



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:18 PM BST

PDB ID : 4JBS  
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2 in complex with PHOSPHINIC PSEUDOTRIPEPTIDE inhibitor.  
Authors : Saridakis, E.; Birtley, J.; Stratikos, E.; Mavridis, I.M.  
Deposited on : 2013-02-20  
Resolution : 2.79 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  
buster-report : 1.1.7 (2018)  
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

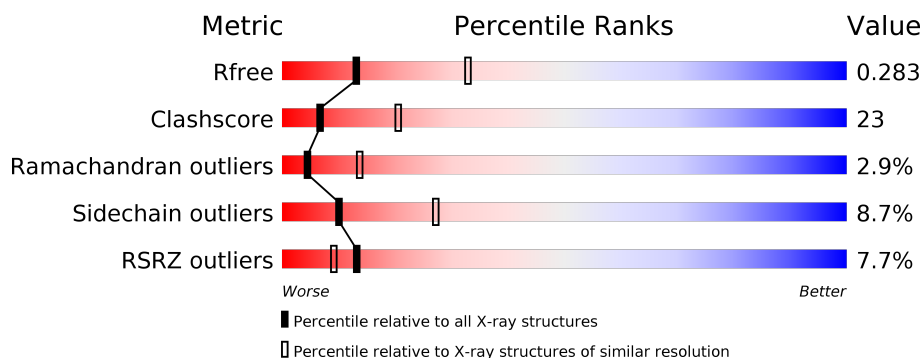
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	967	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>32%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	967	<div> <div>12%</div> <div> <div></div> <div>43%</div> <div>41%</div> <div>5%</div> <div>12%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
3	E	4	<div> <div></div> <div>25%</div> <div>75%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14457 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	2	2	0
			7045	4547	1170	1301	27			
1	B	854	Total	C	N	O	S	0	0	0
			6831	4416	1130	1259	26			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q6P179
A	2	VAL	-	cloning artifact	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	1	MET	-	cloning artifact	UNP Q6P179
B	2	VAL	-	cloning artifact	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

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



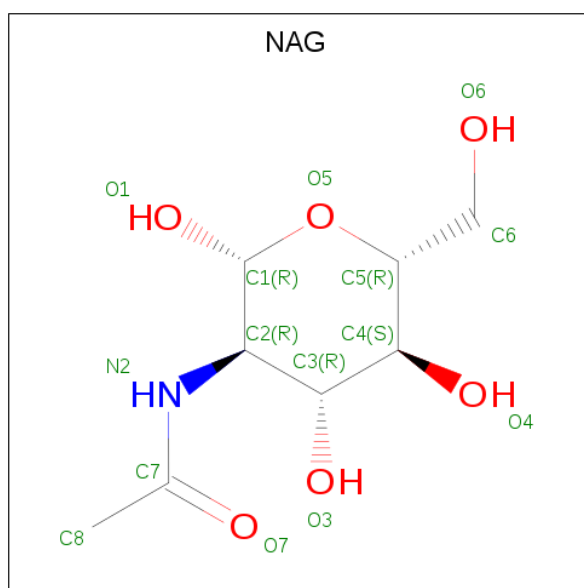
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

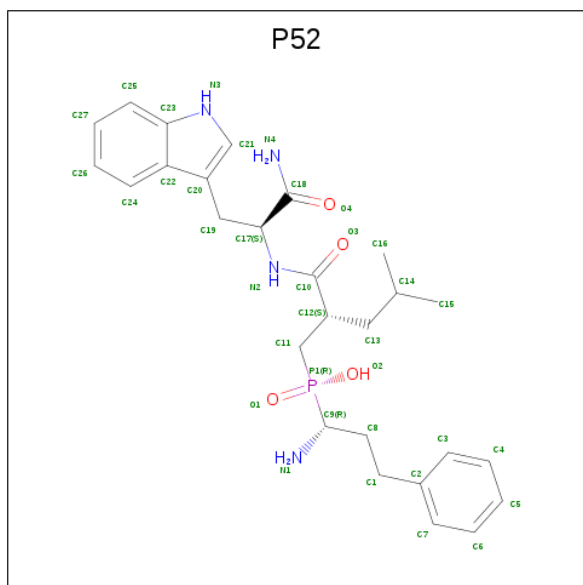


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

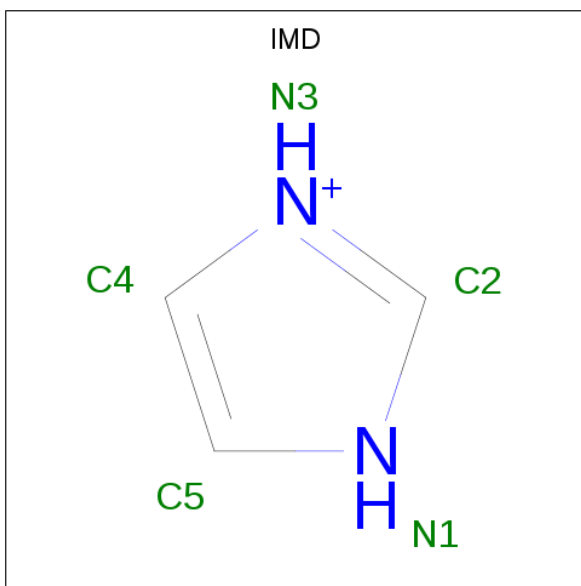
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is Nalpha-[(2S)-2-{[[[(1R)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]methyl}-4-methylpentanoyl]-L-tryptophanamide (three-letter code: P52) (formula: C<sub>27</sub>H<sub>37</sub>N<sub>4</sub>O<sub>4</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	1	0
			36	27	4	4	1		
6	B	1	Total	C	N	O	P	1	0
			36	27	4	4	1		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).

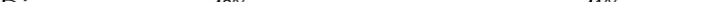


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			5	3	2		
7	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	207	Total	O	0	0
			207	207		
8	B	86	Total	O	0	0
			86	86		



Chain B:  12% 43% 41% 5% 12%





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

Chain C: 100%



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

Chain D: 50%



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

Chain F: 50%



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

Chain E: 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.15Å 134.77Å 128.73Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	10.99 – 2.79 48.77 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.7 (10.99-2.79) 99.8 (48.77-2.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.206 , 0.278 0.214 , 0.283	Depositor DCC
$R_{free}$ test set	3225 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 65.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.006 for -h,l,k 0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: ZN, MAN, NAG, P52, IMD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/7222	0.46	0/9787
1	B	0.26	0/6995	0.45	0/9488
All	All	0.27	0/14217	0.46	0/19275

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7045	0	6981	282	0
1	B	6831	0	6698	374	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	F	28	0	25	3	0
3	E	50	0	43	4	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	36	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	36	0	35	2	0
7	A	10	0	10	0	0
8	A	207	0	0	6	0
8	B	86	0	0	0	0
All	All	14457	0	13943	658	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 23.

All (658) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:HB1	1:A:57:THR:HA	1.31	1.09
1:B:374:HIS:HE1	1:B:392:LYS:HG2	1.29	0.96
1:B:565:ARG:HD2	1:B:584:TYR:HE2	1.28	0.94
1:B:582:GLU:N	1:B:583:ARG:HB2	1.85	0.92
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.50	0.91
1:B:889:LEU:HD21	1:B:925:GLY:HA2	1.55	0.89
1:A:122:LEU:HB2	1:A:137:LEU:HD21	1.55	0.87
1:B:784:LEU:HD22	1:B:785:ASN:H	1.39	0.87
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.58	0.86
1:B:355:THR:HG21	1:B:820:GLU:HB2	1.58	0.86
1:B:122:LEU:HB2	1:B:137:LEU:HD21	1.57	0.86
1:A:75:PRO:HG3	1:A:211:PHE:CD1	2.11	0.85
1:A:118:THR:O	1:A:119:ASN:HB2	1.75	0.84
1:A:56:ALA:CB	1:A:57:THR:HA	2.07	0.84
1:A:355:THR:HG21	1:A:820:GLU:HB2	1.60	0.83
1:B:374:HIS:CE1	1:B:392:LYS:HG2	2.12	0.83
1:B:104:ALA:H	1:B:158:PRO:HG3	1.43	0.82
1:A:528:LEU:HD23	1:A:529:GLY:HA2	1.59	0.82
1:A:591:THR:HB	1:A:625:VAL:HG23	1.60	0.82
1:B:565:ARG:HD2	1:B:584:TYR:CE2	2.14	0.81
1:B:712:ARG:HA	1:B:866:PRO:HG3	1.64	0.79
1:B:75:PRO:HG3	1:B:211:PHE:CD1	2.16	0.79
1:A:915:LYS:O	1:A:919:GLU:HG2	1.83	0.79
1:A:581:GLN:HG3	1:A:582:GLU:H	1.47	0.78
1:A:662:LEU:HB3	1:A:683:MET:HE1	1.65	0.78
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.18	0.78
1:A:152:VAL:HG21	1:A:156:LEU:HD21	1.64	0.77
1:B:777:TRP:HA	1:B:784:LEU:HB3	1.66	0.77
1:B:152:VAL:HG12	1:B:154:GLU:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TYR:OH	1:A:466:LYS:HD3	1.87	0.75
1:B:911:LEU:O	1:B:915:LYS:HB2	1.87	0.75
1:A:537:MET:O	1:A:540:THR:HG22	1.85	0.74
1:B:640:TRP:CZ3	1:B:666:VAL:HG22	2.21	0.74
1:A:475:GLN:O	1:A:479:ILE:HG12	1.87	0.74
1:B:464:MET:HG3	1:B:629:GLY:HA2	1.70	0.74
1:B:411:LEU:HA	1:B:745:VAL:HG21	1.70	0.73
1:B:56:ALA:HB2	1:B:62:PHE:N	2.04	0.73
1:B:626:ASP:HA	1:B:657:LYS:HB3	1.70	0.73
1:B:338:ASN:HB2	1:B:341:LEU:O	1.89	0.73
1:A:56:ALA:HB1	1:A:57:THR:CA	2.15	0.72
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.70	0.72
1:B:877:ARG:HG3	1:B:917:PHE:CD1	2.24	0.72
1:A:245:GLU:HG2	1:A:246:GLY:H	1.54	0.72
1:B:69:LEU:HD13	1:B:211:PHE:HD2	1.55	0.71
1:A:935:LEU:O	1:A:939:THR:HG23	1.91	0.71
1:B:943:LYS:O	1:B:947:LYS:HB3	1.90	0.71
1:A:551:VAL:HB	1:A:562:GLN:HB2	1.73	0.70
1:B:843:LEU:HD22	1:B:849:VAL:HB	1.73	0.70
1:B:548:PRO:HG3	1:B:586:TRP:CG	2.27	0.70
1:B:889:LEU:HB3	1:B:894:ILE:HG21	1.73	0.70
1:B:632:ILE:HG22	1:B:633:VAL:H	1.57	0.69
1:A:366[B]:ARG:HH21	1:A:397:LYS:NZ	1.91	0.69
1:A:738:SER:O	1:A:751:ARG:HD3	1.92	0.69
1:B:540:THR:HG21	1:B:587:HIS:HB2	1.74	0.68
3:E:3:MAN:H3	3:E:4:MAN:H2	1.75	0.68
1:B:83:HIS:NE2	3:E:1:NAG:H83	2.08	0.68
1:A:615:PRO:O	1:A:616:GLU:HG3	1.93	0.68
1:A:884:LEU:HD21	1:A:889:LEU:HD23	1.75	0.68
1:A:183:THR:HG22	1:A:193:ILE:HG12	1.76	0.68
1:B:843:LEU:O	1:B:846:GLU:HB3	1.93	0.68
1:A:533:GLU:HG2	1:A:536:GLU:HB2	1.76	0.67
1:A:191:THR:H	1:B:191:THR:HB	1.58	0.67
1:A:220:PHE:O	1:A:256:THR:HG23	1.94	0.67
1:B:947:LYS:HG3	1:B:947:LYS:O	1.94	0.67
1:B:442:THR:HG23	1:B:445:GLN:H	1.59	0.67
1:B:419:ASN:HD22	1:B:419:ASN:N	1.93	0.67
1:A:604:ILE:HG22	1:A:605:LEU:H	1.61	0.66
1:B:588:ILE:HG23	1:B:605:LEU:HD23	1.76	0.66
1:B:388:ASP:HB3	1:B:391:LEU:HG	1.76	0.66
1:B:62:PHE:CE1	1:B:142:TYR:HB2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PHE:CD1	1:B:142:TYR:HB2	2.31	0.65
1:B:674:ARG:HH11	1:B:674:ARG:HB3	1.61	0.65
1:B:313:TYR:HE2	1:B:478:ILE:HD11	1.61	0.65
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.79	0.65
1:A:602:ARG:O	1:A:603:HIS:HB2	1.96	0.65
1:A:784:LEU:HD22	1:A:785:ASN:H	1.62	0.65
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.32	0.65
1:B:570:VAL:HB	1:B:943:LYS:HG3	1.78	0.65
1:B:536:GLU:O	1:B:540:THR:HG22	1.97	0.64
1:A:550:LEU:HB3	1:A:633:VAL:HG12	1.79	0.64
1:B:764:ALA:HB3	1:B:765:PRO:HD3	1.80	0.64
1:B:949:LEU:N	1:B:950:PRO:HD2	2.11	0.64
1:A:650:ASN:HB3	1:A:653:LEU:HG	1.79	0.64
1:B:152:VAL:HG21	1:B:156:LEU:HD21	1.80	0.64
1:A:355:THR:CG2	1:A:820:GLU:HB2	2.27	0.64
1:B:594:THR:HA	1:B:620:TRP:O	1.98	0.63
1:B:405:ASN:O	1:B:409:PRO:HG3	1.98	0.63
1:B:398:TYR:OH	1:B:466:LYS:HD3	1.98	0.63
1:B:245:GLU:CG	1:B:246:GLY:H	2.11	0.63
1:B:412:GLN:CD	1:B:746:TRP:HD1	2.02	0.63
1:B:310:TYR:HD1	1:B:314:PHE:CE2	2.16	0.63
1:B:922:GLU:OE1	1:B:922:GLU:HA	1.97	0.63
1:B:57:THR:HB	1:B:58:ASN:CG	2.19	0.63
1:B:431:ASN:HA	1:B:565:ARG:HH22	1.63	0.62
1:B:662:LEU:O	1:B:666:VAL:HG23	1.99	0.62
1:B:678:ASP:HA	1:B:681:LEU:HB2	1.81	0.62
1:B:626:ASP:HA	1:B:657:LYS:CB	2.29	0.62
1:B:635:TYR:HB2	1:B:640:TRP:CD1	2.34	0.62
1:B:767:ILE:O	1:B:767:ILE:HG13	1.98	0.62
1:A:666:VAL:HG21	1:A:683:MET:SD	2.39	0.62
1:B:582:GLU:N	1:B:583:ARG:CB	2.60	0.62
1:B:659:ARG:O	1:B:663:ILE:HG13	1.99	0.62
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.81	0.62
1:B:910:LYS:HD3	1:B:913:GLU:OE2	1.99	0.62
1:A:892:TYR:O	1:A:896:MET:HB3	2.00	0.61
1:A:568:GLN:HG2	1:A:940:LYS:HE2	1.82	0.61
1:B:731:LYS:N	1:B:732:PRO:HD2	2.15	0.61
1:B:906:SER:HB3	1:B:941:ASN:HB3	1.81	0.61
1:A:293:ARG:NH2	3:E:3:MAN:O2	2.33	0.61
1:B:656:PRO:O	1:B:660:VAL:HG23	2.00	0.61
1:A:594:THR:HG22	1:A:621:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:LEU:O	1:A:915:LYS:HB2	2.00	0.61
1:B:802:THR:OG1	1:B:833:HIS:HE1	1.84	0.61
1:A:338:ASN:HB2	1:A:341:LEU:O	2.01	0.61
1:A:385:TRP:HD1	1:A:387:ASN:HD22	1.45	0.61
1:B:565:ARG:O	1:B:567:LEU:HD12	2.01	0.61
1:A:727:LEU:HD21	1:A:761:LEU:HB3	1.82	0.60
1:B:666:VAL:HG21	1:B:683:MET:SD	2.41	0.60
1:B:604:ILE:HG22	1:B:605:LEU:H	1.66	0.60
3:E:3:MAN:C3	3:E:4:MAN:H2	2.31	0.60
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.81	0.60
1:A:382:THR:O	1:A:489:ASN:HA	2.01	0.60
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.81	0.60
1:B:330:ASP:OD1	1:B:851:LYS:HD2	2.00	0.60
1:B:488:ARG:HG2	1:B:489:ASN:H	1.66	0.60
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.84	0.60
1:B:236:MET:HG2	1:B:256:THR:HG22	1.83	0.60
1:B:664:HIS:O	1:B:668:GLN:HG2	2.02	0.60
1:A:213:GLU:HB2	1:A:216:PHE:CD2	2.37	0.60
1:A:581:GLN:HG3	1:A:582:GLU:N	2.17	0.59
1:B:791:LEU:HD11	1:B:795:TYR:CZ	2.36	0.59
1:A:314:PHE:O	1:A:316:ILE:HG13	2.02	0.59
1:A:582:GLU:O	1:A:583:ARG:CB	2.50	0.59
1:B:643:LEU:O	1:B:646:GLN:HB3	2.03	0.59
1:A:119:ASN:O	1:A:166:MET:HA	2.02	0.59
1:A:232:ALA:HB3	1:A:251:ASP:OD2	2.03	0.59
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.85	0.59
1:B:475:GLN:O	1:B:479:ILE:HG12	2.03	0.59
1:B:540:THR:HG21	1:B:587:HIS:H	1.68	0.59
1:B:626:ASP:HB3	1:B:657:LYS:HD3	1.85	0.59
1:A:533:GLU:HG2	1:A:533:GLU:O	2.01	0.58
1:B:140:LEU:HD12	1:B:151:LEU:HD11	1.85	0.58
1:A:500:SER:HB3	1:A:534:VAL:HB	1.85	0.58
1:A:450:PHE:O	1:A:895:ARG:NH2	2.36	0.58
1:A:186:THR:HG23	1:A:190:GLU:O	2.04	0.58
1:A:662:LEU:O	1:A:666:VAL:HG23	2.04	0.58
1:A:640:TRP:CD1	1:A:675:LEU:HD11	2.38	0.58
1:B:484:LYS:HD3	1:B:485:PHE:CZ	2.39	0.58
1:B:491:LYS:HG2	1:B:492:ASN:N	2.19	0.58
1:A:332:ALA:HB3	1:A:333:PRO:HD3	1.86	0.57
1:B:422:PHE:HA	1:B:425:ILE:HD12	1.85	0.57
1:B:468:PHE:CG	1:B:468:PHE:O	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD13	1:A:149:ALA:HA	1.87	0.57
1:B:56:ALA:O	1:B:57:THR:HG23	2.03	0.57
1:B:709:MET:O	1:B:713:ARG:HG2	2.05	0.57
1:A:548:PRO:HG3	1:A:586:TRP:CD2	2.39	0.57
1:B:310:TYR:CD1	1:B:314:PHE:HE2	2.23	0.57
1:B:310:TYR:O	1:B:314:PHE:HB2	2.05	0.57
1:B:419:ASN:HD22	1:B:419:ASN:H	1.51	0.57
1:B:731:LYS:N	1:B:732:PRO:CD	2.68	0.57
1:B:934:VAL:O	1:B:938:ILE:HG13	2.05	0.57
1:A:192:ARG:HA	1:B:190:GLU:HG2	1.86	0.57
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.20	0.57
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.87	0.56
1:A:856:ALA:HB1	1:A:896:MET:HG2	1.87	0.56
1:B:182:SER:OG	1:B:330:ASP:HB2	2.05	0.56
1:A:348:SER:HB3	1:A:367:VAL:HG21	1.87	0.56
1:B:245:GLU:CG	1:B:246:GLY:N	2.68	0.56
1:A:85:ASN:HB3	1:A:88:SER:HB3	1.85	0.56
1:B:236:MET:CE	1:B:256:THR:HA	2.35	0.56
1:B:566:PHE:CE2	1:B:672:ALA:HB2	2.40	0.56
1:B:954:THR:O	1:B:958:VAL:HG23	2.05	0.56
1:A:385:TRP:HD1	1:A:387:ASN:ND2	2.02	0.56
1:A:95:GLU:HG2	1:A:168:PHE:HE1	1.68	0.56
1:B:355:THR:CG2	1:B:820:GLU:HB2	2.34	0.56
1:B:568:GLN:NE2	1:B:671:GLY:HA3	2.21	0.56
1:B:846:GLU:HG3	1:B:848:LYS:H	1.71	0.56
1:A:141:SER:HA	1:A:148:ILE:HG22	1.86	0.56
1:A:240:LYS:HG2	1:A:252:HIS:HB2	1.88	0.56
1:A:475:GLN:HG2	1:A:479:ILE:HD11	1.86	0.56
1:B:245:GLU:CD	1:B:246:GLY:H	2.09	0.56
1:A:125:GLU:HA	1:A:125:GLU:OE1	2.06	0.56
1:A:320:LEU:HD23	1:A:320:LEU:N	2.21	0.56
1:B:468:PHE:CD2	1:B:469:LEU:HG	2.41	0.55
1:B:63:PRO:HB2	1:B:107:PHE:CD1	2.40	0.55
1:B:784:LEU:HD22	1:B:785:ASN:N	2.14	0.55
2:F:1:NAG:H61	2:F:2:NAG:H83	1.86	0.55
1:A:124:SER:HB2	1:A:131:MET:O	2.06	0.55
1:A:487:TYR:HA	8:A:1152:HOH:O	2.06	0.55
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.87	0.55
1:A:748:ARG:HB3	1:A:789:ASP:OD2	2.06	0.55
1:B:703:LEU:HD13	1:B:726:LEU:HD21	1.87	0.55
1:A:245:GLU:HG2	1:A:246:GLY:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:LEU:HD23	1:A:840:LEU:HD21	1.89	0.55
1:B:545:LYS:HG2	1:B:546:GLY:H	1.71	0.55
1:B:697:LEU:HD21	1:B:750:LEU:HA	1.87	0.55
1:A:807:TYR:O	1:A:811[B]:GLN:HG2	2.07	0.55
1:B:318:TYR:CE2	1:B:323:LEU:HB2	2.42	0.55
1:B:731:LYS:HE3	1:B:763:HIS:CE1	2.40	0.55
1:B:777:TRP:CB	1:B:786:ILE:HD11	2.37	0.55
1:B:485:PHE:CZ	1:B:494:ASP:HB3	2.41	0.55
1:A:528:LEU:HD23	1:A:529:GLY:CA	2.35	0.55
1:B:655:ARG:HB2	1:B:658:ASP:OD2	2.07	0.55
1:A:625:VAL:HG12	1:A:655:ARG:HD2	1.87	0.55
1:B:422:PHE:O	1:B:425:ILE:HB	2.07	0.55
1:A:889:LEU:HB2	1:A:928:LEU:HD11	1.88	0.54
1:B:236:MET:HE2	1:B:256:THR:HG22	1.88	0.54
1:A:919:GLU:OE2	1:A:919:GLU:HA	2.06	0.54
1:B:729:TYR:C	1:B:731:LYS:H	2.11	0.54
1:B:889:LEU:HB2	1:B:928:LEU:HD11	1.89	0.54
1:A:784:LEU:HD13	1:A:785:ASN:N	2.23	0.54
1:B:374:HIS:CE1	1:B:392:LYS:CG	2.88	0.54
1:A:236:MET:HE2	1:A:256:THR:HA	1.89	0.54
1:B:58:ASN:ND2	1:B:58:ASN:N	2.55	0.54
1:A:548:PRO:HG3	1:A:586:TRP:CE3	2.43	0.54
1:A:834:GLN:H	1:A:834:GLN:HE21	1.55	0.54
1:A:528:LEU:CD2	1:A:529:GLY:HA2	2.33	0.54
1:B:442:THR:HG22	1:B:445:GLN:CD	2.28	0.54
1:A:100:LEU:HD12	1:A:101:VAL:N	2.22	0.54
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.43	0.54
1:B:298:TYR:CE2	1:B:361:LYS:HD2	2.43	0.54
1:B:540:THR:O	1:B:544:GLN:HG2	2.09	0.53
1:A:236:MET:CE	1:A:256:THR:HA	2.39	0.53
1:A:911:LEU:CD1	1:A:939:THR:HG22	2.37	0.53
1:B:227:GLU:OE1	1:B:229:ARG:HD3	2.09	0.53
1:B:272:HIS:CE1	1:B:290:PRO:HB3	2.44	0.53
1:A:381:VAL:HG21	1:A:482:LEU:HA	1.89	0.53
1:A:731:LYS:N	1:A:732:PRO:CD	2.72	0.53
1:A:764:ALA:HB3	1:A:765:PRO:HD3	1.89	0.53
1:B:659:ARG:HD2	1:B:690:GLU:OE1	2.08	0.53
1:A:156:LEU:HD12	1:A:162:TYR:CE1	2.44	0.53
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.44	0.53
1:B:245:GLU:HG2	1:B:246:GLY:H	1.72	0.53
1:B:56:ALA:HB2	1:B:62:PHE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:TYR:O	1:B:705:SER:HB3	2.08	0.53
1:B:859:LEU:HD23	1:B:897:ILE:HG23	1.91	0.53
1:B:99:VAL:O	1:B:100:LEU:HB2	2.09	0.53
1:B:401:LEU:HA	1:B:413:PHE:CE2	2.44	0.53
1:B:622:LYS:HZ3	1:B:662:LEU:HG	1.72	0.53
1:B:718:ILE:HD11	1:B:952:LEU:HD13	1.91	0.53
1:B:960:THR:O	1:B:960:THR:HG22	2.08	0.53
1:B:559:LEU:O	1:B:611:THR:HG23	2.09	0.53
1:A:278:THR:CG2	1:A:282:VAL:HB	2.39	0.52
1:A:444:THR:HG23	1:A:890:GLY:H	1.73	0.52
1:A:475:GLN:O	1:A:478:ILE:HG12	2.09	0.52
1:B:145:HIS:O	1:B:147:GLN:HG3	2.10	0.52
1:B:245:GLU:HG2	1:B:246:GLY:N	2.23	0.52
1:B:381:VAL:HG13	1:B:485:PHE:HB2	1.91	0.52
1:B:173:GLY:H	1:B:180:TYR:HA	1.74	0.52
1:B:351:PHE:CZ	1:B:361:LYS:HE2	2.45	0.52
1:A:763:HIS:CD2	1:A:765:PRO:HD2	2.45	0.52
1:B:278:THR:HG22	1:B:304:LEU:HD23	1.92	0.52
1:B:384:GLU:HG3	1:B:490:ALA:O	2.09	0.52
1:A:366[B]:ARG:HG3	1:A:400:GLU:OE1	2.09	0.52
1:A:624:ASN:HD21	1:A:629:GLY:H	1.57	0.52
1:B:834:GLN:OE1	1:B:834:GLN:HA	2.09	0.52
1:A:559:LEU:HD12	1:A:612:LEU:O	2.10	0.52
1:A:922:GLU:HA	1:A:926:SER:HB2	1.92	0.52
1:B:173:GLY:N	1:B:180:TYR:HA	2.25	0.52
1:B:780:SER:O	1:B:783:LYS:HD3	2.10	0.52
1:A:889:LEU:HD12	1:A:889:LEU:O	2.09	0.51
1:B:67:LEU:HB3	1:B:145:HIS:CD2	2.44	0.51
1:B:916:LEU:O	1:B:916:LEU:HD13	2.10	0.51
1:B:935:LEU:O	1:B:939:THR:HG23	2.11	0.51
1:A:374:HIS:HA	1:A:377:PHE:O	2.10	0.51
1:B:731:LYS:HE3	1:B:763:HIS:HE1	1.74	0.51
1:A:722:LEU:HD13	1:A:956:LEU:HD11	1.91	0.51
1:B:857:ALA:HA	1:B:896:MET:HE1	1.92	0.51
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.92	0.51
1:A:624:ASN:HD21	1:A:629:GLY:N	2.09	0.51
1:B:465:LEU:HD12	1:B:468:PHE:HD2	1.76	0.51
1:B:568:GLN:O	1:B:569:GLY:O	2.28	0.51
1:B:905:PHE:O	1:B:938:ILE:HG23	2.10	0.51
1:A:388:ASP:HB3	1:A:391:LEU:CD1	2.41	0.51
1:B:605:LEU:HD12	1:B:606:LYS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:CB	1:A:529:GLY:HA2	2.40	0.51
1:B:332:ALA:HB3	1:B:333:PRO:HD3	1.92	0.51
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.76	0.51
1:B:465:LEU:HD11	1:B:534:VAL:HG11	1.93	0.51
1:B:370:HIS:CG	6:B:1010:P52:H25	2.46	0.51
1:B:465:LEU:HD12	1:B:468:PHE:CD2	2.46	0.51
1:B:647:LEU:HA	1:B:651:HIS:HB3	1.92	0.51
1:A:366[B]:ARG:HH21	1:A:397:LYS:HZ2	1.58	0.50
1:A:99:VAL:HG12	1:A:100:LEU:N	2.26	0.50
1:B:80:LEU:HB3	1:B:222:ILE:HD13	1.93	0.50
1:B:808:LEU:HB2	1:B:828:LEU:HD11	1.93	0.50
1:B:912:GLN:NE2	1:B:915:LYS:HD3	2.25	0.50
1:B:955:TRP:O	1:B:958:VAL:HB	2.11	0.50
1:A:213:GLU:HB2	1:A:216:PHE:HD2	1.75	0.50
1:B:491:LYS:HG2	1:B:492:ASN:H	1.76	0.50
1:A:81:PHE:O	1:A:93:ALA:HB1	2.11	0.50
1:A:568:GLN:HG2	1:A:940:LYS:HG3	1.93	0.50
1:B:428:ASP:OD1	1:B:546:GLY:HA2	2.12	0.50
1:B:635:TYR:H	1:B:640:TRP:HE1	1.59	0.50
1:A:436:ILE:HD12	1:A:461:ILE:HD13	1.93	0.50
1:B:635:TYR:HB3	1:B:639:GLY:HA3	1.93	0.50
1:B:786:ILE:HB	1:B:791:LEU:HD13	1.92	0.50
1:B:911:LEU:HG	1:B:911:LEU:O	2.11	0.50
1:A:659:ARG:O	1:A:663:ILE:HG13	2.11	0.49
1:A:674:ARG:O	1:A:675:LEU:HD12	2.10	0.49
1:B:870:GLN:HE22	1:B:910:LYS:NZ	2.10	0.49
1:B:877:ARG:HG3	1:B:917:PHE:CE1	2.47	0.49
1:A:177:GLU:HB3	1:A:203:GLN:HG2	1.94	0.49
1:A:873:TRP:O	1:A:877:ARG:HB2	2.12	0.49
1:B:83:HIS:CE1	1:B:225:ARG:HD2	2.47	0.49
1:A:183:THR:HA	1:A:192:ARG:O	2.12	0.49
1:A:681:LEU:HD21	1:A:952:LEU:HD23	1.94	0.49
1:A:954:THR:O	1:A:958:VAL:HG23	2.13	0.49
1:B:337:GLU:HG3	1:B:374:HIS:HB3	1.93	0.49
1:B:57:THR:HB	1:B:58:ASN:OD1	2.13	0.49
1:B:727:LEU:O	1:B:731:LYS:HD3	2.13	0.49
1:B:849:VAL:HG12	1:B:850:ILE:HG13	1.94	0.49
1:A:873:TRP:CE2	1:A:877:ARG:HD3	2.47	0.49
1:A:718:ILE:HG21	1:A:952:LEU:HD13	1.93	0.49
1:A:323:LEU:HD12	1:A:324:ASP:N	2.27	0.49
1:A:559:LEU:CD1	1:A:612:LEU:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PHE:CD1	1:B:197:THR:HG22	2.48	0.49
1:B:275:SER:HB3	1:B:283:LYS:HE2	1.95	0.49
1:B:725:TYR:O	1:B:729:TYR:HB2	2.12	0.49
1:B:893:ASP:O	1:B:897:ILE:HG13	2.12	0.49
1:A:67:LEU:HD12	1:A:68:ARG:N	2.27	0.48
1:A:887:PHE:HB2	1:A:894:ILE:HG12	1.94	0.48
1:B:386:TRP:HB3	1:B:446:ILE:HG23	1.94	0.48
1:A:622:LYS:HD3	1:A:662:LEU:HD21	1.95	0.48
1:A:793:ILE:HG13	8:A:1128:HOH:O	2.14	0.48
6:A:1009:P52:H11	6:A:1009:P52:H32	1.95	0.48
1:A:325:LEU:N	1:A:325:LEU:HD12	2.29	0.48
1:A:333:PRO:O	1:A:345:ARG:HD2	2.14	0.48
1:B:159:HIS:O	1:B:160:LEU:HD22	2.13	0.48
1:B:186:THR:HG21	1:B:192:ARG:NH1	2.28	0.48
1:B:385:TRP:CG	1:B:386:TRP:N	2.81	0.48
1:B:582:GLU:N	1:B:583:ARG:CA	2.76	0.48
1:B:55:VAL:O	1:B:56:ALA:HB2	2.13	0.48
1:B:647:LEU:HD22	1:B:686:TYR:CE1	2.48	0.48
1:A:67:LEU:HB3	1:A:145:HIS:CD2	2.48	0.48
1:A:537:MET:CE	1:A:589:PRO:HG3	2.44	0.48
1:A:604:ILE:N	1:A:604:ILE:HD12	2.28	0.48
1:B:390:TRP:CG	1:B:436:ILE:HG23	2.48	0.48
1:B:660:VAL:HG22	1:B:695:ALA:CA	2.44	0.48
1:B:730:PHE:C	1:B:732:PRO:HD2	2.34	0.48
1:B:333:PRO:O	1:B:345:ARG:HD2	2.13	0.48
1:A:386:TRP:HB3	1:A:446:ILE:HG23	1.95	0.48
1:A:626:ASP:OD1	1:A:657:LYS:HB2	2.13	0.48
1:B:236:MET:HE2	1:B:256:THR:HA	1.94	0.48
1:B:887:PHE:HB2	1:B:894:ILE:HG12	1.94	0.48
1:B:889:LEU:HA	1:B:890:GLY:HA2	1.59	0.48
1:A:430:LEU:HD21	1:A:940:LYS:HE3	1.94	0.48
1:A:465:LEU:HD22	1:A:496:TRP:HZ3	1.79	0.48
1:B:364:VAL:O	1:B:368:ILE:HG13	2.14	0.48
1:A:659:ARG:HD2	1:A:690:GLU:OE1	2.13	0.48
1:B:738:SER:O	1:B:740:SER:N	2.45	0.48
1:A:731:LYS:N	1:A:732:PRO:HD2	2.29	0.47
1:A:834:GLN:HG3	1:A:871:LEU:HD12	1.95	0.47
1:B:248:LEU:O	1:B:249:LEU:HD23	2.14	0.47
1:B:352:ASP:OD2	1:B:355:THR:HB	2.14	0.47
1:B:622:LYS:NZ	1:B:662:LEU:HG	2.28	0.47
1:B:309:PHE:C	1:B:309:PHE:CD2	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:VAL:HG12	1:B:680:ALA:HB2	1.94	0.47
1:B:236:MET:HB3	1:B:254:GLU:HB3	1.95	0.47
1:A:375:GLN:O	1:A:379:ASN:HB2	2.14	0.47
1:A:681:LEU:HB3	1:A:955:TRP:NE1	2.29	0.47
1:B:156:LEU:HD12	1:B:162:TYR:CE1	2.49	0.47
1:B:436:ILE:HD11	1:B:458:GLY:HA2	1.95	0.47
1:B:857:ALA:HA	1:B:896:MET:CE	2.44	0.47
1:A:533:GLU:O	1:A:535:LYS:N	2.48	0.47
1:B:540:THR:OG1	1:B:586:TRP:HA	2.14	0.47
1:B:614:LEU:C	1:B:616:GLU:H	2.17	0.47
1:B:918:PHE:CD1	1:B:918:PHE:N	2.82	0.47
1:A:479:ILE:HG22	1:A:483:LYS:HE3	1.97	0.47
1:B:100:LEU:HD13	1:B:161:LYS:HG2	1.97	0.47
1:B:902:THR:OG1	1:B:934:VAL:HG11	2.15	0.47
1:B:798:GLY:O	1:B:801:THR:HG22	2.15	0.47
1:A:330:ASP:OD1	1:A:851:LYS:HD2	2.15	0.47
1:B:99:VAL:HG12	1:B:100:LEU:H	1.80	0.47
1:B:278:THR:HG21	1:B:307:LEU:HD23	1.96	0.47
1:A:616:GLU:O	1:A:618:THR:N	2.49	0.46
1:A:889:LEU:HA	1:A:890:GLY:HA2	1.50	0.46
1:A:124:SER:HA	8:A:1231:HOH:O	2.15	0.46
1:A:388:ASP:HB3	1:A:391:LEU:HD12	1.97	0.46
1:B:582:GLU:CA	1:B:583:ARG:HB2	2.44	0.46
1:B:718:ILE:HG13	1:B:956:LEU:HD12	1.97	0.46
1:B:332:ALA:O	1:B:345:ARG:NH1	2.48	0.46
1:B:588:ILE:O	1:B:605:LEU:HB3	2.14	0.46
1:B:870:GLN:HE22	1:B:910:LYS:HE3	1.80	0.46
1:B:257:VAL:HB	2:F:1:NAG:O6	2.15	0.46
1:A:488:ARG:HG2	1:A:489:ASN:N	2.30	0.46
1:B:467:ASP:CG	1:B:602:ARG:HH12	2.19	0.46
1:B:647:LEU:HD13	1:B:686:TYR:CD2	2.51	0.46
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.96	0.46
1:B:828:LEU:HB3	1:B:840:LEU:HD11	1.96	0.46
1:A:919:GLU:O	1:A:920:SER:C	2.54	0.46
1:B:703:LEU:CD1	1:B:726:LEU:HD21	2.45	0.46
1:A:118:THR:O	1:A:119:ASN:CB	2.53	0.46
1:A:647:LEU:O	1:A:651:HIS:HB3	2.16	0.46
1:B:310:TYR:OH	1:B:373:ALA:HB2	2.15	0.46
1:B:58:ASN:N	1:B:58:ASN:HD22	2.14	0.46
1:A:412:GLN:HB3	1:A:746:TRP:HE1	1.80	0.46
1:A:313:TYR:CE2	1:A:478:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:HG2	1:B:134:GLY:HA3	1.98	0.46
1:B:310:TYR:CD1	1:B:314:PHE:CE2	2.96	0.46
1:A:107:PHE:HB3	1:A:151:LEU:HD23	1.98	0.46
1:A:553:LYS:HB3	1:A:560:ARG:HB2	1.98	0.46
1:B:442:THR:HG22	1:B:445:GLN:CG	2.46	0.46
1:B:674:ARG:O	1:B:675:LEU:HD12	2.15	0.46
1:A:786:ILE:CG2	1:A:790:VAL:HG23	2.46	0.46
1:A:409:PRO:HD2	1:A:410:GLU:OE2	2.16	0.45
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.98	0.45
1:B:186:THR:HG23	1:B:190:GLU:O	2.16	0.45
1:B:651:HIS:HD2	1:B:659:ARG:NH1	2.14	0.45
1:A:236:MET:HE1	1:A:320:LEU:HD22	1.98	0.45
1:B:119:ASN:O	1:B:166:MET:HA	2.16	0.45
1:B:537:MET:HA	1:B:587:HIS:CB	2.46	0.45
1:A:959:ASN:C	1:A:961:ARG:H	2.19	0.45
1:A:191:THR:HB	1:B:191:THR:H	1.82	0.45
1:B:375:GLN:O	1:B:379:ASN:HB2	2.16	0.45
1:B:873:TRP:CE3	1:B:873:TRP:HA	2.52	0.45
1:A:366[B]:ARG:HH21	1:A:397:LYS:HZ1	1.64	0.45
1:A:479:ILE:O	1:A:483:LYS:HG3	2.16	0.45
1:B:751:ARG:HG3	1:B:755:LEU:HD12	1.98	0.45
6:A:1009:P52:H26	6:A:1009:P52:H17	1.71	0.45
1:A:267:ILE:HD12	1:A:341:LEU:HD21	1.99	0.45
1:B:77:HIS:HD1	1:B:219:ASN:HB2	1.81	0.45
1:B:445:GLN:O	1:B:449:MET:HG2	2.16	0.45
1:B:535:LYS:O	1:B:538:MET:N	2.48	0.45
1:B:569:GLY:HA2	1:B:570:VAL:HA	1.69	0.45
1:B:707:TYR:HE1	1:B:723:LYS:HB2	1.81	0.45
1:A:592:TYR:CZ	1:A:601:HIS:HB2	2.52	0.45
1:B:729:TYR:HD2	1:B:730:PHE:N	2.15	0.45
1:A:145:HIS:O	1:A:147:GLN:HG3	2.17	0.45
1:A:411:LEU:HA	1:A:745:VAL:HG21	1.99	0.45
1:A:598:ASN:ND2	1:A:598:ASN:H	2.15	0.45
1:B:258:LYS:HG2	2:F:1:NAG:O5	2.16	0.45
1:B:729:TYR:C	1:B:731:LYS:N	2.70	0.45
1:B:729:TYR:CD2	1:B:730:PHE:N	2.84	0.45
1:A:412:GLN:HB3	1:A:746:TRP:NE1	2.32	0.45
1:A:598:ASN:ND2	1:A:598:ASN:N	2.64	0.45
1:B:183:THR:HA	1:B:192:ARG:O	2.17	0.45
1:B:200:GLU:HA	1:B:201:PRO:HA	1.73	0.45
1:B:104:ALA:HB1	1:B:155:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:ASN:HA	1:B:624:ASN:HD22	1.59	0.45
1:A:452:GLU:HG2	1:A:452:GLU:H	1.32	0.45
1:A:68:ARG:HD3	8:A:1114:HOH:O	2.16	0.45
1:A:786:ILE:HB	1:A:791:LEU:HD13	1.99	0.45
1:B:453:VAL:O	1:B:457:LYS:HB3	2.16	0.45
1:B:537:MET:O	1:B:541:TRP:CD1	2.70	0.45
1:B:718:ILE:HG13	1:B:956:LEU:CD1	2.47	0.45
1:A:156:LEU:HD12	1:A:162:TYR:CZ	2.52	0.44
1:A:434:ARG:NH1	1:A:435:PRO:O	2.50	0.44
1:A:598:ASN:N	1:A:598:ASN:HD22	2.13	0.44
1:A:916:LEU:HD22	1:A:916:LEU:HA	1.76	0.44
1:A:925:GLY:O	1:A:926:SER:C	2.54	0.44
1:B:342:ILE:HG22	1:B:344:TYR:CE1	2.51	0.44
1:A:809:LEU:O	1:A:812:TYR:HB3	2.17	0.44
1:B:273:SER:HB3	1:B:287:TYR:CD1	2.52	0.44
1:B:724:ARG:HB3	1:B:728:GLN:NE2	2.33	0.44
1:B:873:TRP:HE3	1:B:873:TRP:HA	1.82	0.44
1:A:624:ASN:HB2	1:A:631:TYR:CE2	2.53	0.44
1:A:860:HIS:CD2	1:A:864:ARG:HD2	2.52	0.44
1:A:926:SER:HA	1:A:927:HIS:HA	1.69	0.44
1:B:156:LEU:HD12	1:B:162:TYR:CZ	2.52	0.44
1:B:374:HIS:HA	1:B:377:PHE:O	2.18	0.44
1:B:774:PHE:CG	1:B:798:GLY:HA3	2.53	0.44
1:A:181:LYS:HE2	1:A:181:LYS:HB3	1.59	0.44
1:A:559:LEU:HD12	1:A:612:LEU:HB3	2.00	0.44
1:B:75:PRO:HG2	1:B:216:PHE:HB3	2.00	0.44
1:B:378:GLY:HA3	1:B:392:LYS:HG3	2.00	0.44
1:B:538:MET:O	1:B:541:TRP:HB2	2.17	0.44
1:B:588:ILE:HG12	1:B:588:ILE:O	2.16	0.44
1:B:651:HIS:HD2	1:B:659:ARG:HH11	1.65	0.44
1:A:553:LYS:O	1:A:559:LEU:HA	2.18	0.44
1:A:604:ILE:H	1:A:604:ILE:HD12	1.83	0.44
1:A:738:SER:O	1:A:751:ARG:CD	2.63	0.44
1:A:921:LEU:HD12	1:A:931:PHE:CZ	2.53	0.44
1:B:150:LEU:HD13	1:B:164:VAL:HG11	2.00	0.44
1:B:457:LYS:O	1:B:461:ILE:HG23	2.18	0.44
1:A:366[B]:ARG:NH2	1:A:397:LYS:NZ	2.64	0.44
1:A:600:ILE:HG23	1:A:625:VAL:HG21	1.99	0.44
1:A:651:HIS:C	1:A:651:HIS:CD2	2.91	0.44
1:A:660:VAL:HG22	1:A:695:ALA:HA	1.99	0.44
1:A:75:PRO:HG3	1:A:211:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HD13	1:B:166:MET:SD	2.58	0.44
1:B:421:CYS:O	1:B:425:ILE:HG13	2.18	0.44
1:B:217:LYS:HE3	1:B:489:ASN:OD1	2.18	0.44
1:B:651:HIS:CE1	1:B:689:HIS:HB3	2.52	0.44
1:B:832:LYS:HD3	1:B:832:LYS:HA	1.83	0.44
1:A:533:GLU:O	1:A:534:VAL:C	2.56	0.44
1:B:214:PRO:HA	1:B:260:SER:HB3	1.98	0.44
1:B:431:ASN:CA	1:B:565:ARG:HH22	2.29	0.44
1:B:927:HIS:O	1:B:928:LEU:HD23	2.18	0.44
1:B:931:PHE:O	1:B:935:LEU:HG	2.18	0.44
1:A:278:THR:HG23	1:A:282:VAL:HB	2.00	0.43
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.99	0.43
1:B:666:VAL:O	1:B:670:VAL:HG23	2.18	0.43
1:B:676:THR:HG23	1:B:679:LYS:H	1.83	0.43
1:B:729:TYR:O	1:B:731:LYS:N	2.51	0.43
1:B:96:LYS:HE3	1:B:96:LYS:HB3	1.77	0.43
1:B:624:ASN:HD21	1:B:629:GLY:N	2.15	0.43
1:B:713:ARG:HB2	1:B:715:ILE:HG13	1.99	0.43
1:A:366[B]:ARG:NH2	1:A:397:LYS:HZ2	2.15	0.43
1:B:357:SER:H	1:B:360:ASP:HB2	1.83	0.43
1:B:790:VAL:O	1:B:794:VAL:HG23	2.19	0.43
1:B:942:ILE:O	1:B:946:GLU:HG2	2.17	0.43
1:A:434:ARG:HD2	1:A:438:LYS:HD3	1.99	0.43
1:A:442:THR:HG22	1:A:445:GLN:CD	2.39	0.43
1:A:819:ALA:O	1:A:822:ASN:HB3	2.18	0.43
1:B:418:LEU:HA	1:B:418:LEU:HD23	1.88	0.43
1:A:104:ALA:HB1	1:A:155:LYS:HE2	2.00	0.43
1:A:488:ARG:CG	1:A:489:ASN:N	2.81	0.43
1:A:592:TYR:CE1	1:A:601:HIS:HB2	2.53	0.43
1:A:559:LEU:HD12	1:A:612:LEU:C	2.39	0.43
1:B:67:LEU:HB3	1:B:145:HIS:NE2	2.32	0.43
1:B:285:SER:O	1:B:286:ILE:HD13	2.18	0.43
1:B:176:PHE:CD2	1:B:332:ALA:HB2	2.54	0.43
1:B:419:ASN:ND2	1:B:419:ASN:N	2.64	0.43
1:A:386:TRP:CE3	1:A:389:ILE:HD13	2.53	0.43
1:A:792:LYS:HD3	1:A:826:TYR:CD2	2.54	0.43
1:B:95:GLU:HG2	1:B:168:PHE:HE1	1.83	0.43
1:B:479:ILE:O	1:B:483:LYS:HB2	2.18	0.43
1:A:57:THR:HG23	1:A:141:SER:O	2.18	0.43
1:B:545:LYS:CG	1:B:546:GLY:H	2.31	0.43
1:B:545:LYS:HG2	1:B:546:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:SER:HB3	1:B:620:TRP:CE2	2.53	0.43
1:B:647:LEU:HD23	1:B:651:HIS:HB2	2.01	0.43
1:B:78:TYR:HB2	1:B:220:PHE:CD1	2.54	0.43
1:B:79:ASP:O	1:B:95:GLU:HA	2.19	0.43
1:A:832:LYS:HA	1:A:832:LYS:HD3	1.88	0.43
1:B:545:LYS:CG	1:B:546:GLY:N	2.81	0.43
1:B:860:HIS:C	1:B:860:HIS:CD2	2.92	0.43
1:B:724:ARG:HD2	1:B:728:GLN:HE22	1.84	0.43
1:B:797:VAL:O	1:B:800:GLN:HG2	2.19	0.43
1:A:565:ARG:HD3	1:A:581:GLN:HB2	2.00	0.42
1:A:587:HIS:HA	1:A:605:LEU:O	2.19	0.42
1:A:60:GLU:HB3	1:A:61:ARG:H	1.68	0.42
1:B:597:SER:C	1:B:599:VAL:H	2.22	0.42
1:B:624:ASN:CG	1:B:627:SER:HA	2.40	0.42
1:B:870:GLN:HE22	1:B:910:LYS:CE	2.31	0.42
1:A:142:TYR:CE1	1:A:144:ALA:HB3	2.54	0.42
1:A:364:VAL:O	1:A:368:ILE:HG13	2.19	0.42
1:A:873:TRP:CE3	1:A:873:TRP:HA	2.54	0.42
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.82	0.42
1:A:298:TYR:CE2	1:A:361:LYS:HE3	2.54	0.42
1:A:336:MET:O	1:A:342:ILE:HG23	2.18	0.42
1:B:595:SER:HA	1:B:620:TRP:CH2	2.54	0.42
1:B:866:PRO:O	1:B:869:GLN:HG2	2.18	0.42
1:A:457:LYS:O	1:A:461:ILE:HG23	2.19	0.42
1:A:945:LEU:O	1:A:949:LEU:HB2	2.20	0.42
1:B:154:GLU:O	1:B:155:LYS:C	2.58	0.42
1:B:214:PRO:HG3	1:B:386:TRP:CZ2	2.54	0.42
1:B:233:LEU:O	1:B:266:TYR:HA	2.19	0.42
1:B:604:ILE:H	1:B:604:ILE:HD12	1.84	0.42
1:B:695:ALA:HA	1:B:698:GLU:HB3	2.01	0.42
1:A:176:PHE:HE1	1:A:330:ASP:HB3	1.84	0.42
1:A:608:LYS:HD3	1:A:608:LYS:O	2.20	0.42
1:A:888:ASP:HB2	1:A:891:SER:HB3	2.02	0.42
1:B:777:TRP:HB2	1:B:784:LEU:HD12	2.01	0.42
1:A:130:TYR:HB3	1:A:131:MET:H	1.61	0.42
1:A:786:ILE:HG12	1:A:794:VAL:HG11	2.02	0.42
1:B:122:LEU:CB	1:B:137:LEU:HD21	2.39	0.42
1:B:181:LYS:HE2	1:B:181:LYS:HB3	1.80	0.42
1:B:248:LEU:C	1:B:249:LEU:HD23	2.40	0.42
1:B:949:LEU:N	1:B:950:PRO:CD	2.80	0.42
1:A:348:SER:O	1:A:364:VAL:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLU:HB2	1:A:445:GLN:OE1	2.19	0.42
1:A:533:GLU:CG	1:A:533:GLU:O	2.66	0.42
1:A:581:GLN:CG	1:A:582:GLU:H	2.16	0.42
1:A:588:ILE:HA	1:A:589:PRO:HD3	1.83	0.42
1:A:845:MET:SD	1:A:855:LEU:HD11	2.59	0.42
1:B:334:GLY:HA2	1:B:345:ARG:HD3	2.02	0.42
1:B:380:LEU:HD11	1:B:487:TYR:CE2	2.55	0.42
1:B:438:LYS:HG2	1:B:439:PRO:N	2.33	0.42
1:B:906:SER:CB	1:B:941:ASN:HB3	2.47	0.42
1:A:436:ILE:HA	1:A:453:VAL:HG12	2.01	0.42
1:B:429:SER:O	1:B:430:LEU:HD23	2.19	0.42
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.91	0.42
1:A:614:LEU:HA	1:A:615:PRO:HD3	1.87	0.42
1:A:855:LEU:HD22	1:A:859:LEU:HD22	2.02	0.42
1:B:324:ASP:C	1:B:325:LEU:HD12	2.39	0.42
1:B:436:ILE:CD1	1:B:458:GLY:HA2	2.50	0.42
1:B:647:LEU:O	1:B:651:HIS:HB3	2.20	0.42
1:B:726:LEU:O	1:B:729:TYR:O	2.38	0.42
1:B:943:LYS:HD3	1:B:943:LYS:HA	1.71	0.42
1:A:364:VAL:HA	1:A:367:VAL:HG13	2.00	0.42
1:A:488:ARG:CG	1:A:489:ASN:H	2.32	0.42
1:A:667:PHE:CE1	1:A:680:ALA:HB1	2.55	0.42
1:A:681:LEU:HD12	1:A:681:LEU:HA	1.84	0.42
1:B:270:ASP:OD1	1:B:270:ASP:N	2.53	0.42
1:B:469:LEU:O	1:B:473:LYS:HB3	2.20	0.42
1:B:710:MET:O	1:B:713:ARG:O	2.37	0.42
1:A:132:LYS:O	1:A:134:GLY:HA2	2.19	0.41
1:A:231:ILE:O	1:A:268:VAL:HA	2.20	0.41
1:A:588:ILE:HG12	1:A:588:ILE:O	2.20	0.41
1:A:604:ILE:O	1:A:605:LEU:HB2	2.20	0.41
1:A:717:ASP:OD1	1:A:953:ARG:NH1	2.53	0.41
1:B:444:THR:HG23	1:B:890:GLY:H	1.85	0.41
1:A:666:VAL:HG11	1:A:680:ALA:HA	2.01	0.41
1:B:408:TYR:N	1:B:409:PRO:HD3	2.35	0.41
1:B:314:PHE:O	1:B:316:ILE:HG13	2.19	0.41
1:B:770:ALA:HB1	1:B:797:VAL:HG21	2.03	0.41
1:A:117:ILE:CD1	1:A:148:ILE:HD13	2.51	0.41
1:A:479:ILE:H	1:A:479:ILE:HG12	1.64	0.41
1:A:884:LEU:HA	1:A:884:LEU:HD12	1.74	0.41
1:B:832:LYS:HB3	1:B:867:LYS:HE3	2.02	0.41
1:A:959:ASN:C	1:A:961:ARG:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:N	8:A:1231:HOH:O	2.51	0.41
1:A:950:PRO:HG2	8:A:1261:HOH:O	2.21	0.41
1:B:488:ARG:HG2	1:B:489:ASN:N	2.34	0.41
1:B:547:ILE:HA	1:B:548:PRO:HD3	1.81	0.41
1:B:559:LEU:HD12	1:B:612:LEU:O	2.21	0.41
1:B:56:ALA:HB2	1:B:62:PHE:HB2	2.03	0.41
1:B:918:PHE:N	1:B:918:PHE:HD1	2.19	0.41
1:B:93:ALA:HB3	1:B:168:PHE:CE2	2.56	0.41
1:B:382:THR:HB	1:B:489:ASN:OD1	2.21	0.41
1:B:682:ASP:OD1	1:B:955:TRP:NE1	2.47	0.41
1:B:866:PRO:HA	1:B:869:GLN:OE1	2.20	0.41
1:B:888:ASP:O	1:B:891:SER:N	2.53	0.41
1:A:625:VAL:CG1	1:A:655:ARG:HD2	2.51	0.41
1:A:819:ALA:O	1:A:823:LYS:HG3	2.21	0.41
1:B:534:VAL:HG12	1:B:538:MET:HG2	2.03	0.41
1:B:924:GLN:C	1:B:926:SER:H	2.24	0.41
1:A:137:LEU:HD11	1:A:152:VAL:HG22	2.02	0.41
1:A:491:LYS:HE3	1:A:491:LYS:HB2	1.94	0.41
1:A:605:LEU:HD12	1:A:606:LYS:N	2.36	0.41
1:B:239:VAL:HG12	1:B:240:LYS:N	2.36	0.41
1:B:62:PHE:HA	1:B:63:PRO:HD3	1.68	0.41
1:B:918:PHE:HE2	1:B:934:VAL:HB	1.85	0.41
1:A:334:GLY:H	6:A:1009:P52:H18	1.68	0.41
1:B:707:TYR:CE1	1:B:723:LYS:HB2	2.56	0.41
1:A:385:TRP:CD1	1:A:387:ASN:ND2	2.85	0.40
1:A:910:LYS:HA	1:A:910:LYS:HD3	1.84	0.40
1:A:921:LEU:O	1:A:926:SER:OG	2.28	0.40
6:B:1010:P52:H27	6:B:1010:P52:H17	1.87	0.40
1:B:239:VAL:HG12	1:B:240:LYS:HD2	2.03	0.40
1:B:465:LEU:CD1	1:B:534:VAL:HG11	2.51	0.40
1:A:191:THR:O	1:B:190:GLU:HG2	2.21	0.40
1:A:412:GLN:NE2	1:A:745:VAL:HB	2.36	0.40
1:A:419:ASN:O	1:A:423:GLU:HG3	2.20	0.40
1:A:826:TYR:C	1:A:826:TYR:CD2	2.94	0.40
1:B:604:ILE:O	1:B:605:LEU:HB2	2.21	0.40
1:B:677:LEU:HG	1:B:681:LEU:HD22	2.04	0.40
1:B:82:VAL:O	1:B:84:PRO:HD3	2.21	0.40
1:B:838:LEU:HD22	1:B:838:LEU:O	2.21	0.40
1:B:865:ARG:HG2	1:B:865:ARG:H	1.65	0.40
1:A:248:LEU:O	1:A:249:LEU:HD23	2.20	0.40
1:A:614:LEU:HD12	1:A:615:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:GLU:OE2	1:A:702:TYR:HE2	2.03	0.40
1:A:715:ILE:HG21	1:A:718:ILE:HD12	2.02	0.40
1:B:103:ASN:O	1:B:104:ALA:C	2.59	0.40
1:B:355:THR:HG21	1:B:820:GLU:CB	2.41	0.40
1:B:537:MET:HA	1:B:587:HIS:HB2	2.02	0.40
1:B:74:ILE:HA	1:B:75:PRO:HD3	1.64	0.40
1:A:563:GLN:OE1	1:A:585:LEU:HA	2.22	0.40
1:A:882:HIS:O	1:A:882:HIS:ND1	2.54	0.40
1:B:197:THR:HB	1:B:199:PHE:CZ	2.57	0.40
1:B:757:LEU:O	1:B:761:LEU:HD22	2.21	0.40
1:B:898:ILE:HG22	1:B:899:SER:N	2.36	0.40
1:A:697:LEU:HD12	1:A:697:LEU:HA	1.84	0.40
1:B:78:TYR:CD2	1:B:220:PHE:CE1	3.09	0.40
1:B:884:LEU:HD11	1:B:889:LEU:HD23	2.04	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	863/967 (89%)	771 (89%)	76 (9%)	16 (2%)	8	23
1	B	842/967 (87%)	701 (83%)	107 (13%)	34 (4%)	3	8
All	All	1705/1934 (88%)	1472 (86%)	183 (11%)	50 (3%)	4	14

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	583	ARG
1	A	616	GLU
1	A	617	LYS

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Mol	Chain	Res	Type
1	A	922	GLU
1	A	923	ALA
1	B	535	LYS
1	B	545	LYS
1	B	546	GLY
1	B	569	GLY
1	B	596	SER
1	B	926	SER
1	B	948	ASN
1	A	534	VAL
1	A	619	SER
1	B	100	LEU
1	B	216	PHE
1	B	606	LYS
1	B	616	GLU
1	B	649	GLN
1	B	739	TRP
1	B	776	GLN
1	B	860	HIS
1	A	603	HIS
1	A	605	LEU
1	B	72	VAL
1	B	155	LYS
1	B	239	VAL
1	B	245	GLU
1	B	278	THR
1	B	694	PRO
1	A	55	VAL
1	A	155	LYS
1	B	60	GLU
1	B	921	LEU
1	B	945	LEU
1	B	470	GLY
1	B	598	ASN
1	B	720	GLU
1	B	730	PHE
1	B	732	PRO
1	A	60	GLU
1	B	99	VAL
1	B	615	PRO
1	B	692	SER
1	A	715	ILE

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Mol	Chain	Res	Type
1	B	715	ILE
1	A	175	GLY
1	B	898	ILE
1	A	133	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	772/870 (89%)	699 (90%)	73 (10%)	8	23
1	B	733/870 (84%)	675 (92%)	58 (8%)	12	31
All	All	1505/1740 (86%)	1374 (91%)	131 (9%)	10	27

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	PHE
1	A	65	GLN
1	A	67	LEU
1	A	73	VAL
1	A	80	LEU
1	A	92	VAL
1	A	110	LEU
1	A	130	TYR
1	A	145	HIS
1	A	194	LEU
1	A	196	VAL
1	A	229	ARG
1	A	243	GLU
1	A	248	LEU
1	A	261	THR
1	A	278	THR
1	A	320	LEU
1	A	322	LYS
1	A	355	THR

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Mol	Chain	Res	Type
1	A	364	VAL
1	A	367	VAL
1	A	383	MET
1	A	395	PHE
1	A	401	LEU
1	A	426	THR
1	A	437	SER
1	A	442	THR
1	A	452	GLU
1	A	479	ILE
1	A	491	LYS
1	A	493	ASP
1	A	528	LEU
1	A	530	GLU
1	A	533	GLU
1	A	552	VAL
1	A	559	LEU
1	A	563	GLN
1	A	582	GLU
1	A	585	LEU
1	A	588	ILE
1	A	591	THR
1	A	593	SER
1	A	598	ASN
1	A	604	ILE
1	A	613	ASP
1	A	618	THR
1	A	624	ASN
1	A	625	VAL
1	A	645	THR
1	A	676	THR
1	A	681	LEU
1	A	697	LEU
1	A	722	LEU
1	A	729	TYR
1	A	742	LYS
1	A	761	LEU
1	A	762	ASN
1	A	767	ILE
1	A	773	LEU
1	A	801	THR
1	A	802	THR

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Mol	Chain	Res	Type
1	A	825	LEU
1	A	834	GLN
1	A	835	GLU
1	A	855	LEU
1	A	859	LEU
1	A	877	ARG
1	A	896	MET
1	A	909	ASP
1	A	916	LEU
1	A	926	SER
1	A	927	HIS
1	A	952	LEU
1	B	58	ASN
1	B	73	VAL
1	B	76	LEU
1	B	80	LEU
1	B	99	VAL
1	B	106	GLN
1	B	110	LEU
1	B	145	HIS
1	B	155	LYS
1	B	169	GLN
1	B	194	LEU
1	B	196	VAL
1	B	215	LEU
1	B	240	LYS
1	B	245	GLU
1	B	261	THR
1	B	268	VAL
1	B	322	LYS
1	B	352	ASP
1	B	364	VAL
1	B	367	VAL
1	B	383	MET
1	B	395	PHE
1	B	401	LEU
1	B	419	ASN
1	B	433	SER
1	B	434	ARG
1	B	436	ILE
1	B	468	PHE
1	B	533	GLU

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Mol	Chain	Res	Type
1	B	540	THR
1	B	559	LEU
1	B	585	LEU
1	B	588	ILE
1	B	598	ASN
1	B	604	ILE
1	B	610	ASP
1	B	621	VAL
1	B	624	ASN
1	B	625	VAL
1	B	633	VAL
1	B	650	ASN
1	B	674	ARG
1	B	675	LEU
1	B	681	LEU
1	B	686	TYR
1	B	697	LEU
1	B	761	LEU
1	B	767	ILE
1	B	825	LEU
1	B	834	GLN
1	B	855	LEU
1	B	871	LEU
1	B	873	TRP
1	B	888	ASP
1	B	909	ASP
1	B	911	LEU
1	B	952	LEU

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

Mol	Chain	Res	Type
1	A	159	HIS
1	A	169	GLN
1	A	412	GLN
1	A	554	GLN
1	A	562	GLN
1	A	587	HIS
1	A	598	ASN
1	A	624	ASN
1	A	648	ASN
1	A	651	HIS

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Mol	Chain	Res	Type
1	A	664	HIS
1	A	806	ASN
1	A	834	GLN
1	A	854	ASN
1	A	860	HIS
1	A	869	GLN
1	A	870	GLN
1	A	904	HIS
1	A	927	HIS
1	A	959	ASN
1	B	58	ASN
1	B	159	HIS
1	B	203	GLN
1	B	301	GLN
1	B	412	GLN
1	B	419	ASN
1	B	563	GLN
1	B	598	ASN
1	B	624	ASN
1	B	651	HIS
1	B	689	HIS
1	B	728	GLN
1	B	763	HIS
1	B	811	GLN
1	B	822	ASN
1	B	833	HIS
1	B	860	HIS
1	B	870	GLN
1	B	879	ASN
1	B	912	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 ⓘ

10 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	0.58	0	17,19,21	0.89	1 (5%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	0.85	0
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	0.95	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.49	0	17,19,21	1.95	3 (17%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	1.43	1 (5%)
3	MAN	E	3	3	11,11,12	0.59	0	15,15,17	2.02	4 (26%)
3	MAN	E	4	3	11,11,12	0.53	0	15,15,17	2.01	3 (20%)
2	NAG	F	1	1,2	14,14,15	0.54	0	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.59	0	17,19,21	1.08	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	6.30	120.72	112.19
3	E	1	NAG	C1-O5-C5	5.18	119.21	112.19
3	E	2	NAG	C1-O5-C5	4.62	118.45	112.19
3	E	3	MAN	C2-C3-C4	4.34	118.41	110.89
3	E	1	NAG	C4-C3-C2	-4.00	105.16	111.02
3	E	3	MAN	C1-C2-C3	3.71	114.23	109.67
2	F	2	NAG	C1-O5-C5	3.56	117.02	112.19
3	E	1	NAG	C1-C2-N2	2.96	115.54	110.49
3	E	3	MAN	C1-O5-C5	2.94	116.18	112.19
3	E	4	MAN	C6-C5-C4	-2.64	106.82	113.00
3	E	4	MAN	C2-C3-C4	-2.54	106.50	110.89
3	E	3	MAN	C3-C4-C5	2.29	114.33	110.24
2	D	2	NAG	O5-C5-C6	2.17	110.60	107.20
2	D	2	NAG	C1-O5-C5	2.14	115.10	112.19
2	C	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	C	2	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

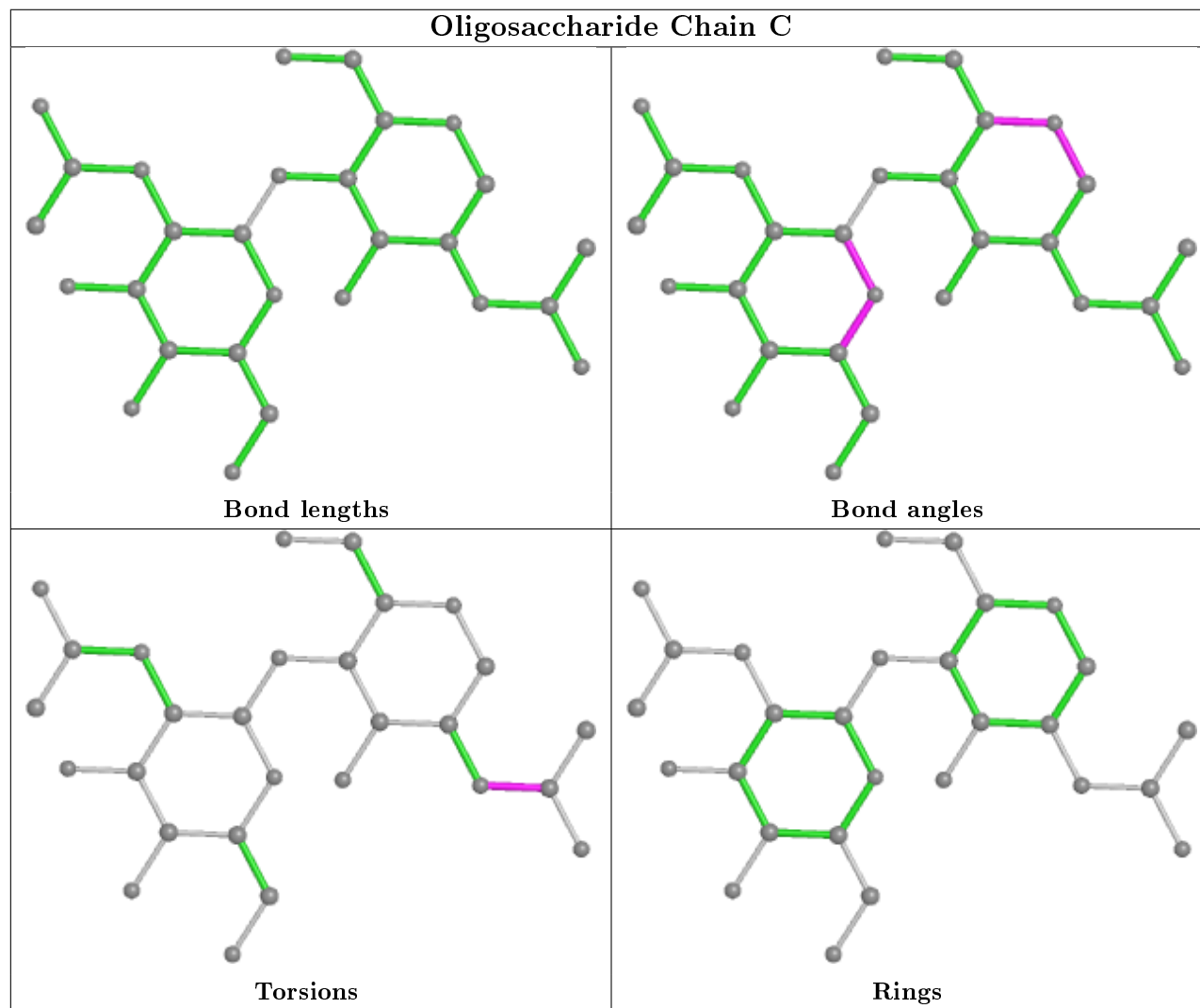
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C1-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	3	MAN	C4-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2

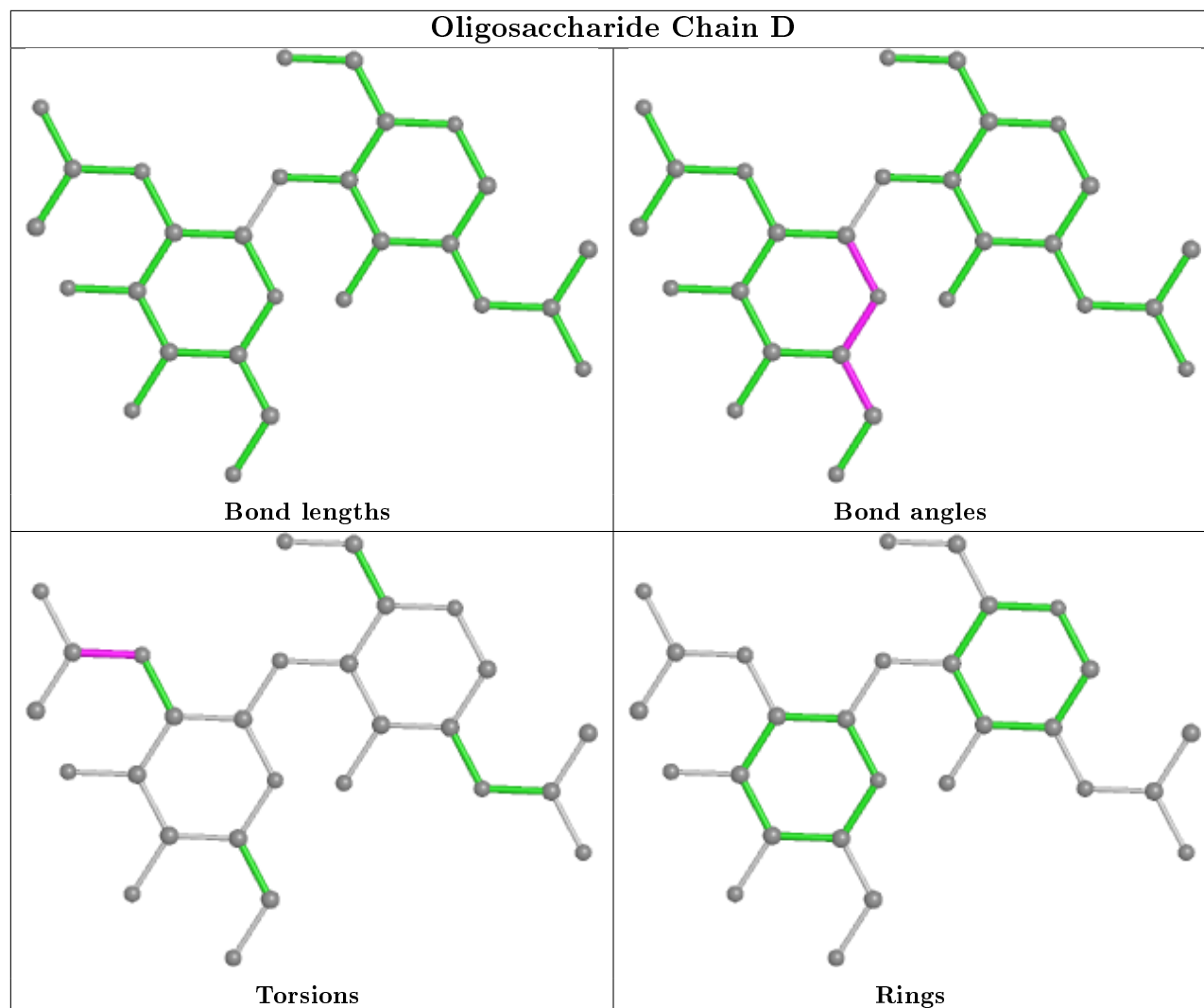
There are no ring outliers.

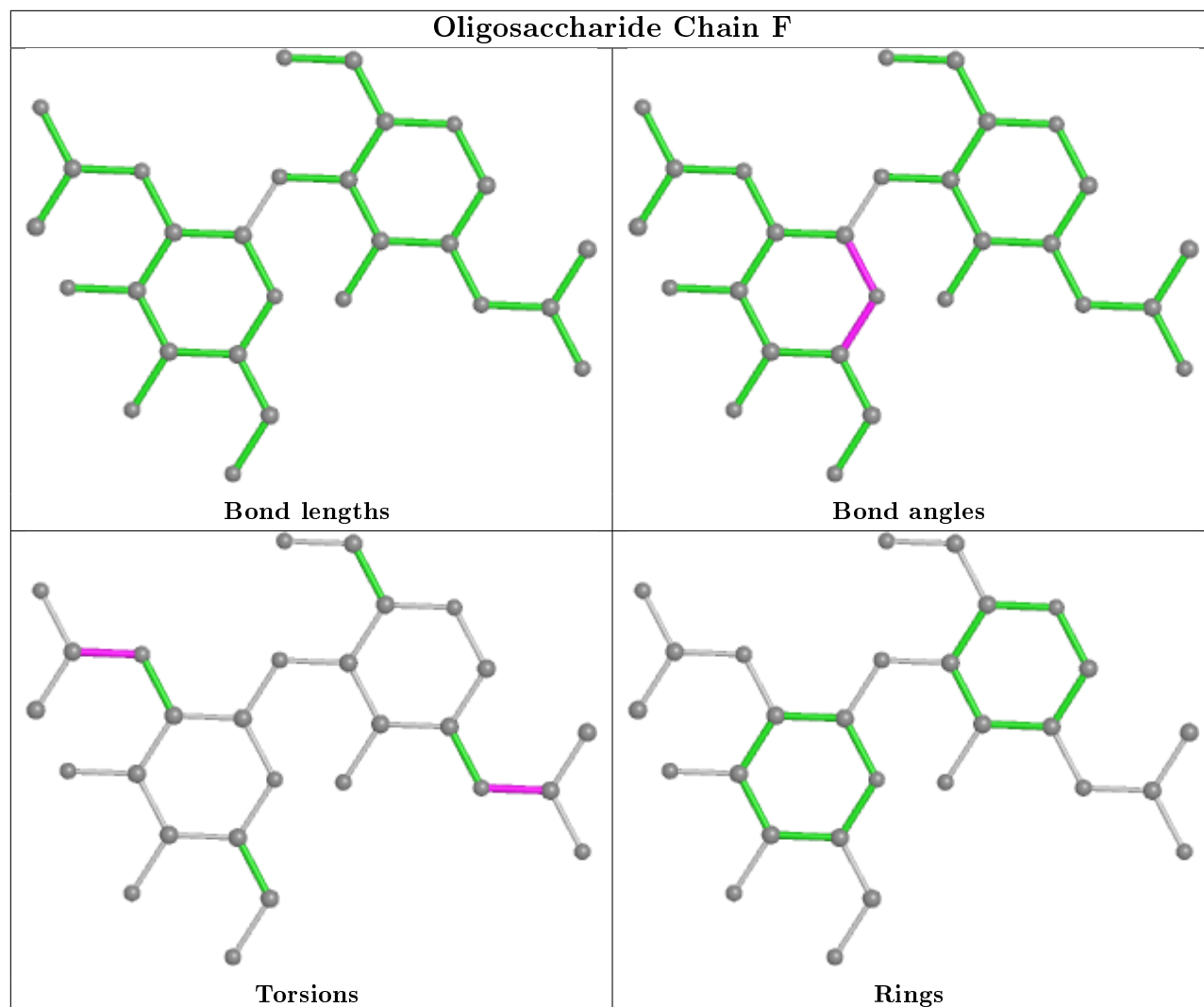
5 monomers are involved in 7 short contacts:

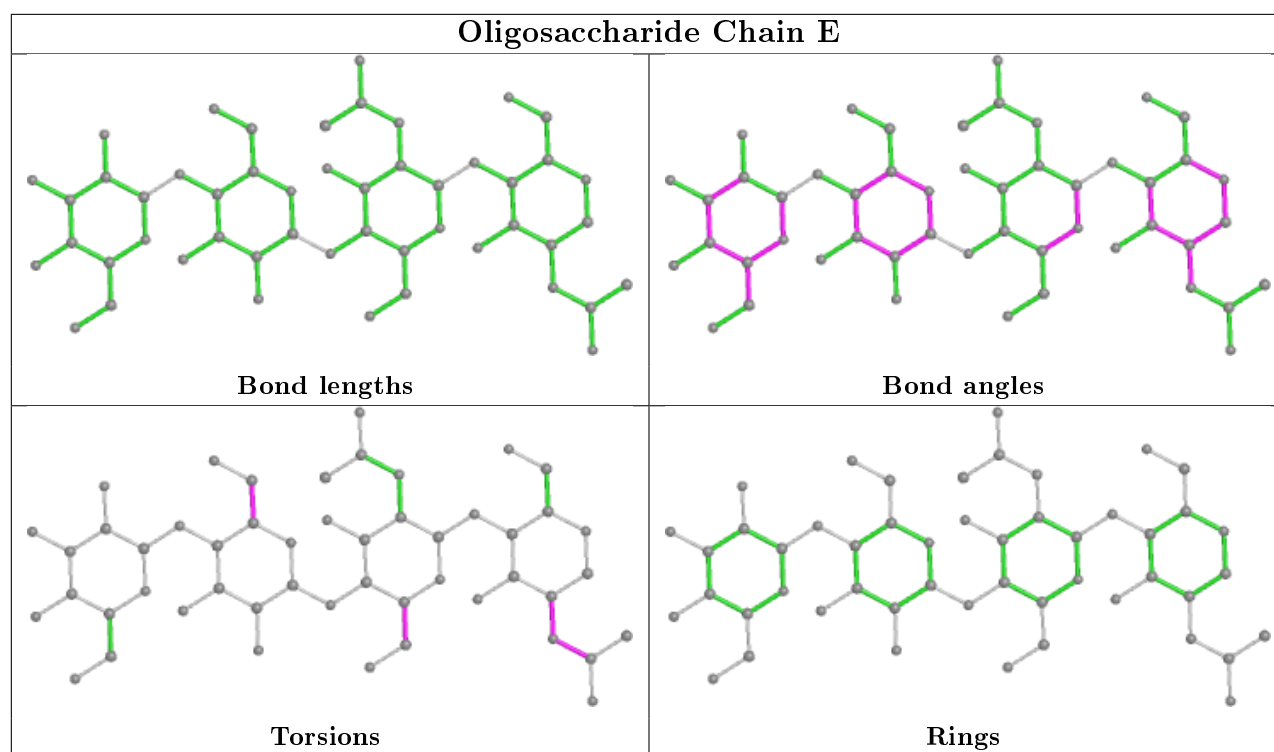
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	MAN	2	0
3	E	3	MAN	3	0
3	E	1	NAG	1	0
2	F	1	NAG	3	0
2	F	2	NAG	1	0

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	P52	B	1010	5	33,38,38	3.83	5 (15%)	38,53,53	2.93	5 (13%)
4	NAG	A	1005	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
7	IMD	A	1011	-	3,5,5	0.38	0	4,5,5	0.49	0
4	NAG	B	1007	1	14,14,15	0.57	0	17,19,21	1.23	1 (5%)
6	P52	A	1009	5	33,38,38	3.84	5 (15%)	38,53,53	2.27	5 (13%)
7	IMD	A	1010	-	3,5,5	0.36	0	4,5,5	0.65	0
4	NAG	A	1007	1	14,14,15	0.48	0	17,19,21	0.97	1 (5%)
4	NAG	B	1008	1	14,14,15	0.48	0	17,19,21	0.79	1 (5%)
4	NAG	A	1006	1	14,14,15	0.77	0	17,19,21	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IMD	A	1010	-	-	-	0/1/1/1
6	P52	B	1010	5	-	14/29/36/36	0/3/3/3
4	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
7	IMD	A	1011	-	-	-	0/1/1/1
4	NAG	B	1007	1	-	4/6/23/26	0/1/1/1
6	P52	A	1009	5	-	11/29/36/36	0/3/3/3
4	NAG	B	1008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1009	P52	P1-C11	-19.75	1.60	1.79
6	B	1010	P52	P1-C11	-19.67	1.60	1.79
6	B	1010	P52	C9-N1	-6.77	1.29	1.48
6	A	1009	P52	C9-N1	-6.72	1.29	1.48
6	B	1010	P52	C18-N4	4.40	1.44	1.32
6	A	1009	P52	C10-N2	4.29	1.43	1.34
6	A	1009	P52	C18-N4	4.15	1.43	1.32
6	B	1010	P52	C10-N2	3.99	1.42	1.34
6	B	1010	P52	P1-O1	-2.02	1.46	1.49
6	A	1009	P52	P1-O1	-2.01	1.46	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1010	P52	C17-N2-C10	16.40	156.83	121.67
6	A	1009	P52	C17-N2-C10	11.86	147.10	121.67
4	B	1007	NAG	O5-C1-C2	3.55	116.89	111.29
4	A	1005	NAG	C1-O5-C5	2.87	116.08	112.19
6	A	1009	P52	O3-C10-N2	-2.65	118.02	122.93
6	B	1010	P52	O4-C18-N4	-2.60	118.49	123.00
4	A	1007	NAG	C1-O5-C5	2.55	115.64	112.19
6	B	1010	P52	C5-C4-C3	2.52	124.02	120.19
6	A	1009	P52	O4-C18-N4	-2.37	118.88	123.00
6	B	1010	P52	O3-C10-N2	-2.36	118.56	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1009	P 52	C5-C4-C3	2.33	123.74	120.19
6	B	1010	P 52	C12-C10-N2	2.28	120.15	116.21
6	A	1009	P 52	C12-C10-N2	2.23	120.06	116.21
4	B	1008	NAG	C1-O5-C5	2.18	115.15	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1010	P 52	C1-C8-C9-N1
6	B	1010	P 52	C8-C9-P1-O1
6	B	1010	P 52	O3-C10-C12-C13
6	B	1010	P 52	N2-C10-C12-C13
6	B	1010	P 52	O3-C10-N2-C17
6	B	1010	P 52	C12-C10-N2-C17
6	B	1010	P 52	P1-C11-C12-C10
6	B	1010	P 52	C12-C11-P1-O1
6	B	1010	P 52	C12-C11-P1-O2
6	B	1010	P 52	C10-C12-C13-C14
6	B	1010	P 52	C11-C12-C13-C14
4	B	1007	NAG	C8-C7-N2-C2
4	B	1007	NAG	O7-C7-N2-C2
6	A	1009	P 52	O3-C10-C12-C13
6	A	1009	P 52	N2-C10-C12-C13
6	A	1009	P 52	O3-C10-N2-C17
6	A	1009	P 52	C12-C10-N2-C17
6	A	1009	P 52	C12-C11-P1-O1
6	A	1009	P 52	C12-C11-P1-O2
6	A	1009	P 52	C10-C12-C13-C14
6	A	1009	P 52	C11-C12-C13-C14
4	B	1008	NAG	O7-C7-N2-C2
4	A	1007	NAG	C8-C7-N2-C2
4	A	1007	NAG	O7-C7-N2-C2
4	B	1008	NAG	C8-C7-N2-C2
6	A	1009	P 52	C12-C13-C14-C15
6	A	1009	P 52	C12-C13-C14-C16
6	B	1010	P 52	C19-C17-N2-C10
4	B	1007	NAG	O5-C5-C6-O6
4	B	1007	NAG	C4-C5-C6-O6
4	A	1005	NAG	C8-C7-N2-C2
4	A	1005	NAG	O7-C7-N2-C2
4	A	1007	NAG	O5-C5-C6-O6

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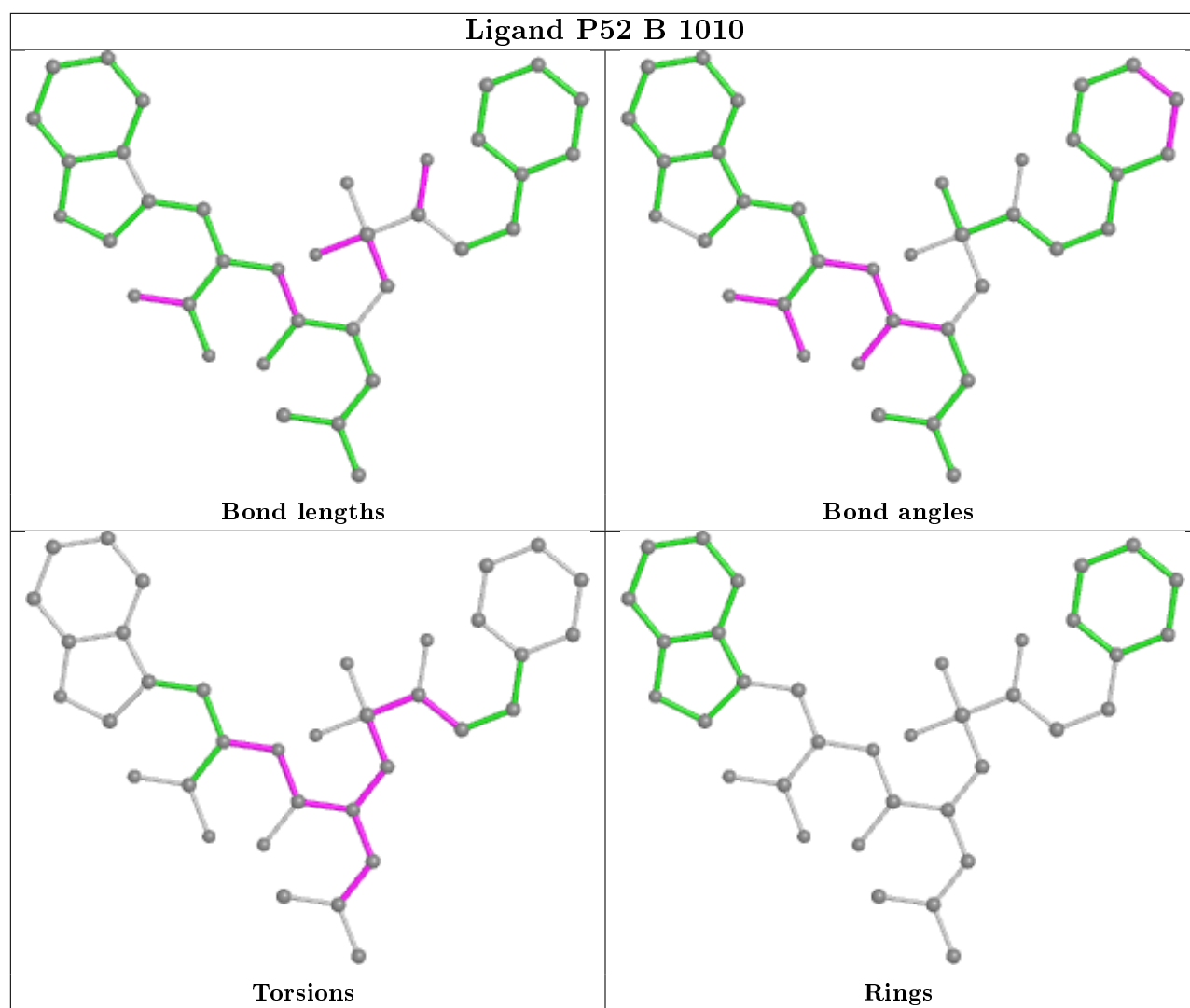
Mol	Chain	Res	Type	Atoms
4	A	1007	NAG	C4-C5-C6-O6
6	B	1010	P52	P1-C11-C12-C13
4	A	1006	NAG	C8-C7-N2-C2
6	B	1010	P52	C12-C13-C14-C16
4	A	1006	NAG	O7-C7-N2-C2
6	A	1009	P52	C1-C8-C9-N1

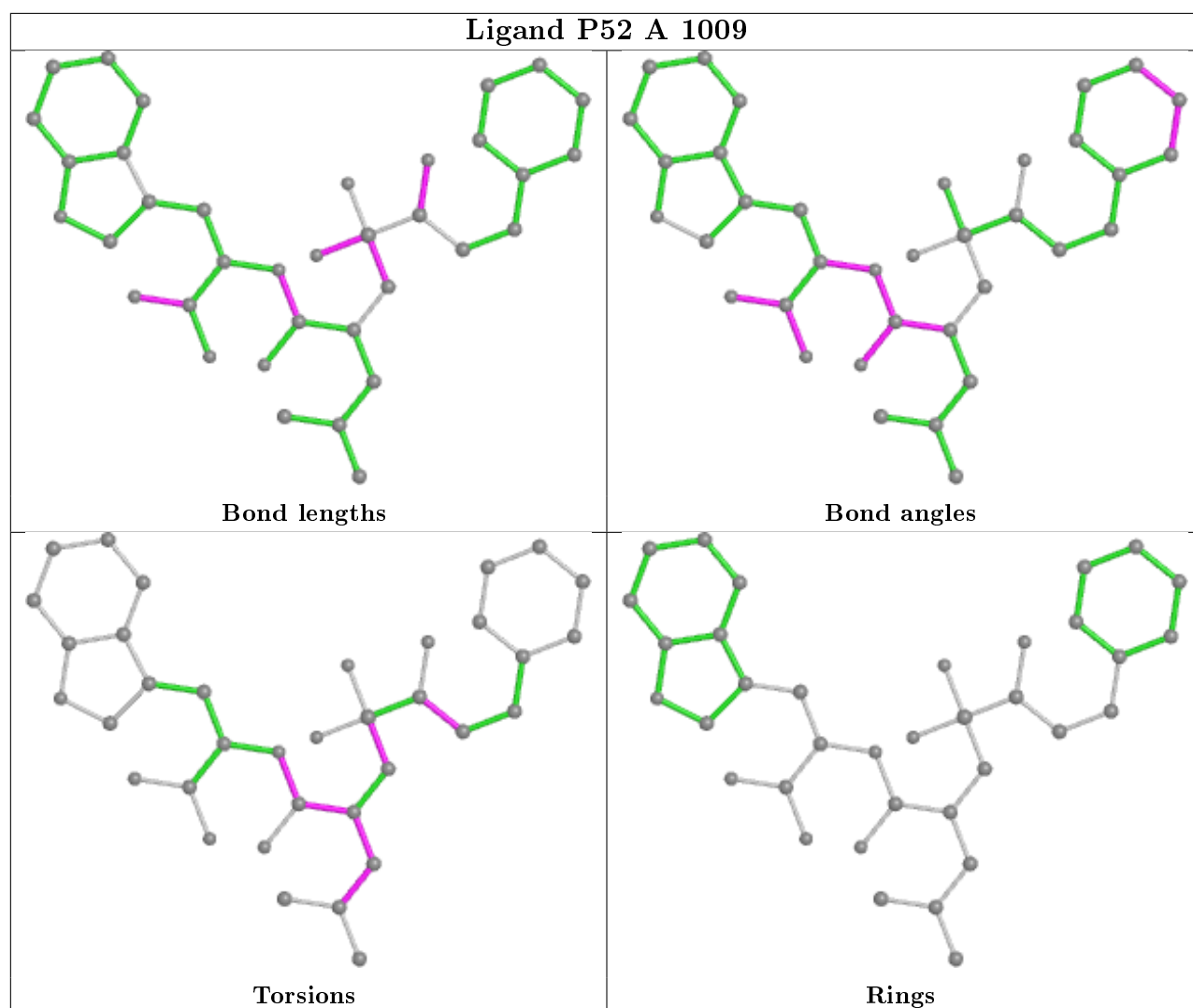
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1010	P52	2	0
6	A	1009	P52	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	869/967 (89%)	-0.01	15 (1%) 70 67	21, 48, 86, 115	2 (0%)
1	B	854/967 (88%)	0.76	117 (13%) 3 2	29, 84, 120, 144	0
All	All	1723/1934 (89%)	0.37	132 (7%) 13 9	21, 62, 112, 144	2 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	TRP	12.1
1	B	570	VAL	8.9
1	B	559	LEU	8.4
1	B	687	LEU	7.4
1	B	603	HIS	6.6
1	B	537	MET	6.3
1	B	602	ARG	5.7
1	B	534	VAL	5.5
1	B	550	LEU	5.5
1	B	611	THR	5.3
1	B	72	VAL	5.3
1	B	623	PHE	5.2
1	B	635	TYR	5.2
1	B	561	LEU	5.2
1	B	634	HIS	5.2
1	B	105	THR	5.0
1	B	153	PRO	4.9
1	B	681	LEU	4.8
1	B	609	THR	4.6
1	B	622	LYS	4.6
1	B	610	ASP	4.4
1	B	607	SER	4.3
1	B	73	VAL	4.3
1	B	797	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	637	GLY	4.2
1	B	152	VAL	4.2
1	B	613	ASP	4.2
1	B	666	VAL	4.2
1	B	555	ASP	4.1
1	B	924	GLN	4.1
1	B	956	LEU	4.0
1	B	107	PHE	4.0
1	B	651	HIS	3.9
1	B	569	GLY	3.8
1	B	108	ILE	3.8
1	B	767	ILE	3.8
1	B	831	SER	3.7
1	B	606	LYS	3.7
1	B	620	TRP	3.6
1	B	952	LEU	3.6
1	B	944	TRP	3.6
1	B	734	ILE	3.6
1	B	837	LEU	3.5
1	B	106	GLN	3.5
1	B	532	ALA	3.5
1	A	779	GLU	3.5
1	A	614	LEU	3.5
1	B	500	SER	3.5
1	A	559	LEU	3.3
1	B	633	VAL	3.3
1	A	556	GLY	3.3
1	B	416	TYR	3.2
1	B	590	LEU	3.2
1	B	549	LEU	3.2
1	B	465	LEU	3.2
1	B	677	LEU	3.2
1	B	838	LEU	3.1
1	B	768	GLN	3.1
1	B	667	PHE	3.1
1	A	72	VAL	3.0
1	B	648	ASN	3.0
1	B	380	LEU	3.0
1	B	600	ILE	3.0
1	B	832	LYS	3.0
1	A	784	LEU	3.0
1	B	120	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	638	HIS	2.9
1	A	618	THR	2.9
1	B	784	LEU	2.9
1	B	719	SER	2.9
1	B	162	TYR	2.9
1	B	621	VAL	2.9
1	B	598	ASN	2.9
1	B	750	LEU	2.8
1	B	689	HIS	2.8
1	B	680	ALA	2.8
1	B	612	LEU	2.8
1	B	66	GLU	2.7
1	A	619	SER	2.7
1	B	541	TRP	2.7
1	B	536	GLU	2.7
1	B	670	VAL	2.7
1	B	724	ARG	2.7
1	B	639	GLY	2.7
1	B	945	LEU	2.7
1	B	156	LEU	2.6
1	B	647	LEU	2.6
1	B	142	TYR	2.6
1	B	686	TYR	2.6
1	B	597	SER	2.6
1	B	150	LEU	2.6
1	A	162	TYR	2.5
1	A	612	LEU	2.5
1	B	866	PRO	2.5
1	B	614	LEU	2.5
1	B	74	ILE	2.5
1	B	556	GLY	2.5
1	B	101	VAL	2.5
1	B	723	LYS	2.5
1	B	538	MET	2.5
1	B	775	SER	2.5
1	B	721	ASN	2.5
1	B	100	LEU	2.4
1	B	644	ILE	2.4
1	B	366	ARG	2.4
1	B	588	ILE	2.4
1	B	605	LEU	2.4
1	B	684	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	641	ASP	2.4
1	B	102	SER	2.4
1	B	954	THR	2.3
1	B	774	PHE	2.3
1	A	647	LEU	2.3
1	B	671	GLY	2.3
1	B	828	LEU	2.3
1	A	555	ASP	2.3
1	B	865	ARG	2.3
1	A	617	LYS	2.3
1	A	552	VAL	2.3
1	B	599	VAL	2.2
1	B	64	TRP	2.2
1	B	696	LEU	2.2
1	B	799	ALA	2.2
1	B	636	GLU	2.1
1	B	615	PRO	2.1
1	B	727	LEU	2.1
1	B	739	TRP	2.1
1	B	560	ARG	2.1
1	B	441	GLU	2.1
1	B	619	SER	2.0
1	A	108	ILE	2.0
1	B	643	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

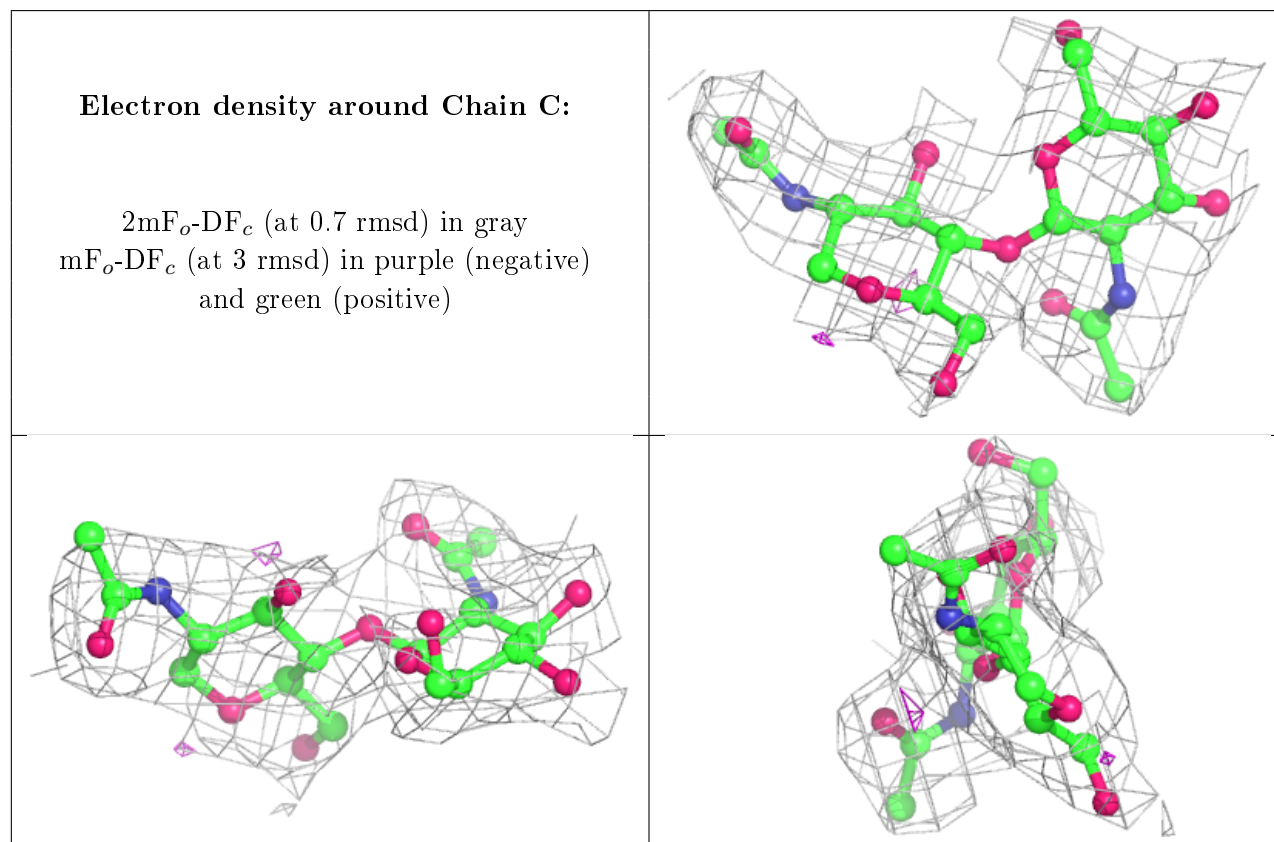
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	E	4	11/12	0.70	0.33	91,109,129,132	0
3	MAN	E	3	11/12	0.83	0.17	70,86,98,107	0
2	NAG	F	2	14/15	0.86	0.20	62,94,102,102	0
2	NAG	C	2	14/15	0.88	0.21	62,80,91,93	0

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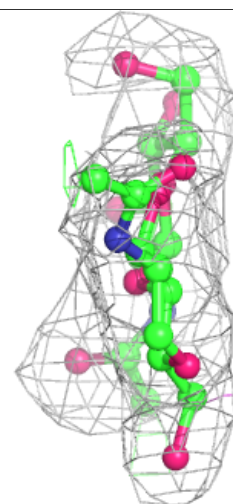
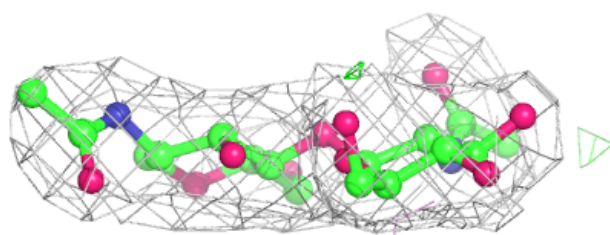
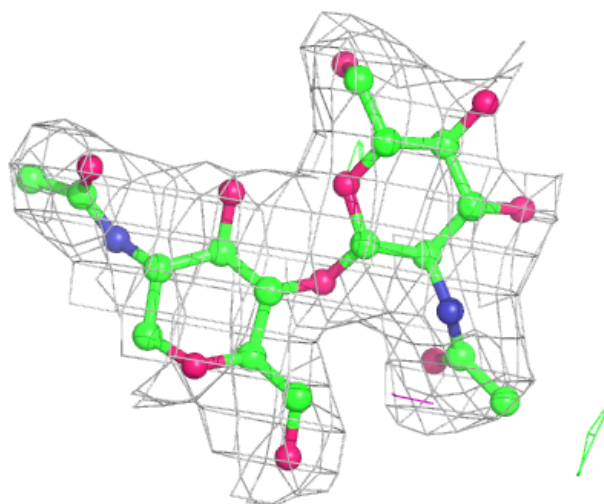
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	2	14/15	0.90	0.16	48,71,91,97	0
2	NAG	F	1	14/15	0.91	0.16	67,85,101,103	0
2	NAG	D	2	14/15	0.94	0.14	50,63,70,72	0
3	NAG	E	1	14/15	0.94	0.14	36,53,63,63	0
2	NAG	C	1	14/15	0.95	0.19	39,61,68,68	0
2	NAG	D	1	14/15	0.97	0.14	40,47,62,64	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.



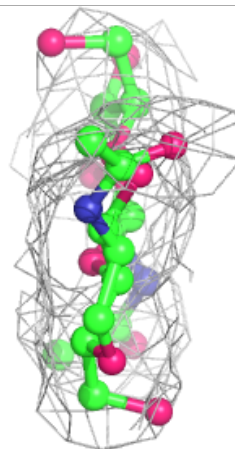
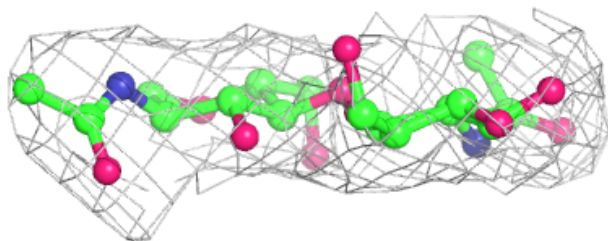
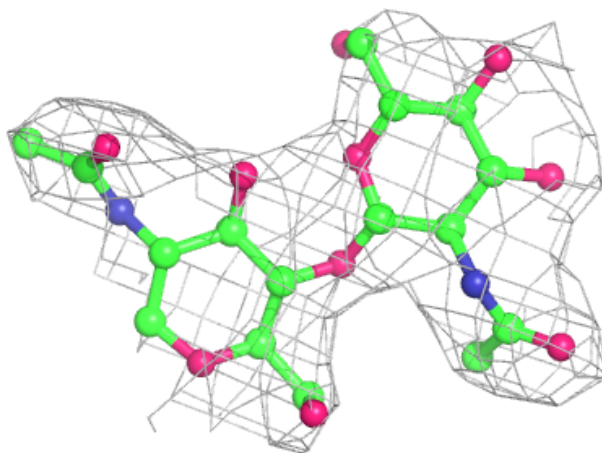
**Electron density around Chain D:**

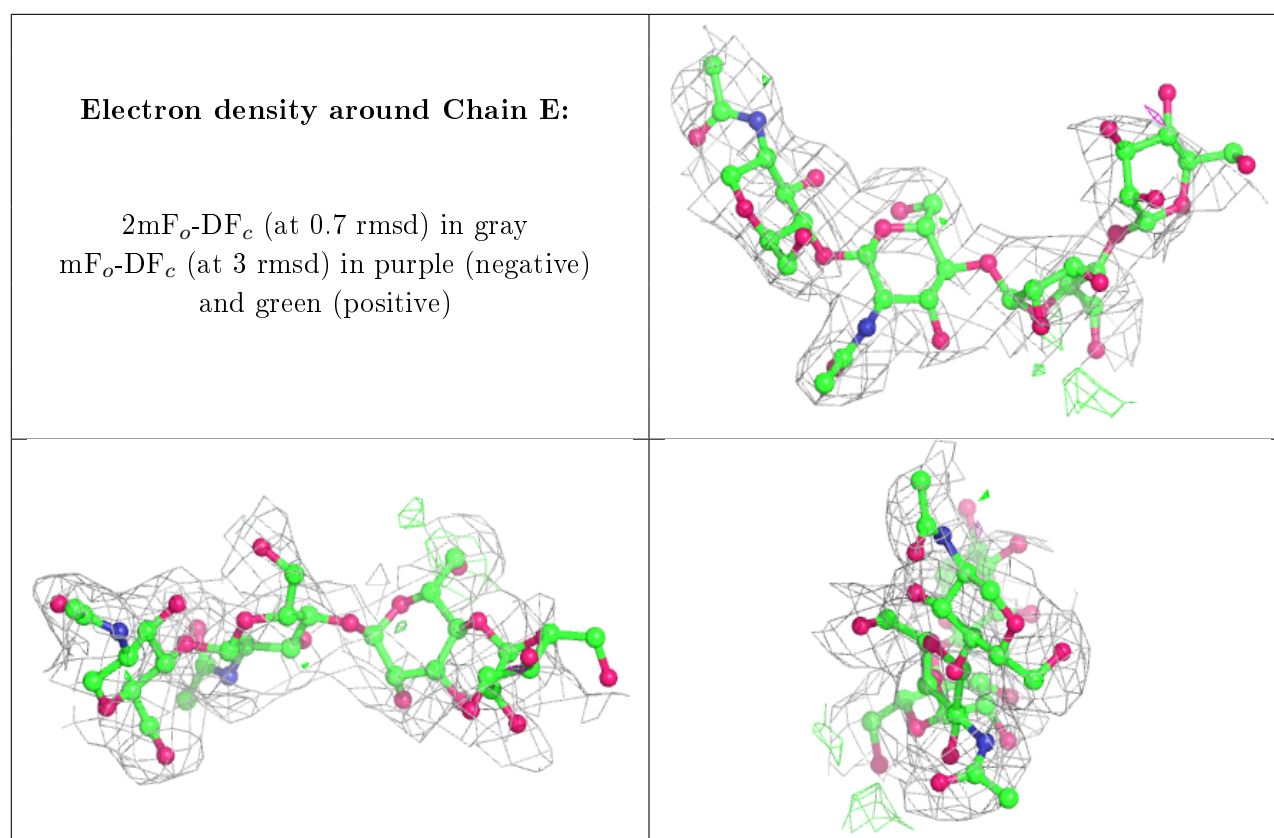
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain F:**

$2mF_o-DF_c$  (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.

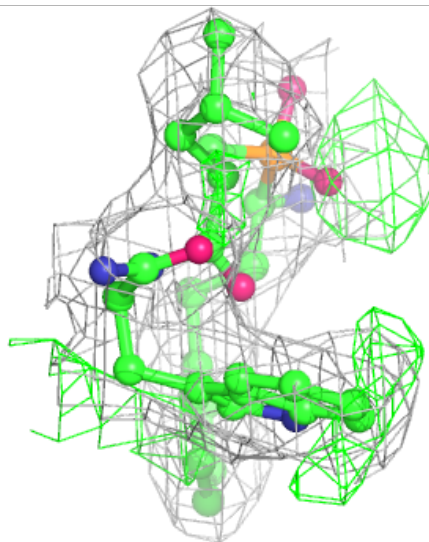
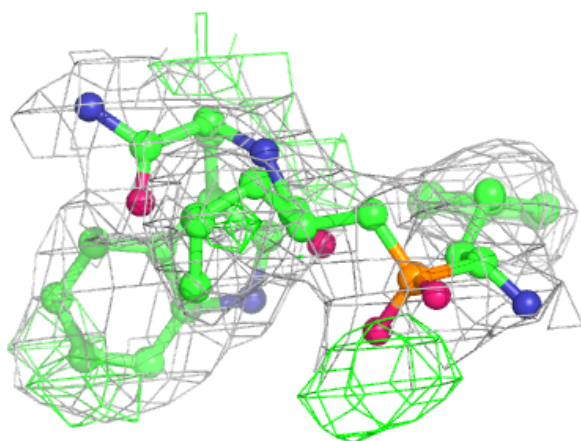
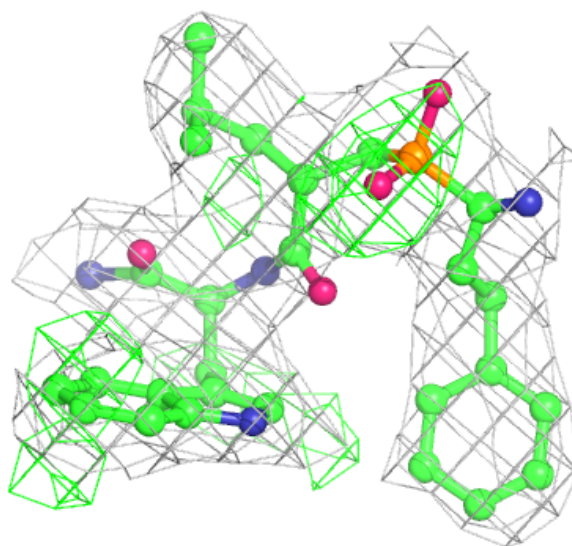
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	1007	14/15	0.77	0.27	85,112,123,137	0
7	IMD	A	1010	5/5	0.79	0.24	64,68,69,80	0
4	NAG	B	1008	14/15	0.83	0.29	79,109,118,122	0
4	NAG	A	1007	14/15	0.85	0.18	80,105,111,113	0
4	NAG	A	1006	14/15	0.88	0.26	76,88,106,106	0
7	IMD	A	1011	5/5	0.91	0.22	57,60,69,70	0
4	NAG	A	1005	14/15	0.94	0.17	65,78,82,84	0
6	P52	A	1009	36/36	0.95	0.31	25,38,60,66	3
6	P52	B	1010	36/36	0.95	0.32	33,57,88,90	4
5	ZN	B	1009	1/1	0.98	0.23	47,47,47,47	0
5	ZN	A	1008	1/1	0.99	0.22	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

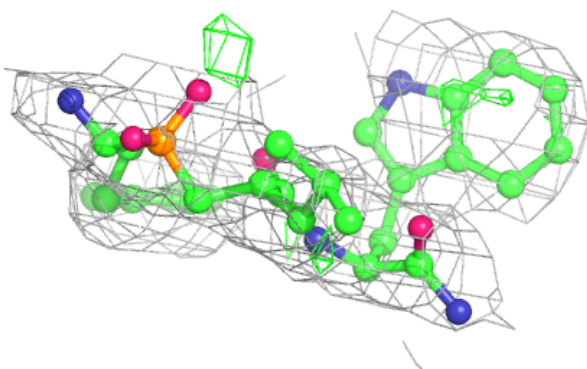
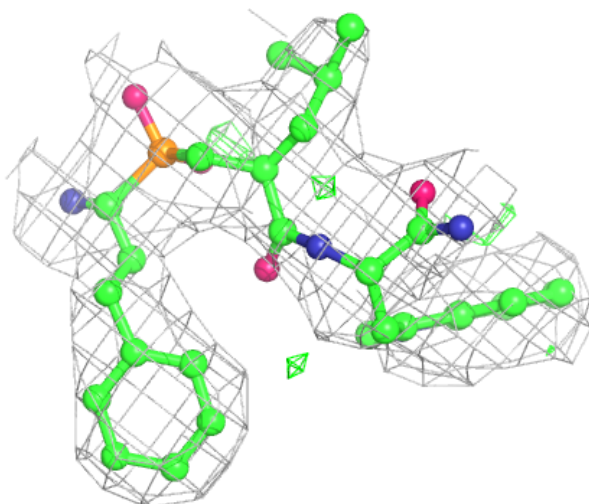
**Electron density around P52 A 1009:**

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



**Electron density around P52 B 1010:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.