEU:HD12	1.75	0.69
1:B:346:PHE:HA	1:B:352:SER:OG	1.92	0.69
1:A:265:ASN:CG	1:A:266:ASP:H	1.96	0.69
1:A:494:ASP:OD2	1:A:496:LYS:HB3	1.92	0.69
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.56	0.69
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.22	0.69
1:B:316:ILE:HD11	1:B:414:LEU:HD12	1.73	0.69
1:B:77:TYR:CE1	1:B:348:LYS:HG3	2.28	0.69
1:B:444:GLY:O	1:B:446:PRO:HD3	1.93	0.68
1:A:327:LEU:HD12	1:A:426:TYR:O	1.92	0.68
1:B:42:MET:O	1:B:44:PRO:HD2	1.93	0.68
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:THR:HB	3:A:1011:SO4:O4	1.94	0.68
1:B:115:LEU:HD23	1:B:198:THR:HB	1.75	0.68
1:B:77:TYR:CE1	1:B:348:LYS:CD	2.77	0.68
1:A:224:ARG:HD3	1:A:325:GLN:HE21	1.59	0.68
1:B:370:VAL:HG13	1:B:374:ALA:HB3	1.76	0.67
1:A:160:ALA:HB2	1:A:169:GLY:HA2	1.75	0.67
1:B:351:GLU:CA	1:B:351:GLU:OE1	2.31	0.67
1:B:50:PRO:CG	1:B:175:ASP:OD1	2.36	0.67
1:B:77:TYR:CE1	1:B:348:LYS:CG	2.77	0.67
1:B:434:ALA:O	1:B:437:LEU:HB2	1.95	0.66
1:A:457:ILE:N	1:A:458:PRO:CD	2.59	0.66
1:B:433:ARG:NH2	1:B:439:TRP:O	2.27	0.66
1:A:183:VAL:O	1:A:187:VAL:HG12	1.96	0.66
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.11	0.66
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.31	0.65
1:A:114:VAL:CG2	1:A:145:VAL:HB	2.26	0.65
1:A:197:VAL:HG12	1:A:222:PHE:HA	1.76	0.65
1:B:32:PHE:CD2	1:B:32:PHE:N	2.64	0.65
1:B:488:ASP:OD1	1:B:490:ASN:ND2	2.30	0.64
1:B:195:THR:HA	1:B:223:HIS:CE1	2.32	0.64
1:A:425:VAL:C	1:A:426:TYR:HD2	2.02	0.63
1:B:112:THR:HG23	1:B:191:GLY:O	1.99	0.63
1:A:370:VAL:HG13	1:A:374:ALA:HB3	1.80	0.63
1:B:453:PHE:CD1	1:B:453:PHE:N	2.64	0.63
1:B:76:LEU:HD23	1:B:77:TYR:CD2	2.33	0.63
1:A:294:VAL:HG21	1:A:338:PHE:O	1.98	0.62
1:B:354:ILE:HG22	1:B:358:GLU:OE1	1.99	0.62
1:B:137:PHE:CZ	1:B:460:ASP:HB2	2.34	0.62
1:A:381:HIS:HB3	4:A:607:HOH:O	1.99	0.62
1:B:219:ARG:HH11	1:B:219:ARG:HG2	1.65	0.62
1:A:373:LEU:CD2	1:A:539:LEU:HD21	2.29	0.61
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.34	0.61
1:A:468:GLU:HA	1:A:471:ILE:HD12	1.81	0.61
1:B:22:LEU:HD13	1:B:136:ARG:HH21	1.65	0.61
1:B:316:ILE:CD1	1:B:414:LEU:HD12	2.31	0.61
1:B:255:VAL:HG23	1:B:284:HIS:ND1	2.16	0.61
1:B:253:HIS:O	1:B:255:VAL:N	2.33	0.60
1:B:216:PRO:HB2	1:B:217:PRO:HD3	1.83	0.60
1:B:461:PRO:C	1:B:463:ARG:H	2.04	0.60
1:B:87:ASN:HB3	1:B:88:PRO:HD2	1.84	0.60
1:B:12:VAL:HG12	1:B:14:GLY:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ALA:O	1:A:211:MET:HG2	2.01	0.60
1:B:80:PHE:HZ	1:B:438:SER:O	1.84	0.60
1:A:184:GLN:HA	1:A:184:GLN:NE2	2.14	0.60
1:A:19:GLY:CA	1:A:32:PHE:CE1	2.85	0.60
1:B:433:ARG:HH11	1:B:433:ARG:HG3	1.67	0.60
1:A:56:TRP:NE1	1:A:60:VAL:HG23	2.16	0.59
1:B:32:PHE:HD2	1:B:32:PHE:N	2.00	0.59
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.66	0.59
1:A:522:ARG:HH22	1:B:387:HIS:CE1	2.20	0.59
1:B:321:PHE:O	1:B:324:LEU:HB2	2.01	0.59
1:B:203:SER:HB2	1:B:447:HIS:CE1	2.37	0.59
1:B:432:HIS:ND1	1:B:515:LEU:HD11	2.18	0.59
1:A:183:VAL:HG13	1:A:187:VAL:HB	1.84	0.59
1:B:200:PHE:CB	1:B:226:VAL:HB	2.32	0.59
1:A:466:THR:O	1:A:469:GLU:HB2	2.03	0.59
1:B:342:GLY:O	1:B:344:PRO:HD3	2.02	0.59
1:B:54:GLN:HE21	1:B:55:PRO:CD	2.15	0.59
1:A:344:PRO:HB2	1:A:358:GLU:HG2	1.86	0.58
1:A:413:GLN:HE21	1:A:533:ASN:HB3	1.68	0.58
1:B:84:GLU:HA	1:B:87:ASN:HD22	1.68	0.58
1:A:114:VAL:HG21	1:A:187:VAL:HG21	1.86	0.57
1:B:172:GLY:O	1:B:175:ASP:HB2	2.03	0.57
1:A:115:LEU:HD23	1:A:198:THR:HB	1.86	0.57
1:B:270:VAL:O	1:B:273:LEU:HB3	2.04	0.57
1:B:65:PHE:HB2	1:B:90:ARG:NH1	2.18	0.57
1:A:192:GLY:O	1:A:194:PRO:HD3	2.05	0.57
1:B:77:TYR:CE1	1:B:348:LYS:HD2	2.39	0.57
1:A:200:PHE:CB	1:A:226:VAL:HB	2.35	0.57
1:A:203:SER:HB2	1:A:447:HIS:NE2	2.20	0.57
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.87	0.57
1:B:77:TYR:CD1	1:B:348:LYS:CE	2.88	0.57
1:B:453:PHE:H	1:B:453:PHE:HD1	1.51	0.57
1:B:102:TRP:HB3	1:B:139:VAL:HG21	1.87	0.56
1:A:119:TYR:CE1	1:A:151:TYR:CE2	2.94	0.56
1:B:31:ALA:C	1:B:32:PHE:CD2	2.79	0.56
1:A:227:LEU:HD12	1:A:227:LEU:N	2.20	0.56
1:B:491:GLU:OE1	1:B:492:PRO:HD3	2.06	0.56
1:B:68:VAL:HG22	1:B:127:ALA:CB	2.36	0.56
1:A:256:GLY:O	1:A:257:CYS:CB	2.53	0.56
1:A:106:PRO:O	1:A:107:ARG:C	2.43	0.55
1:B:37:PHE:HD1	1:B:178:LEU:HD23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG11	1:B:443:MET:CE	2.36	0.55
1:A:193:ASP:OD1	1:A:195:THR:N	2.36	0.55
1:A:490:ASN:N	1:A:490:ASN:ND2	2.53	0.55
1:A:106:PRO:HG2	1:A:143:ARG:NH1	2.21	0.55
1:B:20:ILE:CG2	1:B:63:THR:HA	2.37	0.55
1:B:278:ALA:O	1:B:280:VAL:N	2.40	0.55
1:B:77:TYR:CD1	1:B:348:LYS:NZ	2.75	0.55
1:A:114:VAL:HG22	1:A:145:VAL:HB	1.89	0.55
1:A:80:PHE:CD1	1:A:348:LYS:HE2	2.42	0.55
1:B:213:LEU:HD23	1:B:222:PHE:HZ	1.72	0.55
1:B:202:GLU:HA	1:B:228:GLN:O	2.07	0.55
1:A:162:PRO:HD2	1:A:245:ARG:NH1	2.22	0.54
1:B:453:PHE:HD1	1:B:453:PHE:N	2.05	0.54
1:A:120:GLY:HA2	1:A:205:GLY:H	1.73	0.54
1:B:102:TRP:CB	1:B:139:VAL:HG21	2.38	0.54
1:B:213:LEU:HD23	1:B:222:PHE:CZ	2.42	0.54
1:A:257:CYS:CB	1:A:272:CYS:SG	2.95	0.54
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.90	0.54
1:A:5:ASP:O	1:A:7:GLU:N	2.40	0.54
1:B:54:GLN:NE2	1:B:55:PRO:CD	2.65	0.54
1:B:389:GLU:OE1	1:B:389:GLU:HA	2.08	0.53
1:A:387:HIS:CE1	1:B:522:ARG:HH22	2.26	0.53
1:A:210:GLY:HA3	1:A:232:PRO:HD3	1.90	0.53
1:B:113:PRO:HG2	1:B:144:THR:HG22	1.91	0.53
1:B:312:PRO:O	1:B:316:ILE:HB	2.08	0.53
1:A:496:LYS:HD2	1:A:496:LYS:C	2.28	0.53
1:A:114:VAL:CG1	1:A:197:VAL:HG22	2.35	0.53
1:A:291:GLN:OE1	1:A:369:GLN:HB3	2.09	0.53
1:B:539:LEU:HD23	1:B:539:LEU:C	2.30	0.53
1:A:450:GLU:HG2	1:A:451:ILE:N	2.24	0.53
1:A:265:ASN:CG	1:A:266:ASP:N	2.62	0.52
1:A:246:ARG:HH21	1:A:250:GLN:HG2	1.73	0.52
1:B:339:LEU:C	1:B:341:TYR:H	2.13	0.52
1:A:24:THR:HG22	1:A:26:GLY:N	2.15	0.52
1:A:36:PRO:HB2	1:A:53:LYS:HG2	1.91	0.52
1:B:339:LEU:O	1:B:341:TYR:N	2.42	0.52
1:A:203:SER:HB2	1:A:447:HIS:CE1	2.45	0.52
1:B:160:ALA:HB2	1:B:169:GLY:HA2	1.91	0.52
1:A:457:ILE:N	1:A:458:PRO:HD2	2.23	0.52
1:A:426:TYR:HE1	1:A:489:PRO:HD2	1.65	0.52
1:B:13:ARG:NH2	1:B:185:GLU:HG2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:HG3	1:B:485:ARG:HG2	1.91	0.52
1:B:528:ALA:N	3:B:1016:SO4:O3	2.43	0.52
1:B:37:PHE:CD2	1:B:99:LEU:HD23	2.45	0.51
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.92	0.51
1:A:227:LEU:CD1	1:A:227:LEU:N	2.73	0.51
1:B:137:PHE:HZ	1:B:460:ASP:HB2	1.75	0.51
1:B:24:THR:HG22	1:B:26:GLY:H	1.76	0.51
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.46	0.51
1:A:29:VAL:HG22	1:A:140:GLN:HB2	1.93	0.51
1:A:543:THR:HG22	1:B:543:THR:HG22	1.91	0.51
1:B:250:GLN:HE21	1:B:288:VAL:HA	1.74	0.51
1:A:12:VAL:HG12	1:A:14:GLY:H	1.75	0.51
1:A:488:ASP:OD1	1:A:490:ASN:ND2	2.44	0.51
1:B:382:TYR:CG	1:B:401:VAL:HG22	2.45	0.51
1:B:307:PHE:HD1	1:B:308:LEU:HD13	1.74	0.51
1:B:472:PHE:CE1	1:B:514:ASP:O	2.64	0.51
1:B:138:LEU:HD23	1:B:146:LEU:HD23	1.91	0.51
1:B:325:GLN:HE21	1:B:487:GLY:HA3	1.74	0.51
1:A:266:ASP:O	1:A:269:LEU:N	2.44	0.51
1:B:250:GLN:HG3	1:B:288:VAL:HG12	1.93	0.51
1:B:124:TYR:CD1	1:B:125:SER:HB3	2.45	0.51
1:A:195:THR:O	1:A:196:SER:C	2.50	0.50
1:B:482:ASN:ND2	1:B:492:PRO:HG3	2.26	0.50
1:A:202:GLU:HG3	1:A:451:ILE:HD11	1.94	0.50
1:B:257:CYS:HB2	1:B:258:PRO:HA	1.93	0.50
1:B:417:ARG:CZ	4:B:649:HOH:O	2.30	0.50
1:A:162:PRO:HG2	1:A:241:MET:HB3	1.93	0.50
1:B:110:SER:O	1:B:112:THR:HG22	2.11	0.50
1:B:355:SER:O	1:B:356:ARG:C	2.48	0.50
1:A:226:VAL:C	1:A:227:LEU:HD12	2.31	0.50
1:A:138:LEU:HD12	1:A:477:MET:HB3	1.92	0.50
1:B:84:GLU:HA	1:B:87:ASN:ND2	2.26	0.50
1:A:333:ASP:OD2	1:A:444:GLY:HA3	2.12	0.50
1:A:122:GLY:O	1:A:123:PHE:HB2	2.12	0.49
1:A:44:PRO:O	1:A:274:ARG:NH1	2.45	0.49
1:B:13:ARG:NH1	1:B:185:GLU:HG2	2.27	0.49
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.95	0.49
1:A:161:LEU:HD13	1:A:248:ALA:HB3	1.95	0.49
1:B:328:VAL:O	1:B:427:ALA:HA	2.13	0.49
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.47	0.49
1:A:141:ALA:O	1:A:142:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:NAG:O3	2:D:2:NAG:O5	2.29	0.49
1:B:383:THR:HG22	1:B:384:ASP:N	2.28	0.49
1:B:316:ILE:HD11	1:B:414:LEU:CD1	2.43	0.48
1:B:433:ARG:HH21	1:B:441:LEU:CA	2.23	0.48
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.48	0.48
1:A:256:GLY:O	1:A:257:CYS:HB3	2.12	0.48
1:B:10:VAL:CG1	1:B:11:THR:N	2.76	0.48
1:B:292:GLU:O	1:B:365:VAL:HG23	2.14	0.48
1:B:77:TYR:CE1	1:B:348:LYS:CE	2.96	0.48
1:B:5:ASP:O	1:B:7:GLU:N	2.46	0.48
1:A:426:TYR:N	1:A:426:TYR:HD2	2.11	0.48
1:B:255:VAL:O	1:B:255:VAL:HG13	2.13	0.48
1:B:467:ALA:O	1:B:471:ILE:HD12	2.13	0.48
1:B:61:ASP:OD2	1:B:63:THR:HG23	2.14	0.48
1:A:197:VAL:H	1:A:223:HIS:HD2	1.61	0.48
1:B:472:PHE:O	1:B:475:ARG:N	2.47	0.48
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.49	0.48
1:B:195:THR:HA	1:B:223:HIS:HE1	1.77	0.48
1:B:237:ALA:O	1:B:301:PRO:HD2	2.14	0.48
1:A:202:GLU:HA	1:A:228:GLN:O	2.13	0.48
1:B:400:ASP:O	1:B:401:VAL:C	2.49	0.48
1:B:382:TYR:CD2	1:B:401:VAL:HG22	2.48	0.48
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.49	0.48
1:B:201:GLY:O	1:B:228:GLN:HB2	2.14	0.48
1:B:162:PRO:HG2	1:B:241:MET:HB3	1.96	0.48
1:B:193:ASP:O	1:B:195:THR:N	2.47	0.48
1:B:374:ALA:O	1:B:377:ALA:HB3	2.14	0.48
1:B:81:GLU:HB2	1:B:438:SER:HB3	1.95	0.48
1:B:46:ARG:O	1:B:47:PHE:HB2	2.13	0.48
1:B:80:PHE:CZ	1:B:438:SER:O	2.67	0.47
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.95	0.47
1:A:317:ASN:O	1:A:421:GLN:NE2	2.46	0.47
1:B:42:MET:O	1:B:44:PRO:CD	2.62	0.47
1:B:351:GLU:HB3	1:B:353:LEU:HG	1.96	0.47
1:A:112:THR:OG1	1:A:113:PRO:HD2	2.14	0.47
1:A:426:TYR:N	1:A:426:TYR:CD2	2.82	0.47
1:B:24:THR:O	1:B:26:GLY:N	2.48	0.47
1:B:402:VAL:O	1:B:406:ASN:HB2	2.14	0.47
1:B:354:ILE:HD11	1:B:395:ARG:HA	1.96	0.47
1:B:79:GLY:HA2	1:B:84:GLU:HG3	1.97	0.47
1:A:384:ASP:C	1:A:384:ASP:OD1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:SER:O	1:B:337:TYR:C	2.51	0.47
1:A:246:ARG:NH2	1:A:250:GLN:HG2	2.28	0.47
1:B:373:LEU:HD23	1:B:543:THR:HG21	1.97	0.47
1:A:118:ILE:HG22	1:A:205:GLY:HA2	1.96	0.47
1:A:197:VAL:H	1:A:223:HIS:CD2	2.33	0.47
1:B:135:GLY:O	1:B:136:ARG:C	2.53	0.47
1:A:29:VAL:HG12	1:A:103:THR:O	2.15	0.46
1:B:294:VAL:HG21	1:B:338:PHE:O	2.14	0.46
1:A:106:PRO:HG2	1:A:143:ARG:HH12	1.80	0.46
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.95	0.46
1:B:13:ARG:CZ	1:B:185:GLU:HG2	2.45	0.46
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.79	0.46
1:A:522:ARG:NH2	1:B:387:HIS:CE1	2.84	0.46
1:B:491:GLU:HB3	1:B:494:ASP:OD1	2.15	0.46
1:B:536:LEU:N	1:B:537:PRO:CD	2.78	0.46
1:A:8:LEU:HD23	1:A:8:LEU:N	2.31	0.46
1:B:54:GLN:CA	1:B:54:GLN:NE2	2.55	0.46
1:A:429:VAL:O	1:A:429:VAL:HG12	2.15	0.46
1:A:457:ILE:H	1:A:458:PRO:CD	2.28	0.46
1:B:433:ARG:HG2	1:B:433:ARG:NH1	2.27	0.46
1:B:68:VAL:HG22	1:B:127:ALA:HB1	1.97	0.46
1:A:467:ALA:HA	1:A:470:LYS:HG3	1.96	0.46
1:B:463:ARG:NH1	1:B:463:ARG:CG	2.77	0.46
1:B:149:MET:HG2	1:B:150:ASN:N	2.25	0.46
1:B:197:VAL:HB	1:B:222:PHE:HA	1.98	0.46
1:B:340:VAL:CG1	1:B:443:MET:CE	2.93	0.46
1:A:337:TYR:HA	1:A:443:MET:CE	2.46	0.46
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.51	0.46
1:A:77:TYR:CE1	1:A:348:LYS:HG2	2.50	0.46
1:A:28:PRO:HG2	1:A:105:TYR:CD1	2.52	0.45
1:B:149:MET:H	1:B:149:MET:HE3	1.81	0.45
1:B:202:GLU:O	1:B:205:GLY:N	2.49	0.45
1:B:228:GLN:HG2	1:B:428:TYR:OH	2.16	0.45
1:B:398:LEU:O	1:B:398:LEU:HG	2.16	0.45
1:A:353:LEU:HD22	1:A:391:PRO:HB2	1.97	0.45
1:A:251:LEU:HA	1:A:254:LEU:HD12	1.99	0.45
1:A:433:ARG:NH2	1:A:441:LEU:HA	2.32	0.45
1:A:113:PRO:HG2	1:A:144:THR:HG22	1.98	0.45
1:A:511:VAL:HG11	1:A:518:LEU:HD13	1.96	0.45
1:B:80:PHE:CD2	1:B:348:LYS:NZ	2.82	0.45
1:B:29:VAL:HG13	1:B:103:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.31	0.45
1:B:253:HIS:C	1:B:255:VAL:H	2.19	0.45
1:A:32:PHE:CD2	1:A:190:PHE:HE1	2.35	0.45
1:B:164:SER:C	1:B:166:GLU:H	2.20	0.45
1:B:274:ARG:CG	1:B:274:ARG:HH11	2.30	0.45
1:B:77:TYR:CE1	1:B:348:LYS:HE3	2.51	0.45
1:A:193:ASP:O	1:A:195:THR:O	2.34	0.45
1:B:44:PRO:HA	1:B:274:ARG:HD3	1.99	0.45
1:B:536:LEU:HB3	1:B:537:PRO:HD3	1.99	0.45
1:A:497:ALA:HB1	1:A:498:PRO:HD2	1.98	0.44
1:A:430:PHE:CD1	1:A:430:PHE:C	2.91	0.44
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.60	0.44
1:B:276:ARG:HG2	1:B:276:ARG:NH1	2.31	0.44
1:B:93:SER:OG	1:B:95:ASP:N	2.49	0.44
1:B:370:VAL:HG13	1:B:374:ALA:CB	2.45	0.44
1:B:187:VAL:HG22	1:B:192:GLY:HA3	2.00	0.44
1:A:178:LEU:HA	1:A:181:GLN:HG3	1.99	0.44
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.33	0.44
1:B:336:SER:HA	1:B:339:LEU:HD12	1.99	0.44
1:B:458:PRO:HG2	1:B:473:ALA:CB	2.44	0.44
1:A:333:ASP:OD2	1:A:445:VAL:N	2.48	0.44
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.42	0.44
1:A:166:GLU:HB3	1:A:270:VAL:HG11	1.99	0.44
1:B:316:ILE:HD13	1:B:316:ILE:HG21	1.60	0.44
1:A:316:ILE:CD1	1:A:414:LEU:HD12	2.48	0.44
1:B:106:PRO:O	1:B:107:ARG:C	2.57	0.44
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.77	0.44
1:B:238:THR:HG22	1:B:301:PRO:HB2	1.99	0.44
1:B:454:ILE:HD13	1:B:476:LEU:HB3	2.00	0.44
1:A:24:THR:O	1:A:25:PRO:C	2.57	0.43
1:A:492:PRO:HD2	1:A:493:ARG:H	1.82	0.43
1:B:359:PHE:CG	1:B:394:LEU:HD22	2.53	0.43
1:A:19:GLY:N	1:A:32:PHE:HE1	2.16	0.43
1:B:336:SER:OG	1:B:337:TYR:N	2.51	0.43
1:B:37:PHE:CD1	1:B:178:LEU:HD23	2.52	0.43
1:B:275:THR:O	1:B:276:ARG:C	2.54	0.43
1:B:324:LEU:HA	1:B:324:LEU:HD23	1.67	0.43
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.81	0.43
1:B:465:TYR:HD2	1:B:469:GLU:OE1	2.01	0.43
1:A:118:ILE:O	1:A:118:ILE:HG22	2.18	0.43
1:A:195:THR:CA	1:A:223:HIS:NE2	2.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HA	1:A:36:PRO:HD2	1.89	0.43
1:A:459:LEU:N	1:A:459:LEU:HD23	2.33	0.43
1:B:274:ARG:HH11	1:B:274:ARG:HG2	1.84	0.43
1:B:387:HIS:N	1:B:388:PRO:HD3	2.34	0.43
1:A:203:SER:OG	1:A:204:ALA:N	2.51	0.43
1:A:139:VAL:HG22	1:A:144:THR:O	2.19	0.43
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.54	0.43
1:A:45:ARG:O	1:A:48:LEU:HB2	2.19	0.43
1:B:372:ASP:OD1	1:B:372:ASP:N	2.52	0.43
1:A:187:VAL:HG22	1:A:192:GLY:HA3	2.00	0.43
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.79	0.43
1:B:167:ALA:HA	1:B:168:PRO:HD3	1.80	0.43
1:B:226:VAL:HA	1:B:327:LEU:O	2.19	0.43
1:A:107:ARG:O	1:A:108:PRO:C	2.57	0.43
1:A:265:ASN:O	1:A:267:THR:N	2.52	0.43
1:B:371:SER:O	1:B:374:ALA:HB3	2.19	0.43
1:B:82:GLY:N	1:B:438:SER:OG	2.48	0.43
1:A:195:THR:C	1:A:223:HIS:CD2	2.92	0.42
1:A:5:ASP:C	1:A:7:GLU:H	2.22	0.42
1:B:286:TRP:CD1	1:B:286:TRP:N	2.87	0.42
1:B:336:SER:O	1:B:338:PHE:N	2.52	0.42
1:B:80:PHE:CG	1:B:348:LYS:NZ	2.78	0.42
1:A:364:ARG:HD2	1:A:364:ARG:HA	1.69	0.42
1:B:457:ILE:O	1:B:458:PRO:C	2.56	0.42
1:B:527:GLN:HE21	1:B:527:GLN:HB3	1.53	0.42
1:A:426:TYR:HD1	1:A:489:PRO:CG	2.32	0.42
1:B:200:PHE:HB3	1:B:226:VAL:HB	2.00	0.42
1:B:243:GLU:OE2	1:B:247:ARG:NE	2.40	0.42
1:B:268:GLU:O	1:B:272:CYS:HB2	2.19	0.42
1:B:525:ARG:NH1	4:B:620:HOH:O	2.51	0.42
1:A:293:SER:HA	1:A:365:VAL:HG23	2.01	0.42
1:B:193:ASP:C	1:B:195:THR:N	2.73	0.42
1:B:354:ILE:H	1:B:354:ILE:HG13	1.60	0.42
1:A:140:GLN:C	1:A:140:GLN:CD	2.78	0.42
1:A:493:ARG:O	1:A:494:ASP:HB2	2.19	0.42
1:A:510:TYR:HE1	1:A:523:GLY:O	2.02	0.42
1:B:77:TYR:HE1	1:B:348:LYS:HG3	1.82	0.42
1:B:319:GLY:H	1:B:421:GLN:HE22	1.67	0.42
1:B:460:ASP:OD1	1:B:462:SER:HB3	2.20	0.42
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.54	0.42
1:B:123:PHE:CZ	1:B:204:ALA:HB1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:CG2	1:B:338:PHE:O	2.67	0.42
1:A:124:TYR:CD1	1:A:124:TYR:C	2.93	0.42
1:B:115:LEU:CD2	1:B:198:THR:HB	2.46	0.42
1:B:424:ARG:HB2	1:B:424:ARG:HE	1.49	0.42
1:B:432:HIS:CE1	1:B:515:LEU:HD11	2.55	0.42
1:A:158:PHE:CZ	1:A:172:GLY:HA3	2.54	0.42
1:A:243:GLU:OE1	1:A:246:ARG:HD3	2.20	0.42
1:A:307:PHE:HD1	1:A:308:LEU:HD13	1.85	0.42
1:B:87:ASN:CB	1:B:88:PRO:HD2	2.45	0.42
1:A:425:VAL:C	1:A:426:TYR:CD2	2.88	0.41
1:B:77:TYR:CZ	1:B:348:LYS:HG3	2.54	0.41
1:A:522:ARG:NH2	1:B:387:HIS:HE1	2.18	0.41
1:A:182:TRP:O	1:A:186:ASN:HB2	2.20	0.41
1:A:452:GLU:O	1:A:457:ILE:HG12	2.20	0.41
1:B:22:LEU:HD22	1:B:23:LYS:HE3	2.02	0.41
1:B:31:ALA:C	1:B:32:PHE:HD2	2.20	0.41
1:A:271:ALA:HA	1:A:274:ARG:HD2	2.02	0.41
1:A:337:TYR:HA	1:A:443:MET:HE2	2.03	0.41
1:B:16:ARG:HD2	1:B:59:VAL:HG12	2.02	0.41
1:B:252:ALA:CB	1:B:269:LEU:HD21	2.50	0.41
1:B:280:VAL:O	1:B:283:ASN:HB2	2.20	0.41
1:B:479:TYR:HA	1:B:489:PRO:O	2.20	0.41
1:A:32:PHE:CD2	1:A:190:PHE:CE1	3.09	0.41
1:B:315:LEU:HA	1:B:315:LEU:HD12	1.66	0.41
1:B:339:LEU:HA	1:B:339:LEU:HD23	1.68	0.41
1:A:251:LEU:HD21	1:A:281:LEU:HD22	2.03	0.41
1:A:458:PRO:HG3	1:A:465:TYR:CD2	2.56	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.56	0.41
1:B:276:ARG:HB3	1:B:280:VAL:HG21	2.03	0.41
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.86	0.41
1:B:393:ARG:O	1:B:395:ARG:N	2.54	0.41
1:B:20:ILE:HG22	1:B:63:THR:HA	2.03	0.41
1:A:200:PHE:HB3	1:A:226:VAL:HB	2.02	0.41
1:B:339:LEU:HD11	1:B:399:SER:HA	2.02	0.41
1:B:494:ASP:C	1:B:496:LYS:H	2.24	0.41
1:A:370:VAL:HG22	1:A:540:LEU:HD21	2.03	0.40
1:A:12:VAL:HG13	1:A:186:ASN:OD1	2.21	0.40
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.43	0.40
1:B:193:ASP:C	1:B:195:THR:H	2.24	0.40
1:A:24:THR:HA	1:A:25:PRO:HD2	1.94	0.40
1:A:346:PHE:CD2	1:A:352:SER:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:TYR:CD1	1:A:489:PRO:CG	3.05	0.40
1:B:152:ARG:O	1:B:157:GLY:HA3	2.20	0.40
1:B:77:TYR:CZ	1:B:348:LYS:CG	3.04	0.40
1:A:316:ILE:HD11	1:A:414:LEU:HD12	2.03	0.40
1:B:123:PHE:CE2	1:B:204:ALA:HB1	2.56	0.40
1:B:282:VAL:H	1:B:282:VAL:HG23	1.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/540 (98%)	456 (86%)	56 (11%)	18 (3%)	3	24
1	B	526/540 (97%)	422 (80%)	77 (15%)	27 (5%)	2	15
All	All	1056/1080 (98%)	878 (83%)	133 (13%)	45 (4%)	2	20

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA
1	A	28	PRO
1	A	257	CYS
1	B	6	ALA
1	B	189	ALA
1	B	241	MET
1	B	254	LEU
1	B	257	CYS
1	B	340	VAL
1	B	385	TRP
1	B	462	SER
1	A	196	SER

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Mol	Chain	Res	Type
1	A	267	THR
1	A	352	SER
1	B	25	PRO
1	B	122	GLY
1	B	143	ARG
1	B	242	GLY
1	B	356	ARG
1	B	397	ALA
1	B	452	GLU
1	B	473	ALA
1	A	61	ASP
1	A	188	ALA
1	A	256	GLY
1	A	266	ASP
1	A	494	ASP
1	B	28	PRO
1	B	81	GLU
1	B	136	ARG
1	B	278	ALA
1	A	241	MET
1	A	317	ASN
1	A	369	GLN
1	A	464	ASN
1	B	279	GLN
1	B	524	LEU
1	B	272	CYS
1	B	466	THR
1	A	404	ASP
1	B	121	GLY
1	B	194	PRO
1	B	239	VAL
1	A	461	PRO
1	A	25	PRO

### 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	433/436 (99%)	369 (85%)	64 (15%)	3	14
1	B	432/436 (99%)	358 (83%)	74 (17%)	2	10
All	All	865/872 (99%)	727 (84%)	138 (16%)	2	11

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	VAL
1	A	18	ARG
1	A	20	ILE
1	A	23	LYS
1	A	30	SER
1	A	48	LEU
1	A	49	PRO
1	A	63	THR
1	A	70	TYR
1	A	75	THR
1	A	83	THR
1	A	85	MET
1	A	91	GLU
1	A	103	THR
1	A	132	VAL
1	A	143	ARG
1	A	144	THR
1	A	161	LEU
1	A	184	GLN
1	A	195	THR
1	A	200	PHE
1	A	203	SER
1	A	208	SER
1	A	211	MET
1	A	219	ARG
1	A	241	MET
1	A	245	ARG
1	A	246	ARG
1	A	254	LEU
1	A	255	VAL
1	A	266	ASP
1	A	285	GLU
1	A	295	PHE
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	311	THR
1	A	324	LEU
1	A	325	GLN
1	A	332	LYS
1	A	333	ASP
1	A	348	LYS
1	A	365	VAL
1	A	370	VAL
1	A	372	ASP
1	A	389	GLU
1	A	396	GLU
1	A	414	LEU
1	A	424	ARG
1	A	436	THR
1	A	437	LEU
1	A	441	LEU
1	A	450	GLU
1	A	463	ARG
1	A	490	ASN
1	A	491	GLU
1	A	496	LYS
1	A	502	PRO
1	A	504	THR
1	A	509	GLN
1	A	512	SER
1	A	522	ARG
1	A	525	ARG
1	A	534	ARG
1	A	536	LEU
1	B	9	LEU
1	B	12	VAL
1	B	23	LYS
1	B	32	PHE
1	B	54	GLN
1	B	59	VAL
1	B	60	VAL
1	B	70	TYR
1	B	83	THR
1	B	100	ASN
1	B	105	TYR
1	B	112	THR
1	B	114	VAL

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Mol	Chain	Res	Type
1	B	132	VAL
1	B	143	ARG
1	B	144	THR
1	B	146	LEU
1	B	149	MET
1	B	159	LEU
1	B	161	LEU
1	B	200	PHE
1	B	203	SER
1	B	211	MET
1	B	216	PRO
1	B	219	ARG
1	B	239	VAL
1	B	241	MET
1	B	246	ARG
1	B	250	GLN
1	B	254	LEU
1	B	255	VAL
1	B	269	LEU
1	B	283	ASN
1	B	291	GLN
1	B	294	VAL
1	B	295	PHE
1	B	296	ARG
1	B	308	LEU
1	B	309	SER
1	B	311	THR
1	B	316	ILE
1	B	324	LEU
1	B	325	GLN
1	B	326	VAL
1	B	332	LYS
1	B	344	PRO
1	B	347	SER
1	B	348	LYS
1	B	351	GLU
1	B	352	SER
1	B	353	LEU
1	B	354	ILE
1	B	360	LEU
1	B	364	ARG
1	B	370	VAL

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Mol	Chain	Res	Type
1	B	372	ASP
1	B	376	GLU
1	B	386	LEU
1	B	414	LEU
1	B	424	ARG
1	B	433	ARG
1	B	436	THR
1	B	437	LEU
1	B	441	LEU
1	B	453	PHE
1	B	462	SER
1	B	463	ARG
1	B	464	ASN
1	B	466	THR
1	B	478	ARG
1	B	490	ASN
1	B	515	LEU
1	B	525	ARG
1	B	534	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	228	GLN
1	A	322	HIS
1	A	325	GLN
1	A	369	GLN
1	A	387	HIS
1	A	474	GLN
1	A	490	ASN
1	A	509	GLN
1	B	54	GLN
1	B	184	GLN
1	B	250	GLN
1	B	265	ASN
1	B	283	ASN
1	B	291	GLN
1	B	325	GLN
1	B	369	GLN
1	B	387	HIS
1	B	421	GLN

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Mol	Chain	Res	Type
1	B	482	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
2	NAG	C	1	1,2	14,14,15	1.97	3 (21%)	17,19,21	3.48	8 (47%)
2	NAG	C	2	2	14,14,15	1.75	3 (21%)	17,19,21	2.71	7 (41%)
2	NAG	D	1	1,2	14,14,15	1.97	3 (21%)	17,19,21	3.81	8 (47%)
2	NAG	D	2	2	14,14,15	1.43	2 (14%)	17,19,21	2.03	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C2-N2	5.12	1.55	1.46
2	C	1	NAG	C2-N2	4.85	1.54	1.46
2	C	2	NAG	C1-C2	4.23	1.58	1.52
2	D	2	NAG	C1-C2	3.51	1.57	1.52
2	C	1	NAG	C1-C2	3.46	1.57	1.52
2	C	2	NAG	C2-N2	3.21	1.51	1.46
2	D	1	NAG	C1-C2	3.08	1.56	1.52
2	D	2	NAG	C3-C2	2.46	1.57	1.52
2	C	1	NAG	O5-C1	-2.43	1.39	1.43
2	D	1	NAG	O7-C7	2.09	1.28	1.23
2	C	2	NAG	C3-C2	2.05	1.56	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	10.14	137.34	122.90
2	D	1	NAG	C2-N2-C7	10.01	137.16	122.90
2	D	1	NAG	C1-O5-C5	8.30	123.44	112.19
2	C	2	NAG	C1-O5-C5	6.14	120.51	112.19
2	C	2	NAG	C2-N2-C7	5.39	130.59	122.90
2	C	1	NAG	C1-C2-N2	5.38	119.68	110.49
2	D	1	NAG	C1-C2-N2	4.68	118.48	110.49
2	D	1	NAG	C4-C3-C2	4.53	117.66	111.02
2	D	2	NAG	O3-C3-C2	4.52	118.83	109.47
2	C	1	NAG	O5-C5-C4	-4.45	100.01	110.83
2	C	1	NAG	C4-C3-C2	3.99	116.86	111.02
2	C	2	NAG	O5-C1-C2	3.95	117.52	111.29
2	C	2	NAG	C4-C3-C2	3.94	116.80	111.02
2	D	2	NAG	C2-N2-C7	3.09	127.31	122.90
2	C	1	NAG	C8-C7-N2	3.00	121.17	116.10
2	D	1	NAG	O5-C5-C4	-2.97	103.59	110.83
2	D	1	NAG	O4-C4-C3	2.97	117.21	110.35
2	C	1	NAG	C6-C5-C4	2.68	119.27	113.00
2	D	2	NAG	O6-C6-C5	-2.65	102.20	111.29
2	D	1	NAG	C3-C4-C5	-2.58	105.63	110.24
2	D	2	NAG	O3-C3-C4	-2.55	104.45	110.35
2	C	1	NAG	O3-C3-C2	-2.46	104.37	109.47
2	D	2	NAG	O4-C4-C5	2.30	115.00	109.30
2	D	2	NAG	O5-C5-C6	2.24	110.71	107.20
2	C	2	NAG	C3-C4-C5	2.17	114.12	110.24
2	C	2	NAG	O7-C7-C8	-2.15	118.06	122.06
2	C	2	NAG	O5-C5-C6	2.10	110.50	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C6	2.10	110.50	107.20
2	D	2	NAG	O7-C7-C8	-2.07	118.21	122.06
2	D	1	NAG	C6-C5-C4	2.06	117.82	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1
2	D	1	NAG	C1

All (10) torsion outliers are listed below:

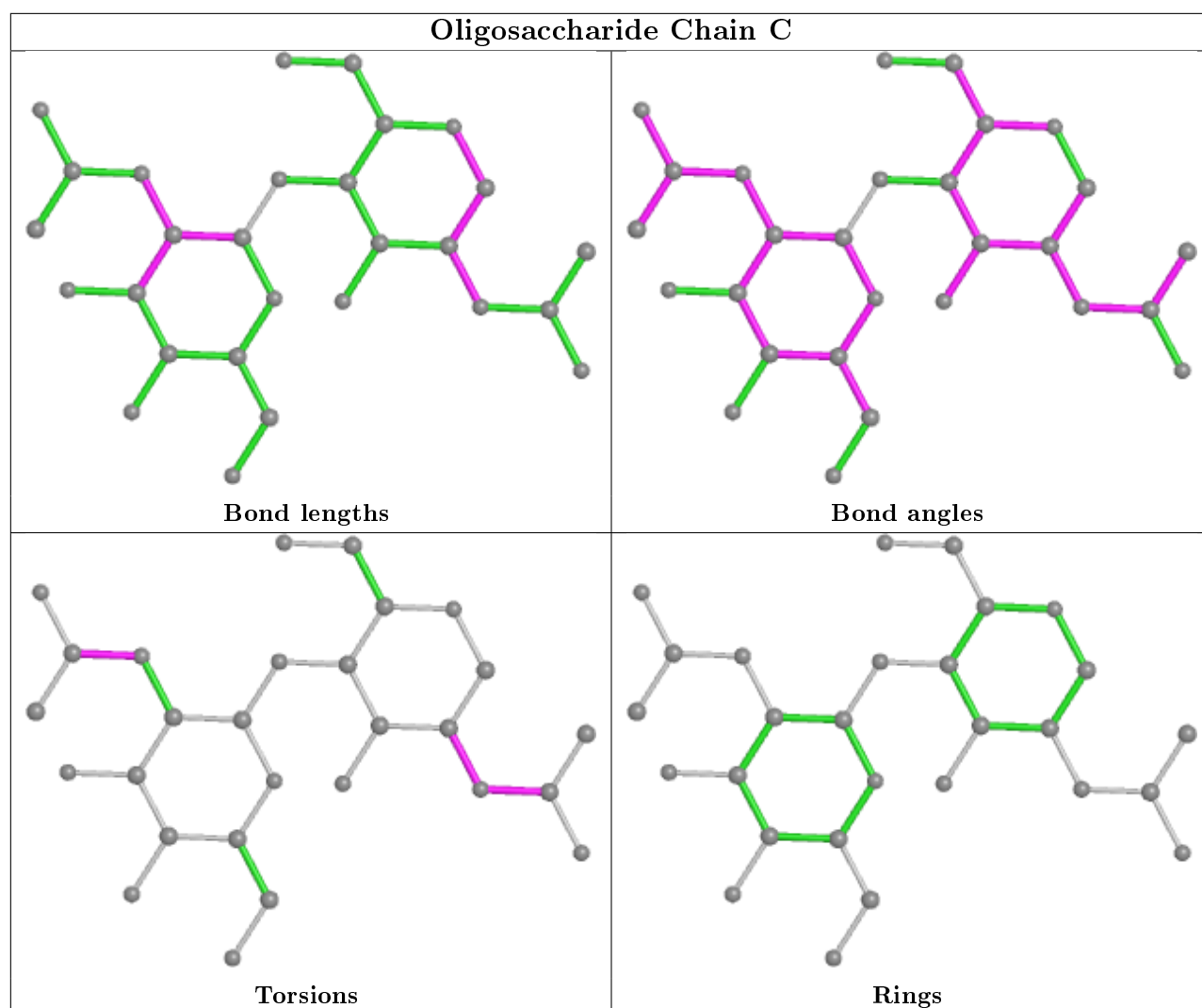
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7

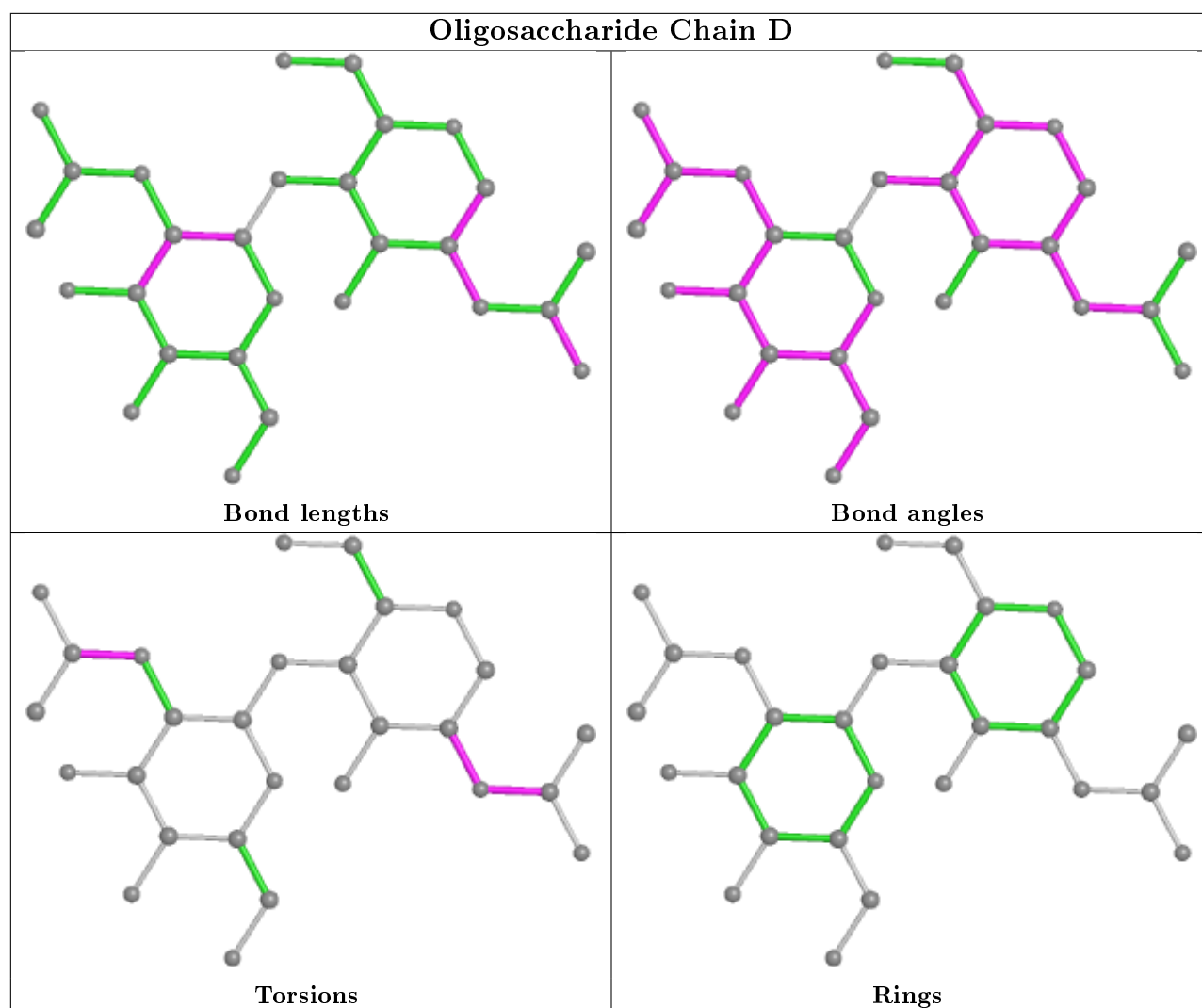
There are no ring outliers.

2 monomers are involved in 1 short contact:

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

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





## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
3	SO4	A	1010	-	4,4,4	0.37	0	6,6,6	0.74	0
3	SO4	B	1015	-	4,4,4	0.13	0	6,6,6	0.24	0
3	SO4	A	1012	-	4,4,4	0.29	0	6,6,6	0.44	0
3	SO4	A	1005	-	4,4,4	0.20	0	6,6,6	0.49	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	1011	-	4,4,4	0.23	0	6,6,6	0.37	0
3	SO4	B	1014	-	4,4,4	0.35	0	6,6,6	0.84	0
3	SO4	A	1013	-	4,4,4	0.27	0	6,6,6	0.56	0
3	SO4	A	1017	-	4,4,4	0.25	0	6,6,6	0.67	0
3	SO4	B	1016	-	4,4,4	0.20	0	6,6,6	0.30	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1011	SO4	1	0
3	B	1016	SO4	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	534/540 (98%)	-0.38	1 (0%) 95 94	47, 69, 97, 114	0
1	B	532/540 (98%)	-0.35	2 (0%) 92 89	49, 79, 112, 137	0
All	All	1066/1080 (98%)	-0.36	3 (0%) 94 92	47, 73, 107, 137	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	PRO	2.6
1	A	78	PRO	2.0
1	B	492	PRO	2.0

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

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

### 6.3 Carbohydrates [i](#)

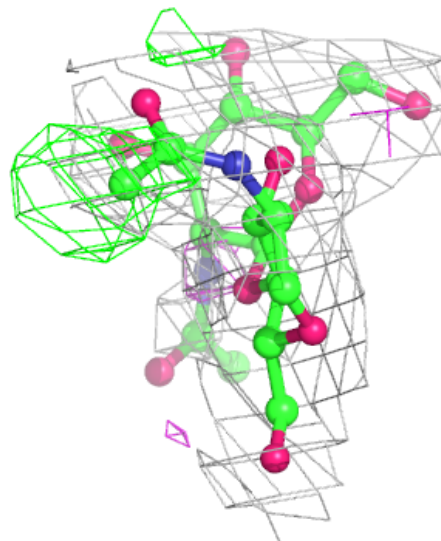
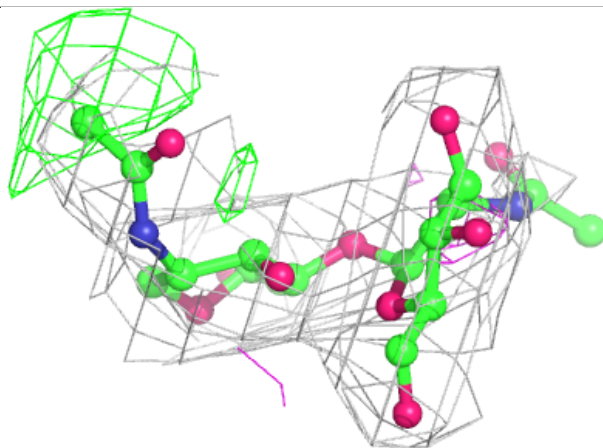
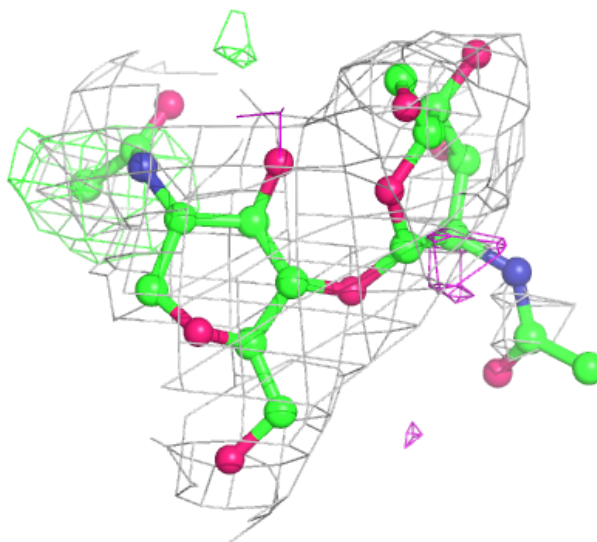
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

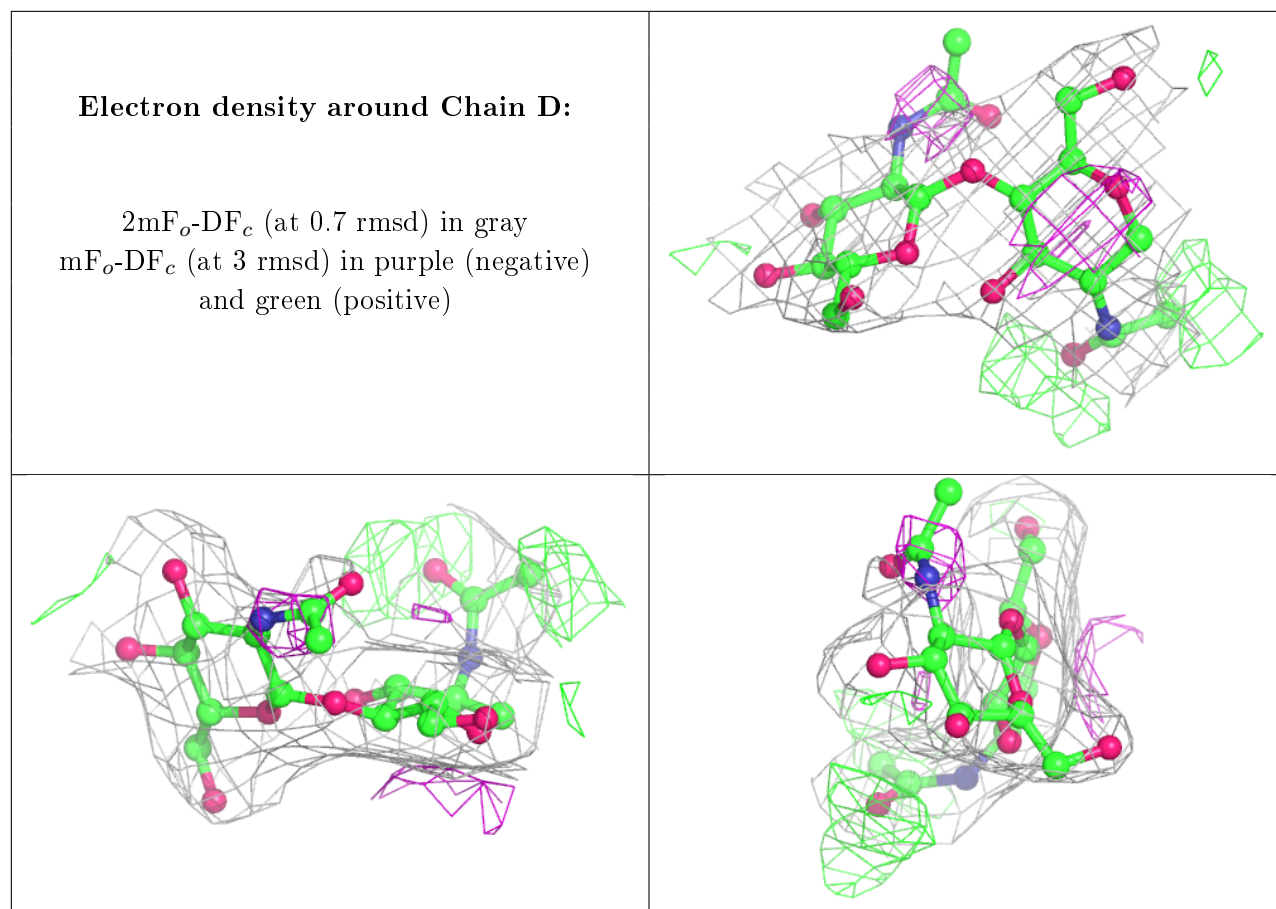
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.77	0.37	107,112,125,125	0
2	NAG	C	2	14/15	0.85	0.33	92,109,119,120	0
2	NAG	C	1	14/15	0.90	0.16	80,85,89,98	0
2	NAG	D	1	14/15	0.90	0.20	79,85,89,98	0

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

**Electron density around Chain C:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	B	1014	5/5	0.84	0.23	119,120,122,123	0
3	SO4	A	1012	5/5	0.86	0.37	128,130,130,131	0
3	SO4	A	1005	5/5	0.88	0.21	131,131,132,133	0
3	SO4	A	1013	5/5	0.91	0.20	130,130,132,132	0
3	SO4	A	1017	5/5	0.91	0.21	112,112,113,114	0
3	SO4	A	1010	5/5	0.92	0.15	112,112,113,115	0
3	SO4	B	1016	5/5	0.93	0.14	130,131,131,132	0
3	SO4	A	1011	5/5	0.94	0.16	115,115,117,117	0
3	SO4	B	1015	5/5	0.95	0.21	107,107,108,108	0

## 6.5 Other polymers

There are no such residues in this entry.