



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:10 AM UTC

PDB ID : 7K66 / pdb_00007k66
Title : Structure of Blood Coagulation Factor VIII in Complex with an Anti-C1 Domain Pathogenic Antibody Inhibitor
Authors : Childers, K.C.; Gish, J.; Jarvis, L.; Peters, S.; Garrels, C.; Smith, I.W.; Spencer, H.T.; Spiegel, P.C.
Deposited on : 2020-09-18
Resolution : 3.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

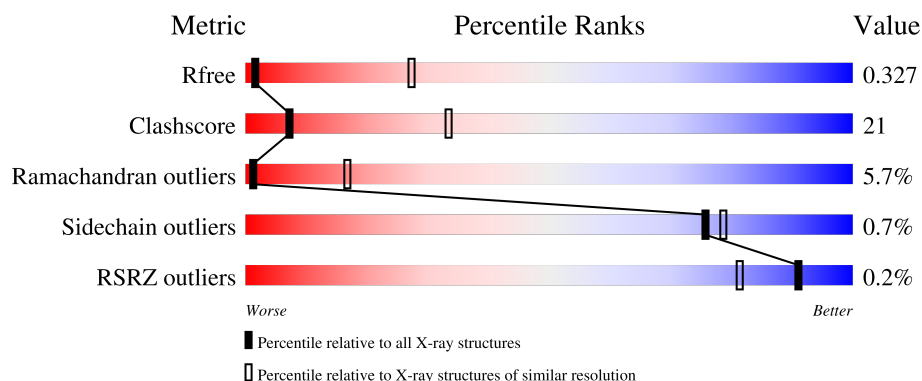
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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

Mol	Chain	Length	Quality of chain
1	A	1467	51% 33% 14%
2	B	223	% 45% 46% .
3	C	213	61% 35% .
4	H	5	100%
5	D	2	100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13606 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 Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1265	Total	C	N	O	S	0	0	0
			10216	6562	1748	1854	52			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1627	ALA	-	linker	UNP P00451
A	1628	GLN	-	linker	UNP P00451
A	1629	ASN	-	linker	UNP P00451
A	1630	SER	-	linker	UNP P00451
A	1631	ARG	-	linker	UNP P00451
A	1632	PRO	-	linker	UNP P00451
A	1633	PRO	-	linker	UNP P00451
A	1634	SER	-	linker	UNP P00451
A	1635	ALA	-	linker	UNP P00451
A	1636	SER	-	linker	UNP P00451

- Molecule 2 is a protein called 2A9 heavy chain.

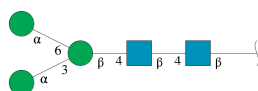
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1649	1048	266	327	8			

- Molecule 3 is a protein called 2A9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1634	1019	271	335	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



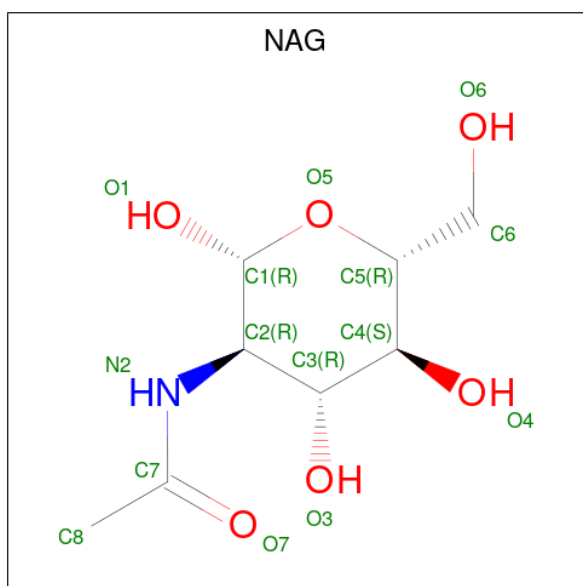
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cu	0	0
			1	1		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		

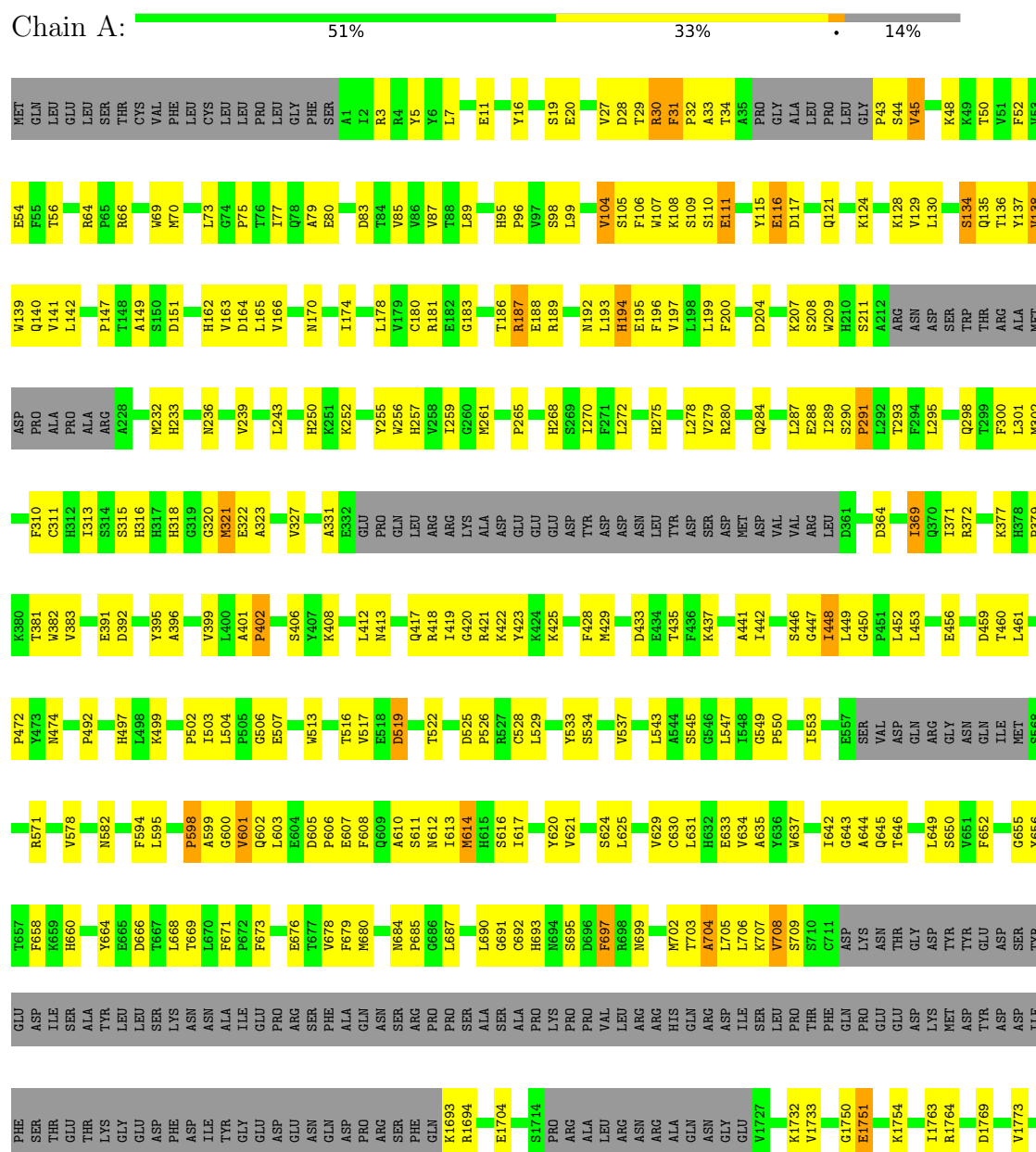
- Molecule 10 is water.

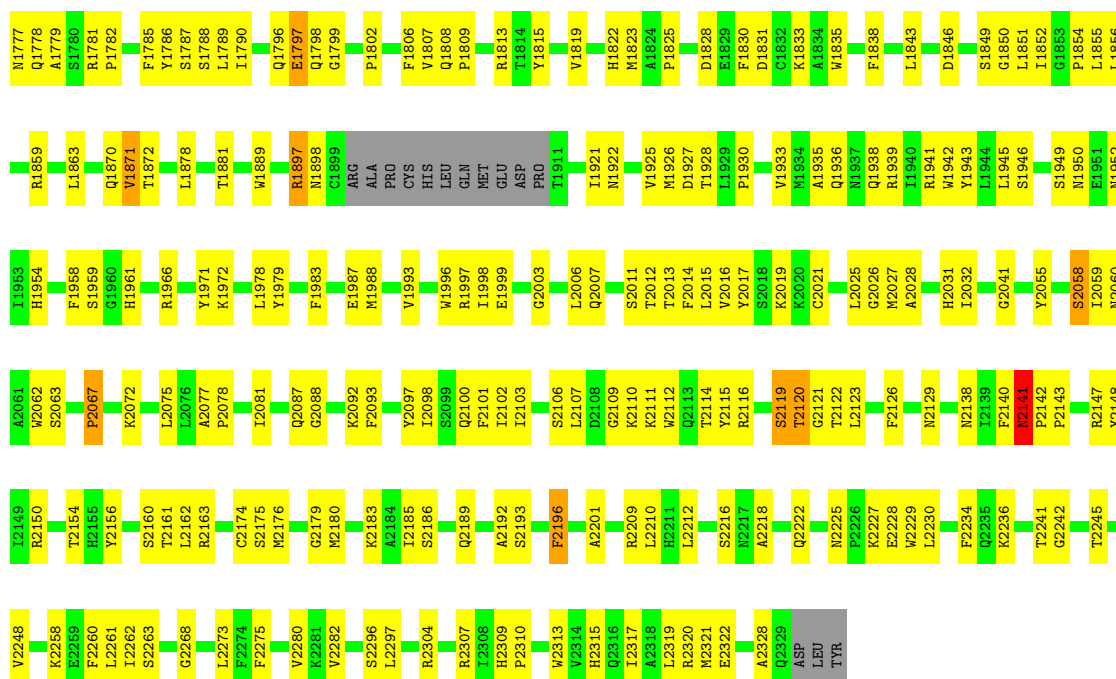
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

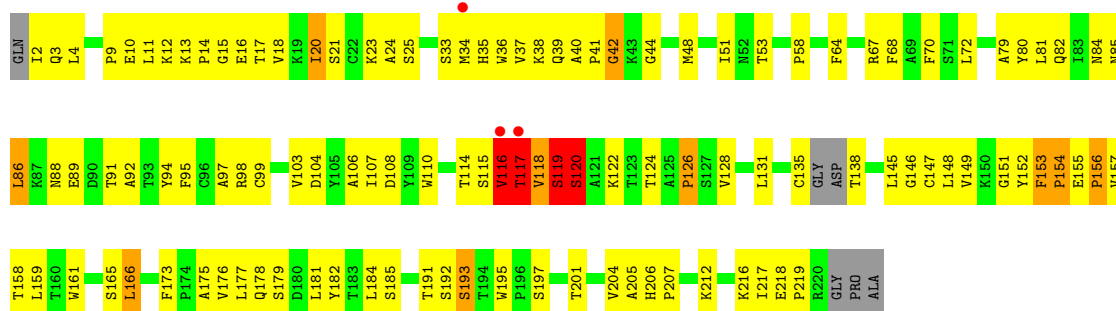
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

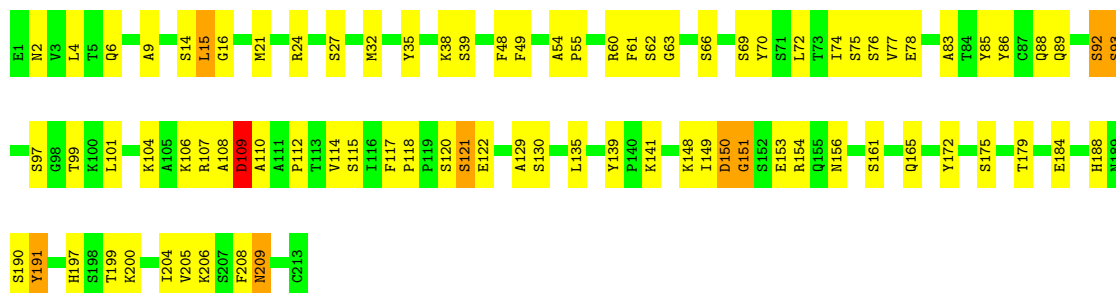




• Molecule 2: 2A9 heavy chain



• Molecule 3: 2A9 light chain



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

nose

Chain H:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 5: 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 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.72Å 116.72Å 371.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 3.92 49.49 – 3.92	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.49-3.92) 97.6 (49.49-3.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.226 , 0.322 0.245 , 0.327	Depositor DCC
R_{free} test set	2000 reflections (8.33%)	wwPDB-VP
Wilson B-factor (Å ²)	147.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 189.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13606	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG, ZN, CU, MAN

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	0.20	0/10502	0.45	2/14238 (0.0%)
2	B	0.35	2/1693 (0.1%)	0.56	2/2312 (0.1%)
3	C	0.20	0/1672	0.51	3/2269 (0.1%)
All	All	0.22	2/13867 (0.0%)	0.47	7/18819 (0.0%)

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
2	B	0	4
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	120	SER	CA-C	6.48	1.58	1.52
2	B	116	VAL	CA-C	-5.69	1.45	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	SER	N-CA-C	-8.10	94.91	108.75
2	B	116	VAL	N-CA-C	-7.38	93.99	109.34
3	C	109	ASP	CA-C-N	-6.25	113.96	122.77
3	C	109	ASP	C-N-CA	-6.25	113.96	122.77
3	C	108	ALA	N-CA-C	5.34	117.53	109.41
1	A	2141	ASN	CA-C-N	-5.15	115.08	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2141	ASN	C-N-CA	-5.15	115.08	120.38

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	HIS	Peptide
2	B	117	THR	Peptide
2	B	119	SER	Mainchain
2	B	120	SER	Peptide
2	B	153	PHE	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	10216	0	9961	360	0
2	B	1649	0	1593	137	0
3	C	1634	0	1560	67	0
4	H	61	0	51	2	0
5	D	28	0	25	0	0
6	A	14	0	13	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	B	1	0	0	0	0
All	All	13606	0	13203	556	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 21.

All (556) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:THR:CB	2:B:117:THR:HG21	1.03	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:THR:CB	2:B:117:THR:CG2	1.98	1.40
2:B:91:THR:OG1	2:B:117:THR:CG2	1.68	1.38
2:B:91:THR:CA	2:B:117:THR:HG21	1.57	1.34
2:B:91:THR:CA	2:B:117:THR:CG2	2.07	1.33
2:B:91:THR:HA	2:B:117:THR:CG2	1.60	1.31
2:B:91:THR:OG1	2:B:117:THR:HG21	1.08	1.26
2:B:88:ASN:O	2:B:118:VAL:HG23	1.36	1.25
2:B:88:ASN:O	2:B:118:VAL:CG2	1.86	1.22
2:B:91:THR:OG1	2:B:117:THR:CB	1.89	1.19
2:B:91:THR:HA	2:B:117:THR:HG22	1.22	1.13
2:B:10:GLU:O	2:B:116:VAL:HG21	1.48	1.12
2:B:11:LEU:HA	2:B:116:VAL:CG1	1.80	1.10
2:B:11:LEU:CB	2:B:116:VAL:HG11	1.87	1.03
1:A:31:PHE:H	1:A:32:PRO:CD	1.70	1.03
2:B:10:GLU:O	2:B:116:VAL:CG2	2.08	1.02
2:B:11:LEU:CD1	2:B:116:VAL:CG1	2.37	1.01
2:B:88:ASN:CA	2:B:118:VAL:CG2	2.39	1.01
2:B:91:THR:CG2	2:B:117:THR:HG21	1.91	1.00
2:B:11:LEU:HA	2:B:116:VAL:HG11	1.41	0.99
2:B:88:ASN:C	2:B:118:VAL:CG2	2.35	0.98
2:B:91:THR:HG23	2:B:117:THR:HG23	1.44	0.97
2:B:88:ASN:HA	2:B:118:VAL:HG22	1.46	0.97
2:B:13:LYS:NZ	2:B:119:SER:OG	1.99	0.95
2:B:11:LEU:CA	2:B:116:VAL:HG11	1.94	0.95
1:A:369:ILE:HG22	1:A:522:THR:HG23	1.49	0.95
1:A:31:PHE:CD1	1:A:32:PRO:HD3	2.02	0.94
2:B:91:THR:CG2	2:B:117:THR:CG2	2.43	0.94
2:B:11:LEU:HD13	2:B:116:VAL:CG1	1.97	0.94
2:B:88:ASN:O	2:B:118:VAL:HG21	1.69	0.93
1:A:1999:GLU:HB3	1:A:2006:LEU:HD11	1.50	0.93
2:B:88:ASN:CA	2:B:118:VAL:HG22	1.97	0.92
1:A:31:PHE:H	1:A:32:PRO:HD3	1.36	0.91
1:A:43:PRO:O	1:A:45:VAL:N	2.04	0.90
2:B:88:ASN:HA	2:B:118:VAL:CG2	2.01	0.90
2:B:11:LEU:HD12	2:B:116:VAL:CG1	2.07	0.85
2:B:88:ASN:HD22	2:B:118:VAL:HG13	1.43	0.83
2:B:11:LEU:CD1	2:B:116:VAL:HG11	2.07	0.83
2:B:91:THR:HG23	2:B:117:THR:CG2	2.05	0.82
1:A:1925:VAL:HG22	1:A:1926:MET:HG3	1.61	0.82
1:A:105:SER:HB3	1:A:140:GLN:HB2	1.61	0.82
1:A:31:PHE:HD1	1:A:32:PRO:HD3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:HIS:HE1	2:B:99:CYS:HB3	1.45	0.81
2:B:91:THR:CA	2:B:117:THR:HG22	1.91	0.81
3:C:61:PHE:CE2	3:C:74:ILE:CD1	2.64	0.81
2:B:11:LEU:HD12	2:B:116:VAL:HG12	1.64	0.79
2:B:88:ASN:C	2:B:118:VAL:HG21	2.05	0.79
3:C:74:ILE:HG21	3:C:77:VAL:HG12	1.66	0.78
1:A:31:PHE:N	1:A:32:PRO:CD	2.42	0.78
2:B:11:LEU:HD13	2:B:116:VAL:HG13	1.65	0.78
2:B:11:LEU:HB2	2:B:116:VAL:HG11	1.64	0.77
1:A:631:LEU:HD11	1:A:685:PRO:HG3	1.68	0.76
1:A:1942:TRP:HE1	1:A:1988:MET:HE2	1.51	0.76
3:C:109:ASP:N	3:C:109:ASP:OD1	2.18	0.74
2:B:13:LYS:HZ3	2:B:119:SER:C	1.96	0.74
2:B:88:ASN:CB	2:B:118:VAL:HG22	2.16	0.74
3:C:200:LYS:HZ2	3:C:204:ILE:CG1	2.00	0.74
1:A:233:HIS:HB3	1:A:321:MET:HG2	1.70	0.74
2:B:91:THR:OG1	2:B:117:THR:OG1	2.06	0.74
2:B:11:LEU:HA	2:B:116:VAL:CB	2.17	0.74
2:B:12:LYS:NZ	2:B:17:THR:O	2.20	0.74
2:B:11:LEU:HD11	2:B:119:SER:OG	1.89	0.73
3:C:200:LYS:HZ2	3:C:204:ILE:HG13	1.54	0.73
1:A:2102:ILE:HD11	2:B:103:VAL:HG11	1.70	0.72
1:A:419:ILE:O	1:A:421:ARG:N	2.22	0.72
2:B:88:ASN:C	2:B:118:VAL:HG23	2.10	0.71
1:A:164:ASP:OD1	1:A:2007:GLN:NE2	2.25	0.70
1:A:73:LEU:HD21	1:A:199:LEU:HB2	1.74	0.70
1:A:1825:PRO:HG3	1:A:1833:LYS:H	1.57	0.70
1:A:189:ARG:HB3	1:A:192:ASN:HB2	1.73	0.70
2:B:145:LEU:HD21	2:B:217:ILE:HG21	1.75	0.68
1:A:2192:ALA:HB2	1:A:2230:LEU:HD12	1.74	0.68
1:A:1789:LEU:HD12	1:A:1855:LEU:HD13	1.75	0.68
3:C:61:PHE:CE2	3:C:74:ILE:HD11	2.27	0.68
1:A:418:ARG:NH1	1:A:607:GLU:O	2.27	0.67
1:A:435:THR:HG23	1:A:437:LYS:H	1.60	0.67
3:C:4:LEU:HD21	3:C:89:GLN:HG2	1.76	0.67
3:C:74:ILE:CG2	3:C:77:VAL:HG12	2.25	0.67
2:B:9:PRO:HB3	2:B:114:THR:HA	1.77	0.66
2:B:88:ASN:CB	2:B:118:VAL:CG2	2.72	0.66
3:C:112:PRO:HB2	3:C:135:LEU:HD22	1.75	0.66
3:C:15:LEU:H	3:C:106:LYS:HB2	1.59	0.66
1:A:5:TYR:HB2	1:A:87:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LEU:HD12	1:A:707:LYS:HG3	1.76	0.65
1:A:3:ARG:NH1	1:A:83:ASP:OD2	2.29	0.65
1:A:1933:VAL:HG22	1:A:2015:LEU:HB3	1.78	0.65
1:A:1782:PRO:HB3	1:A:1809:PRO:HD3	1.78	0.65
1:A:31:PHE:H	1:A:32:PRO:HD2	1.60	0.65
1:A:1808:GLN:HG3	1:A:1809:PRO:HD2	1.78	0.65
1:A:391:GLU:HG2	1:A:392:ASP:H	1.62	0.65
1:A:162:HIS:O	1:A:162:HIS:ND1	2.30	0.64
3:C:130:SER:HA	3:C:179:THR:HB	1.80	0.64
2:B:145:LEU:HD22	2:B:146:GLY:H	1.63	0.64
3:C:60:ARG:HH21	3:C:61:PHE:HE1	1.43	0.64
2:B:2:ILE:HA	2:B:25:SER:HB3	1.79	0.64
2:B:33:SER:O	2:B:34:MET:HG2	1.97	0.63
1:A:16:TYR:HE2	1:A:232:MET:HG3	1.63	0.63
1:A:1733:VAL:HG22	1:A:1851:LEU:HD21	1.80	0.63
2:B:13:LYS:NZ	2:B:119:SER:O	2.23	0.63
3:C:150:ASP:H	3:C:190:SER:HB2	1.64	0.63
3:C:205:VAL:O	3:C:206:LYS:NZ	2.32	0.62
1:A:1939:ARG:NH2	1:A:1987:GLU:OE1	2.32	0.62
1:A:106:PHE:HB2	1:A:110:SER:HB2	1.81	0.62
1:A:2141:ASN:O	1:A:2143:PRO:HD3	2.00	0.61
3:C:24:ARG:HG2	3:C:69:SER:HB2	1.82	0.61
1:A:705:LEU:H	1:A:705:LEU:HD23	1.65	0.61
1:A:69:TRP:HZ3	1:A:197:VAL:H	1.48	0.60
1:A:300:PHE:HD2	1:A:302:MET:HG3	1.65	0.60
1:A:708:VAL:HG23	1:A:709:SER:H	1.66	0.60
3:C:61:PHE:CE2	3:C:74:ILE:HD13	2.36	0.60
1:A:697:PHE:O	1:A:699:ASN:N	2.33	0.60
2:B:51:ILE:HD12	2:B:58:PRO:HG3	1.82	0.60
2:B:151:GLY:HA2	2:B:181:LEU:HD21	1.83	0.60
1:A:2193:SER:OG	1:A:2228:GLU:OE1	2.20	0.60
2:B:11:LEU:HA	2:B:116:VAL:HB	1.82	0.60
1:A:656:TYR:HB3	1:A:680:MET:HE1	1.84	0.59
1:A:1807:VAL:HG22	1:A:1813:ARG:HH11	1.65	0.59
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.84	0.59
2:B:106:ALA:O	2:B:107:ILE:HD12	2.03	0.59
1:A:1949:SER:O	1:A:1952:ASN:ND2	2.36	0.59
1:A:453:LEU:HD23	1:A:513:TRP:HZ3	1.67	0.59
1:A:2101:PHE:HA	1:A:2154:THR:HG23	1.84	0.59
2:B:16:GLU:H	2:B:86:LEU:HD12	1.67	0.59
1:A:1797:GLU:O	1:A:1799:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:O	1:A:195:GLU:N	2.36	0.59
3:C:148:LYS:HA	3:C:153:GLU:HG3	1.84	0.58
1:A:200:PHE:HB3	1:A:321:MET:HE1	1.84	0.58
1:A:525:ASP:N	1:A:525:ASP:OD1	2.36	0.58
1:A:2110:LYS:HA	1:A:2112:TRP:HD1	1.69	0.58
2:B:131:LEU:HD12	3:C:117:PHE:HB3	1.84	0.58
1:A:2141:ASN:HB3	1:A:2142:PRO:HD3	1.86	0.58
3:C:14:SER:HA	3:C:106:LYS:HB2	1.85	0.58
1:A:16:TYR:CE2	1:A:232:MET:HG3	2.39	0.58
1:A:452:LEU:HA	1:A:550:PRO:HG2	1.85	0.58
2:B:175:ALA:HB2	2:B:184:LEU:HB3	1.86	0.58
3:C:149:ILE:O	3:C:151:GLY:N	2.37	0.58
1:A:2110:LYS:HA	1:A:2112:TRP:CD1	2.38	0.57
2:B:91:THR:OG1	2:B:117:THR:HB	1.97	0.57
1:A:1750:GLY:HA2	1:A:1754:LYS:HG3	1.86	0.57
2:B:15:GLY:HA2	2:B:86:LEU:N	2.19	0.57
1:A:31:PHE:CD1	1:A:32:PRO:CD	2.85	0.57
1:A:2114:THR:HG21	1:A:2123:LEU:HD22	1.87	0.57
1:A:200:PHE:HE2	1:A:270:ILE:HG21	1.69	0.57
1:A:634:VAL:HG13	1:A:679:PHE:HE1	1.70	0.57
1:A:2261:LEU:HD22	1:A:2280:VAL:HG12	1.87	0.57
1:A:320:GLY:O	1:A:322:GLU:N	2.36	0.57
1:A:664:TYR:HB2	1:A:1833:LYS:HE3	1.87	0.57
1:A:1870:GLN:OE1	1:A:1941:ARG:NH2	2.37	0.57
2:B:88:ASN:HD22	2:B:118:VAL:CG1	2.17	0.57
1:A:1825:PRO:HD2	1:A:1859:ARG:HB2	1.86	0.56
2:B:88:ASN:HB3	2:B:118:VAL:HG21	1.87	0.56
1:A:503:ILE:HG23	1:A:507:GLU:HB2	1.87	0.56
1:A:2119:SER:C	1:A:2120:THR:HG1	2.13	0.56
3:C:61:PHE:HE2	3:C:74:ILE:HD11	1.71	0.56
3:C:191:TYR:N	3:C:208:PHE:HB2	2.20	0.56
1:A:107:TRP:C	1:A:109:SER:H	2.13	0.56
1:A:166:VAL:O	1:A:170:ASN:ND2	2.36	0.56
1:A:412:LEU:HD22	1:A:421:ARG:HH21	1.70	0.56
1:A:571:ARG:HD3	1:A:635:ALA:HA	1.88	0.56
1:A:2092:LYS:HB3	1:A:2093:PHE:CD1	2.41	0.56
1:A:255:TYR:OH	1:A:364:ASP:O	2.24	0.55
1:A:1838:PHE:HB3	1:A:1852:ILE:HD12	1.87	0.55
2:B:36:TRP:O	2:B:48:MET:HB2	2.06	0.55
2:B:117:THR:OG1	2:B:118:VAL:HB	2.07	0.55
1:A:2261:LEU:HD23	1:A:2282:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:PRO:HA	1:A:413:ASN:HD21	1.70	0.55
1:A:137:TYR:O	1:A:138:VAL:HG12	2.05	0.55
1:A:642:ILE:HD13	1:A:673:PHE:HA	1.89	0.55
1:A:669:THR:HG21	1:A:1979:TYR:HB3	1.89	0.55
1:A:1787:SER:O	1:A:1788:SER:OG	2.17	0.55
3:C:61:PHE:CZ	3:C:74:ILE:HD13	2.41	0.55
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.42	0.55
2:B:205:ALA:HA	2:B:212:LYS:HA	1.89	0.55
1:A:634:VAL:HG13	1:A:679:PHE:CE1	2.42	0.54
3:C:48:PHE:HE1	3:C:54:ALA:HA	1.71	0.54
1:A:497:HIS:CD2	1:A:499:LYS:HG2	2.42	0.54
1:A:516:THR:OG1	1:A:517:VAL:N	2.40	0.54
1:A:2116:ARG:HG2	1:A:2122:THR:O	2.08	0.54
2:B:11:LEU:CG	2:B:116:VAL:HG11	2.37	0.54
3:C:104:LYS:HA	3:C:165:GLN:HE22	1.71	0.54
1:A:2072:LYS:HD3	1:A:2150:ARG:HH21	1.73	0.54
2:B:88:ASN:HB3	2:B:118:VAL:CG2	2.37	0.54
3:C:150:ASP:N	3:C:190:SER:HB2	2.23	0.54
1:A:382:TRP:HB2	1:A:461:LEU:HD12	1.90	0.53
1:A:2067:PRO:HG3	3:C:55:PRO:HD2	1.90	0.53
1:A:2263:SER:HB3	1:A:2273:LEU:HD23	1.89	0.53
3:C:120:SER:OG	3:C:121:SER:N	2.41	0.53
1:A:381:THR:HA	1:A:460:THR:HB	1.90	0.53
1:A:644:ALA:O	1:A:646:THR:N	2.39	0.53
2:B:35:HIS:CE1	2:B:99:CYS:HB3	2.35	0.53
2:B:153:PHE:HB3	2:B:154:PRO:HD2	1.90	0.53
1:A:107:TRP:O	1:A:109:SER:N	2.33	0.53
1:A:1878:LEU:HD11	1:A:1998:ILE:HD13	1.89	0.53
2:B:33:SER:O	2:B:34:MET:CG	2.55	0.53
1:A:313:ILE:HG22	1:A:315:SER:H	1.73	0.53
1:A:134:SER:OG	1:A:135:GLN:N	2.38	0.53
2:B:157:VAL:HG21	2:B:204:VAL:HG13	1.91	0.53
3:C:104:LYS:HA	3:C:165:GLN:NE2	2.23	0.53
1:A:1751:GLU:H	1:A:1754:LYS:HE2	1.74	0.53
2:B:11:LEU:CA	2:B:116:VAL:CG1	2.61	0.53
1:A:2242:GLY:HA2	1:A:2297:LEU:HG	1.91	0.53
1:A:301:LEU:HB3	1:A:327:VAL:HG11	1.91	0.52
2:B:135:CYS:O	2:B:138:THR:N	2.42	0.52
1:A:187:ARG:NH1	1:A:189:ARG:HD3	2.24	0.52
1:A:165:LEU:HD23	1:A:2003:GLY:HA2	1.90	0.52
1:A:165:LEU:HD22	1:A:2006:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASN:OD1	1:A:612:ASN:ND2	2.41	0.52
1:A:104:VAL:HG12	1:A:141:VAL:HG12	1.91	0.52
1:A:111:GLU:OE2	1:A:1959:SER:OG	2.25	0.52
1:A:399:VAL:HG11	1:A:421:ARG:HD3	1.90	0.52
1:A:1878:LEU:HD23	1:A:1922:ASN:HD21	1.73	0.52
1:A:2234:PHE:C	1:A:2236:LYS:H	2.17	0.52
1:A:1961:HIS:HE2	1:A:1996:TRP:CD1	2.27	0.52
1:A:2063:SER:HA	1:A:2160:SER:O	2.09	0.52
1:A:2106:SER:HB2	1:A:2112:TRP:CE2	2.45	0.52
2:B:53:THR:HG22	2:B:72:LEU:HD21	1.92	0.52
1:A:293:THR:HG22	1:A:295:LEU:HD13	1.91	0.52
1:A:616:SER:HA	1:A:621:VAL:HG12	1.92	0.52
2:B:107:ILE:HB	3:C:35:TYR:OH	2.10	0.52
3:C:66:SER:HA	3:C:70:TYR:CZ	2.45	0.52
1:A:2115:TYR:OH	1:A:2142:PRO:O	2.28	0.52
1:A:371:ILE:HG12	1:A:517:VAL:HG21	1.92	0.52
1:A:1946:SER:HB2	1:A:1978:LEU:HB3	1.91	0.52
1:A:2106:SER:HB2	1:A:2112:TRP:CD2	2.44	0.52
2:B:98:ARG:NH2	2:B:108:ASP:OD2	2.34	0.52
1:A:601:VAL:HG12	1:A:602:GLN:H	1.75	0.51
1:A:1925:VAL:O	1:A:1928:THR:OG1	2.17	0.51
1:A:243:LEU:HB3	1:A:323:ALA:HB1	1.93	0.51
3:C:88:GLN:OE1	3:C:97:SER:OG	2.27	0.51
2:B:34:MET:SD	2:B:97:ALA:O	2.68	0.51
3:C:61:PHE:CD2	3:C:74:ILE:HG12	2.46	0.51
1:A:270:ILE:O	1:A:287:LEU:N	2.41	0.51
3:C:6:GLN:HE21	3:C:101:LEU:HD12	1.74	0.51
1:A:279:VAL:HG22	1:A:284:GLN:HG3	1.93	0.51
1:A:650:SER:O	1:A:693:HIS:HB2	2.10	0.51
2:B:195:TRP:HA	2:B:197:SER:H	1.76	0.51
1:A:2062:TRP:O	1:A:2161:THR:HA	2.10	0.51
1:A:2114:THR:HG22	1:A:2115:TYR:H	1.75	0.51
2:B:18:VAL:O	2:B:82:GLN:HA	2.10	0.51
3:C:21:MET:SD	3:C:101:LEU:HD13	2.51	0.51
1:A:7:LEU:HD21	1:A:52:PHE:HB3	1.92	0.51
1:A:106:PHE:HB3	1:A:139:TRP:HD1	1.76	0.51
1:A:268:HIS:HB2	1:A:289:ILE:HG12	1.91	0.51
3:C:191:TYR:H	3:C:208:PHE:HB2	1.76	0.51
1:A:192:ASN:OD1	1:A:252:LYS:HD2	2.10	0.50
1:A:474:ASN:HB2	1:A:537:VAL:HG13	1.94	0.50
1:A:1732:LYS:HB3	1:A:1849:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLU:O	2:B:84:ASN:HA	2.12	0.50
1:A:208:SER:OG	1:A:209:TRP:N	2.45	0.50
1:A:687:LEU:HD22	1:A:1802:PRO:HG3	1.93	0.50
2:B:173:PHE:CG	3:C:175:SER:HB2	2.47	0.50
2:B:152:TYR:OH	2:B:184:LEU:HD22	2.11	0.50
2:B:157:VAL:HG12	2:B:206:HIS:HA	1.93	0.50
1:A:608:PHE:O	1:A:611:SER:OG	2.29	0.50
1:A:637:TRP:HB2	1:A:678:VAL:HG23	1.94	0.50
1:A:116:GLU:HB3	1:A:2013:THR:HG21	1.94	0.50
1:A:642:ILE:HD13	1:A:673:PHE:HD1	1.76	0.50
1:A:2058:SER:OG	1:A:2059:ILE:N	2.43	0.50
1:A:1958:PHE:HB2	1:A:1961:HIS:HB2	1.94	0.49
2:B:88:ASN:ND2	2:B:118:VAL:HG22	2.27	0.49
1:A:11:GLU:HB3	1:A:48:LYS:HE2	1.94	0.49
1:A:80:GLU:O	1:A:83:ASP:HB2	2.12	0.49
1:A:517:VAL:O	1:A:519:ASP:N	2.41	0.49
1:A:422:LYS:HD2	1:A:594:PHE:HZ	1.77	0.49
1:A:423:TYR:OH	1:A:612:ASN:HB3	2.11	0.49
3:C:154:ARG:HE	3:C:156:ASN:HB2	1.77	0.49
3:C:9:ALA:O	3:C:101:LEU:HA	2.13	0.49
1:A:188:GLU:HB2	1:A:193:LEU:HD22	1.93	0.49
1:A:311:CYS:SG	1:A:313:ILE:HG12	2.53	0.49
1:A:504:LEU:HB2	1:A:507:GLU:HG2	1.93	0.49
1:A:2106:SER:HB3	1:A:2148:TYR:HB2	1.94	0.49
1:A:1935:ALA:HA	1:A:2017:TYR:CE1	2.48	0.49
1:A:2218:ALA:HB2	1:A:2248:VAL:HG11	1.94	0.49
1:A:2098:ILE:HD11	1:A:2162:LEU:HB2	1.95	0.49
2:B:37:VAL:HG21	2:B:110:TRP:CZ3	2.48	0.49
1:A:1942:TRP:NE1	1:A:1988:MET:HE2	2.24	0.48
1:A:2261:LEU:HD21	1:A:2282:VAL:HG22	1.94	0.48
2:B:39:GLN:NE2	2:B:44:GLY:O	2.46	0.48
1:A:637:TRP:CD1	1:A:680:MET:HG2	2.48	0.48
1:A:664:TYR:CZ	1:A:1822:HIS:HB2	2.48	0.48
2:B:10:GLU:O	2:B:116:VAL:CB	2.59	0.48
2:B:177:LEU:HB2	2:B:182:TYR:HE1	1.77	0.48
3:C:63:GLY:HA3	3:C:72:LEU:HA	1.95	0.48
1:A:128:LYS:HG2	1:A:163:VAL:HG12	1.95	0.48
1:A:1870:GLN:O	1:A:1872:THR:N	2.43	0.48
2:B:33:SER:C	2:B:34:MET:HG2	2.38	0.48
1:A:418:ARG:NH1	1:A:611:SER:HB3	2.28	0.48
1:A:425:LYS:HB3	1:A:545:SER:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:GLN:NE2	3:C:85:TYR:O	2.45	0.48
2:B:191:THR:O	2:B:193:SER:N	2.44	0.48
3:C:2:ASN:OD1	3:C:27:SER:OG	2.30	0.48
1:A:2228:GLU:O	1:A:2310:PRO:HD2	2.13	0.48
2:B:218:GLU:HG3	2:B:219:PRO:HD2	1.95	0.48
1:A:652:PHE:HE1	1:A:691:GLY:HA3	1.78	0.48
1:A:2141:ASN:HD22	1:A:2141:ASN:C	2.21	0.48
1:A:453:LEU:HD22	1:A:533:TYR:CE2	2.49	0.48
2:B:148:LEU:HD23	2:B:185:SER:HB3	1.95	0.48
1:A:1789:LEU:HD22	1:A:1823:MET:HG2	1.95	0.48
1:A:2021:CYS:HB2	1:A:2176:MET:SD	2.54	0.48
1:A:50:THR:HG21	1:A:95:HIS:CE1	2.49	0.47
1:A:660:HIS:NE2	1:A:676:GLU:OE1	2.43	0.47
1:A:690:LEU:HB2	1:A:704:ALA:O	2.14	0.47
1:A:2186:SER:OG	1:A:2189:GLN:OE1	2.26	0.47
2:B:88:ASN:ND2	2:B:118:VAL:HG13	2.19	0.47
1:A:417:GLN:HA	1:A:595:LEU:HD11	1.97	0.47
1:A:2055:TYR:H	1:A:2163:ARG:HH11	1.60	0.47
3:C:92:SER:OG	3:C:93:SER:N	2.47	0.47
1:A:504:LEU:O	1:A:506:GLY:N	2.48	0.47
1:A:2026:GLY:HA3	1:A:2031:HIS:HB3	1.95	0.47
1:A:1786:TYR:OH	1:A:1788:SER:HB3	2.14	0.47
1:A:2059:ILE:HD12	1:A:2059:ILE:O	2.15	0.47
1:A:1789:LEU:HD11	1:A:1835:TRP:CG	2.50	0.47
1:A:2116:ARG:HA	1:A:2123:LEU:HA	1.96	0.47
1:A:99:LEU:HB3	1:A:137:TYR:CE2	2.50	0.47
1:A:666:ASP:OD2	1:A:1788:SER:OG	2.32	0.47
1:A:2141:ASN:HB3	1:A:2142:PRO:CD	2.44	0.47
3:C:184:GLU:O	3:C:188:HIS:HB2	2.15	0.47
1:A:1785:PHE:HB3	1:A:1815:TYR:CE2	2.50	0.47
2:B:3:GLN:O	2:B:25:SER:OG	2.15	0.47
2:B:23:LYS:HG3	2:B:24:ALA:N	2.30	0.47
1:A:1764:ARG:HD3	1:A:1863:LEU:HD11	1.97	0.47
2:B:89:GLU:C	2:B:91:THR:H	2.22	0.47
1:A:310:PHE:HB2	1:A:322:GLU:HG2	1.96	0.47
1:A:2141:ASN:C	1:A:2141:ASN:ND2	2.72	0.47
1:A:1777:ASN:ND2	1:A:1809:PRO:HA	2.30	0.46
1:A:630:CYS:HB2	1:A:633:GLU:CD	2.41	0.46
2:B:92:ALA:O	2:B:115:SER:HB3	2.16	0.46
3:C:38:LYS:HA	3:C:83:ALA:HB1	1.98	0.46
1:A:525:ASP:HB2	1:A:526:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2236:LYS:O	1:A:2304:ARG:HG3	2.13	0.46
1:A:272:LEU:HD23	1:A:275:HIS:HB2	1.97	0.46
1:A:396:ALA:O	1:A:399:VAL:HG13	2.14	0.46
1:A:631:LEU:C	1:A:633:GLU:H	2.22	0.46
1:A:1790:ILE:HD12	1:A:1790:ILE:O	2.15	0.46
1:A:80:GLU:HA	1:A:180:CYS:O	2.16	0.46
1:A:178:LEU:HD11	1:A:257:HIS:CD2	2.50	0.46
1:A:391:GLU:HG2	1:A:392:ASP:N	2.27	0.46
1:A:1831:ASP:OD1	1:A:1859:ARG:NH2	2.48	0.46
1:A:2156:TYR:HD2	1:A:2160:SER:OG	1.98	0.46
2:B:115:SER:O	2:B:116:VAL:HG23	2.16	0.46
1:A:447:GLY:C	1:A:449:LEU:H	2.23	0.46
1:A:1997:ARG:NE	1:A:2011:SER:OG	2.49	0.46
1:A:1870:GLN:C	1:A:1872:THR:H	2.23	0.46
1:A:1993:VAL:HA	1:A:2016:VAL:HG23	1.98	0.46
2:B:155:GLU:HG2	2:B:156:PRO:HA	1.97	0.46
1:A:417:GLN:NE2	1:A:418:ARG:HH21	2.14	0.46
1:A:433:ASP:N	1:A:433:ASP:OD1	2.49	0.46
1:A:655:GLY:H	1:A:1786:TYR:HE1	1.64	0.46
2:B:40:ALA:C	2:B:42:GLY:H	2.24	0.46
1:A:603:LEU:C	1:A:605:ASP:H	2.24	0.46
1:A:278:LEU:HB2	1:A:298:GLN:HG2	1.97	0.45
1:A:1704:GLU:OE1	1:A:1779:ALA:HA	2.15	0.45
1:A:1750:GLY:HA3	1:A:2116:ARG:HD2	1.97	0.45
1:A:2174:CYS:HB3	1:A:2241:THR:HG21	1.98	0.45
1:A:19:SER:OG	1:A:20:GLU:N	2.49	0.45
1:A:121:GLN:HA	1:A:124:LYS:HB2	1.98	0.45
2:B:20:ILE:HG22	2:B:21:SER:H	1.80	0.45
1:A:412:LEU:HD23	1:A:421:ARG:HA	1.99	0.45
1:A:50:THR:HG21	1:A:95:HIS:NE2	2.32	0.45
1:A:115:TYR:O	1:A:117:ASP:N	2.48	0.45
2:B:122:LYS:HD3	2:B:124:THR:OG1	2.16	0.45
1:A:543:LEU:HD21	1:A:643:GLY:HA2	1.99	0.45
1:A:2101:PHE:HE2	1:A:2103:ILE:HD11	1.82	0.45
1:A:16:TYR:O	1:A:239:VAL:HG22	2.17	0.45
1:A:649:LEU:HG	1:A:692:CYS:SG	2.56	0.45
1:A:1935:ALA:HB3	1:A:1938:GLN:HB2	1.99	0.45
1:A:2241:THR:O	1:A:2297:LEU:N	2.49	0.45
2:B:126:PRO:HG3	2:B:204:VAL:HG12	1.99	0.45
1:A:1843:LEU:HD12	1:A:1843:LEU:H	1.81	0.45
1:A:2258:LYS:H	1:A:2313:TRP:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:HD2	1:A:1971:TYR:HE2	1.82	0.44
1:A:2077:ALA:O	1:A:2147:ARG:HB3	2.17	0.44
1:A:28:ASP:OD2	1:A:30:ARG:HB2	2.17	0.44
1:A:578:VAL:HG23	1:A:645:GLN:HG2	1.99	0.44
1:A:1998:ILE:HG13	1:A:2014:PHE:CD1	2.52	0.44
1:A:2110:LYS:HB2	1:A:2110:LYS:HE3	1.71	0.44
1:A:2119:SER:O	1:A:2121:GLY:N	2.51	0.44
2:B:159:LEU:HD13	2:B:184:LEU:HD11	1.98	0.44
2:B:173:PHE:CD2	3:C:175:SER:HB2	2.52	0.44
2:B:178:GLN:HA	2:B:179:SER:HA	1.66	0.44
3:C:39:SER:O	3:C:39:SER:OG	2.32	0.44
1:A:456:GLU:HB2	1:A:459:ASP:OD1	2.17	0.44
1:A:614:MET:HE3	1:A:621:VAL:HG11	1.99	0.44
3:C:14:SER:O	3:C:16:GLY:N	2.51	0.44
2:B:11:LEU:HD11	2:B:119:SER:CB	2.46	0.44
1:A:318:HIS:CD2	1:A:318:HIS:N	2.85	0.44
1:A:1778:GLN:HB3	1:A:1779:ALA:H	1.48	0.44
1:A:54:GLU:HB2	1:A:75:PRO:HG2	1.99	0.44
1:A:85:VAL:O	1:A:138:VAL:HA	2.18	0.44
1:A:2087:GLN:HG2	1:A:2088:GLY:H	1.83	0.44
1:A:280:ARG:HD2	1:A:1971:TYR:CE2	2.53	0.44
1:A:290:SER:O	1:A:291:PRO:C	2.60	0.44
2:B:64:PHE:HB3	2:B:68:PHE:CE1	2.53	0.44
3:C:110:ALA:HB3	3:C:139:TYR:N	2.33	0.44
1:A:2115:TYR:OH	1:A:2140:PHE:HB2	2.18	0.44
2:B:11:LEU:HD13	2:B:116:VAL:HG11	1.80	0.44
3:C:9:ALA:O	3:C:101:LEU:HD23	2.18	0.44
1:A:529:LEU:HD23	1:A:529:LEU:H	1.82	0.44
1:A:1773:VAL:HG11	1:A:1785:PHE:CZ	2.53	0.44
3:C:141:LYS:HB3	3:C:172:TYR:CG	2.52	0.44
2:B:33:SER:O	2:B:34:MET:SD	2.76	0.43
1:A:121:GLN:HA	1:A:124:LYS:HD2	2.00	0.43
1:A:435:THR:O	1:A:437:LYS:HG2	2.18	0.43
1:A:447:GLY:O	1:A:448:ILE:HG22	2.17	0.43
1:A:605:ASP:HA	1:A:606:PRO:HD3	1.81	0.43
1:A:605:ASP:HB3	1:A:608:PHE:CD2	2.53	0.43
1:A:610:ALA:HA	1:A:613:ILE:HG12	2.00	0.43
1:A:2027:MET:N	1:A:2032:ILE:HD12	2.32	0.43
1:A:5:TYR:CZ	1:A:77:ILE:HG23	2.53	0.43
3:C:16:GLY:HA2	3:C:76:SER:HA	1.99	0.43
1:A:290:SER:O	1:A:293:THR:OG1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1856:LEU:HD11	1:A:1943:TYR:CE2	2.53	0.43
2:B:48:MET:HE1	2:B:68:PHE:CD2	2.52	0.43
1:A:528:CYS:HA	1:A:553:ILE:O	2.18	0.43
1:A:2260:PHE:HE2	1:A:2262:ILE:HD11	1.83	0.43
1:A:174:ILE:HD12	1:A:261:MET:SD	2.58	0.43
1:A:2019:LYS:NZ	4:H:2:NAG:O7	2.52	0.43
1:A:2210:LEU:HB3	1:A:2322:GLU:HB2	2.00	0.43
2:B:3:GLN:H	2:B:25:SER:HB3	1.82	0.43
2:B:37:VAL:O	2:B:94:TYR:HA	2.19	0.43
2:B:67:ARG:HB3	2:B:84:ASN:O	2.18	0.43
1:A:1704:GLU:HG2	1:A:1733:VAL:HB	2.01	0.43
1:A:1763:ILE:HG23	1:A:1855:LEU:HA	2.01	0.43
1:A:2075:LEU:C	1:A:2077:ALA:H	2.27	0.43
3:C:38:LYS:HD2	3:C:83:ALA:HB2	2.01	0.43
3:C:114:VAL:O	3:C:115:SER:OG	2.33	0.43
1:A:300:PHE:CD2	1:A:302:MET:HG3	2.50	0.43
1:A:418:ARG:HH11	1:A:611:SER:HB3	1.84	0.43
1:A:617:ILE:HG22	1:A:625:LEU:HD23	2.00	0.43
1:A:2307:ARG:HD3	1:A:2309:HIS:HE1	1.84	0.43
2:B:88:ASN:CG	2:B:118:VAL:HG22	2.43	0.43
1:A:2100:GLN:HB3	1:A:2154:THR:HG1	1.84	0.43
1:A:2209:ARG:O	1:A:2320:ARG:HB3	2.19	0.43
1:A:379:PRO:HB2	1:A:459:ASP:HA	2.00	0.42
1:A:1996:TRP:HB2	1:A:2014:PHE:CE1	2.54	0.42
1:A:2055:TYR:O	1:A:2060:ASN:HB2	2.18	0.42
1:A:2310:PRO:HG3	1:A:2317:ILE:HD13	2.00	0.42
1:A:107:TRP:C	1:A:109:SER:N	2.77	0.42
1:A:2087:GLN:HA	1:A:2129:ASN:ND2	2.33	0.42
1:A:115:TYR:CE2	1:A:1997:ARG:HB2	2.54	0.42
1:A:136:THR:HG22	1:A:137:TYR:H	1.85	0.42
1:A:620:TYR:HB3	1:A:624:SER:OG	2.19	0.42
1:A:2059:ILE:H	1:A:2059:ILE:HG13	1.67	0.42
1:A:2072:LYS:HD3	1:A:2150:ARG:NH2	2.34	0.42
1:A:2201:ALA:HB1	1:A:2216:SER:HB3	2.01	0.42
2:B:13:LYS:NZ	2:B:119:SER:C	2.73	0.42
1:A:1781:ARG:HD3	1:A:1889:TRP:HB3	2.00	0.42
1:A:1808:GLN:HG3	1:A:1809:PRO:CD	2.46	0.42
1:A:2209:ARG:HB2	1:A:2212:LEU:HB2	2.01	0.42
1:A:170:ASN:HB3	1:A:204:ASP:O	2.20	0.42
1:A:406:SER:OG	1:A:408:LYS:HG2	2.19	0.42
2:B:147:CYS:HB2	2:B:161:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HB3	1:A:1997:ARG:NH2	2.35	0.42
1:A:147:PRO:HB2	1:A:181:ARG:HH21	1.83	0.42
1:A:395:TYR:CD2	1:A:614:MET:HG3	2.54	0.42
1:A:598:PRO:O	1:A:600:GLY:N	2.40	0.42
2:B:11:LEU:CD1	2:B:119:SER:CB	2.97	0.42
2:B:38:LYS:HD3	2:B:64:PHE:CZ	2.54	0.42
1:A:2126:PHE:HD2	1:A:2138:ASN:HB3	1.84	0.42
1:A:134:SER:O	1:A:135:GLN:HB3	2.20	0.42
1:A:288:GLU:HB3	1:A:671:PHE:CE2	2.55	0.42
1:A:605:ASP:HB3	1:A:608:PHE:CE2	2.54	0.42
1:A:1928:THR:O	1:A:1930:PRO:HD3	2.20	0.42
2:B:18:VAL:HG12	2:B:86:LEU:HD11	2.01	0.42
2:B:37:VAL:HB	2:B:95:PHE:HB2	2.01	0.42
2:B:165:SER:OG	2:B:166:LEU:N	2.53	0.42
1:A:199:LEU:HD12	1:A:259:ILE:O	2.20	0.42
1:A:252:LYS:HE3	1:A:252:LYS:HB2	1.72	0.42
1:A:1693:LYS:HB2	1:A:1694:ARG:HG3	2.02	0.42
1:A:1945:LEU:HB2	1:A:1983:PHE:CE1	2.54	0.42
2:B:70:PHE:CE1	2:B:81:LEU:HD13	2.54	0.42
3:C:6:GLN:HG2	3:C:101:LEU:HD12	2.01	0.42
1:A:56:THR:HG22	1:A:64:ARG:HE	1.85	0.42
3:C:32:MET:HE2	3:C:70:TYR:HB2	2.01	0.42
1:A:1897:ARG:HB3	1:A:1898:ASN:H	1.62	0.41
1:A:1949:SER:OG	1:A:1950:ASN:N	2.53	0.41
1:A:2081:ILE:HG22	1:A:2140:PHE:HZ	1.84	0.41
1:A:2273:LEU:HB2	1:A:2275:PHE:CE1	2.54	0.41
2:B:158:THR:O	2:B:158:THR:OG1	2.35	0.41
1:A:66:ARG:NH2	1:A:73:LEU:O	2.46	0.41
1:A:2025:LEU:HD13	1:A:2075:LEU:HD11	2.02	0.41
2:B:13:LYS:HA	2:B:13:LYS:HD3	1.79	0.41
3:C:60:ARG:HH12	3:C:78:GLU:HB2	1.85	0.41
1:A:149:ALA:C	1:A:151:ASP:H	2.29	0.41
1:A:1769:ASP:O	1:A:1819:VAL:HG12	2.20	0.41
1:A:1828:ASP:O	1:A:1966:ARG:HD3	2.21	0.41
1:A:1972:LYS:HE2	1:A:1972:LYS:HB2	1.80	0.41
2:B:156:PRO:HB2	2:B:157:VAL:H	1.55	0.41
2:B:201:THR:HA	2:B:216:LYS:HA	2.02	0.41
3:C:141:LYS:HB3	3:C:172:TYR:CD2	2.54	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.70	0.41
1:A:428:PHE:O	1:A:450:GLY:HA2	2.20	0.41
1:A:1846:ASP:HA	1:A:1849:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1881:THR:HA	1:A:1954:HIS:HE2	1.85	0.41
1:A:2141:ASN:HB2	4:H:1:NAG:H3	2.01	0.41
3:C:154:ARG:NE	3:C:156:ASN:O	2.53	0.41
1:A:3:ARG:NH1	1:A:79:ALA:HA	2.36	0.41
1:A:96:PRO:HB3	1:A:130:LEU:HG	2.01	0.41
1:A:629:VAL:HG22	1:A:706:LEU:HD11	2.03	0.41
1:A:105:SER:O	1:A:140:GLN:N	2.47	0.41
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.86	0.41
1:A:428:PHE:HE2	1:A:534:SER:HA	1.85	0.41
1:A:1952:ASN:HB3	1:A:1954:HIS:HE2	1.85	0.41
1:A:2183:LYS:HA	1:A:2209:ARG:NH1	2.36	0.41
1:A:11:GLU:HG2	1:A:50:THR:HB	2.03	0.41
1:A:684:ASN:O	1:A:708:VAL:HG21	2.20	0.41
1:A:2154:THR:HA	3:C:49:PHE:HD2	1.84	0.41
3:C:208:PHE:O	3:C:209:ASN:HB2	2.20	0.41
1:A:98:SER:OG	1:A:162:HIS:N	2.45	0.41
1:A:472:PRO:HB2	1:A:502:PRO:HB2	2.02	0.41
1:A:2196:PHE:CD1	1:A:2222:GLN:HA	2.56	0.41
1:A:2321:MET:HE3	1:A:2321:MET:HB2	1.88	0.41
3:C:197:HIS:ND1	3:C:199:THR:HG23	2.36	0.41
1:A:89:LEU:HD23	1:A:129:VAL:HG21	2.02	0.41
1:A:382:TRP:HE3	1:A:383:VAL:H	1.69	0.41
1:A:658:PHE:CE2	1:A:668:LEU:HB2	2.56	0.41
1:A:1933:VAL:HA	1:A:2015:LEU:O	2.21	0.41
1:A:2225:ASN:OD1	1:A:2227:LYS:HB2	2.21	0.41
2:B:128:VAL:HA	2:B:149:VAL:HG23	2.03	0.41
2:B:176:VAL:HG23	3:C:161:SER:HB2	2.01	0.41
3:C:121:SER:OG	3:C:122:GLU:N	2.53	0.41
3:C:200:LYS:HZ3	3:C:204:ILE:HD12	0.95	0.41
1:A:31:PHE:N	1:A:32:PRO:HD3	2.15	0.41
1:A:196:PHE:HB2	1:A:256:TRP:HZ3	1.85	0.41
1:A:207:LYS:HE2	1:A:207:LYS:HB3	1.91	0.41
1:A:1870:GLN:O	1:A:1871:VAL:HG22	2.20	0.41
2:B:79:ALA:C	2:B:80:TYR:HD1	2.29	0.41
1:A:428:PHE:CZ	1:A:547:LEU:HD22	2.57	0.40
1:A:1921:ILE:HD12	1:A:2012:THR:HG22	2.03	0.40
1:A:70:MET:O	1:A:236:ASN:HB3	2.21	0.40
1:A:186:THR:O	1:A:188:GLU:N	2.54	0.40
1:A:194:HIS:HB3	1:A:196:PHE:CE1	2.55	0.40
1:A:429:MET:HE1	1:A:442:ILE:HD13	2.04	0.40
1:A:655:GLY:HA2	1:A:1788:SER:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:THR:HB	1:A:704:ALA:H	1.65	0.40
1:A:2087:GLN:HA	1:A:2129:ASN:HD21	1.87	0.40
1:A:2106:SER:OG	1:A:2107:LEU:N	2.54	0.40
3:C:6:GLN:HE22	3:C:86:TYR:HA	1.86	0.40
1:A:43:PRO:C	1:A:45:VAL:N	2.71	0.40
1:A:2111:LYS:HB2	1:A:2111:LYS:HE3	1.86	0.40
1:A:2180:MET:HG2	1:A:2185:ILE:HD12	2.03	0.40
2:B:4:LEU:HB2	2:B:110:TRP:O	2.22	0.40
1:A:200:PHE:CE2	1:A:270:ILE:HG13	2.56	0.40
1:A:2015:LEU:HD23	1:A:2016:VAL:C	2.46	0.40
2:B:88:ASN:HA	2:B:118:VAL:HG23	1.96	0.40
3:C:6:GLN:NE2	3:C:101:LEU:HB2	2.37	0.40
1:A:104:VAL:HB	1:A:105:SER:H	1.67	0.40
1:A:301:LEU:HD13	1:A:327:VAL:HG12	2.03	0.40
1:A:310:PHE:CB	1:A:322:GLU:HG2	2.50	0.40
1:A:453:LEU:HD23	1:A:513:TRP:CZ3	2.53	0.40
1:A:1993:VAL:HA	1:A:2016:VAL:CG2	2.52	0.40
1:A:2092:LYS:HB3	1:A:2093:PHE:HD1	1.84	0.40
1:A:2229:TRP:HB3	1:A:2309:HIS:ND1	2.37	0.40
1:A:2245:THR:HB	1:A:2319:LEU:HD11	2.03	0.40
2:B:67:ARG:HG2	2:B:85:ASN:HB3	2.04	0.40
2:B:131:LEU:CD2	2:B:148:LEU:H	2.33	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	1249/1467 (85%)	962 (77%)	222 (18%)	65 (5%)	1	18
2	B	213/223 (96%)	139 (65%)	58 (27%)	16 (8%)	1	13
3	C	211/213 (99%)	149 (71%)	48 (23%)	14 (7%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1673/1903 (88%)	1250 (75%)	328 (20%)	95 (6%)	1	17

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	187	ARG
1	A	250	HIS
1	A	265	PRO
1	A	291	PRO
1	A	420	GLY
1	A	448	ILE
1	A	492	PRO
1	A	598	PRO
1	A	601	VAL
1	A	708	VAL
1	A	1797	GLU
1	A	1871	VAL
2	B	104	ASP
2	B	118	VAL
2	B	154	PRO
2	B	156	PRO
1	A	33	ALA
1	A	45	VAL
1	A	116	GLU
1	A	138	VAL
1	A	321	MET
1	A	331	ALA
1	A	372	ARG
1	A	446	SER
1	A	519	ASP
1	A	1751	GLU
1	A	1806	PHE
1	A	2058	SER
1	A	2067	PRO
1	A	2120	THR
2	B	86	LEU
2	B	193	SER
3	C	107	ARG
3	C	129	ALA
3	C	150	ASP
3	C	191	TYR

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Mol	Chain	Res	Type
1	A	31	PHE
1	A	111	GLU
1	A	142	LEU
1	A	183	GLY
1	A	211	SER
1	A	695	SER
1	A	697	PHE
1	A	704	ALA
1	A	1798	GLN
1	A	2028	ALA
1	A	2119	SER
1	A	2268	GLY
2	B	14	PRO
2	B	117	THR
2	B	207	PRO
3	C	15	LEU
3	C	62	SER
3	C	99	THR
1	A	599	ALA
1	A	614	MET
1	A	1796	GLN
1	A	1830	PHE
1	A	1936	GLN
1	A	2097	TYR
1	A	2175	SER
1	A	2179	GLY
1	A	2196	PHE
1	A	2328	ALA
2	B	166	LEU
3	C	92	SER
3	C	121	SER
1	A	104	VAL
1	A	108	LYS
1	A	134	SER
1	A	401	ALA
1	A	441	ALA
1	A	1897	ARG
1	A	2315	HIS
2	B	192	SER
3	C	209	ASN
1	A	194	HIS
1	A	702	MET

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Mol	Chain	Res	Type
1	A	1850	GLY
3	C	75	SER
3	C	118	PRO
1	A	2041	GLY
1	A	2078	PRO
1	A	2109	GLY
2	B	20	ILE
2	B	116	VAL
2	B	126	PRO
1	A	1854	PRO
1	A	369	ILE
2	B	41	PRO
2	B	42	GLY
3	C	151	GLY
1	A	402	PRO
3	C	93	SER

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	1118/1301 (86%)	1111 (99%)	7 (1%)	78	80
2	B	186/189 (98%)	184 (99%)	2 (1%)	65	74
3	C	186/186 (100%)	185 (100%)	1 (0%)	81	82
All	All	1490/1676 (89%)	1480 (99%)	10 (1%)	76	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	29	THR
1	A	30	ARG
1	A	34	THR
1	A	377	LYS
1	A	2141	ASN

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Mol	Chain	Res	Type
1	A	2296	SER
2	B	119	SER
2	B	120	SER
3	C	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	HIS
1	A	298	GLN
1	A	306	GLN
1	A	317	HIS
1	A	324	HIS
1	A	592	GLN
1	A	1777	ASN
1	A	1822	HIS
1	A	2007	GLN
1	A	2100	GLN
1	A	2141	ASN
1	A	2224	ASN
2	B	6	GLN
2	B	35	HIS
2	B	82	GLN
2	B	84	ASN
2	B	88	ASN
3	C	6	GLN
3	C	36	GLN
3	C	137	ASN
3	C	189	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 ⓘ

7 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
5	NAG	D	1	1,5	14,14,15	1.29	1 (7%)	17,19,21	1.28	1 (5%)
5	NAG	D	2	5	14,14,15	1.23	1 (7%)	17,19,21	1.25	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.38	0	17,19,21	0.61	0
4	NAG	H	2	4	14,14,15	0.35	0	17,19,21	0.50	0
4	BMA	H	3	4	11,11,12	0.95	0	15,15,17	1.51	3 (20%)
4	MAN	H	4	4	11,11,12	1.13	2 (18%)	15,15,17	1.11	2 (13%)
4	MAN	H	5	4	11,11,12	0.94	1 (9%)	15,15,17	1.47	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	1/1/1/1
4	MAN	H	5	4	-	1/2/19/22	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	NAG	O5-C1	4.50	1.51	1.43
5	D	2	NAG	O5-C1	3.77	1.50	1.43
4	H	5	MAN	O5-C5	2.62	1.48	1.43
4	H	4	MAN	C1-C2	2.48	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	4	MAN	O5-C5	2.25	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	MAN	C1-O5-C5	4.72	118.51	112.19
5	D	1	NAG	C1-O5-C5	4.59	118.34	112.19
4	H	3	BMA	C3-C4-C5	3.41	116.41	110.23
5	D	2	NAG	C1-O5-C5	3.05	116.27	112.19
4	H	4	MAN	C1-O5-C5	3.03	116.25	112.19
4	H	3	BMA	C1-O5-C5	2.52	115.57	112.19
4	H	5	MAN	O2-C2-C3	-2.36	105.26	110.15
4	H	3	BMA	O2-C2-C3	-2.02	105.98	110.15
4	H	4	MAN	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2	NAG	C4-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	H	5	MAN	O5-C5-C6-O6
4	H	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C4-C5-C6-O6

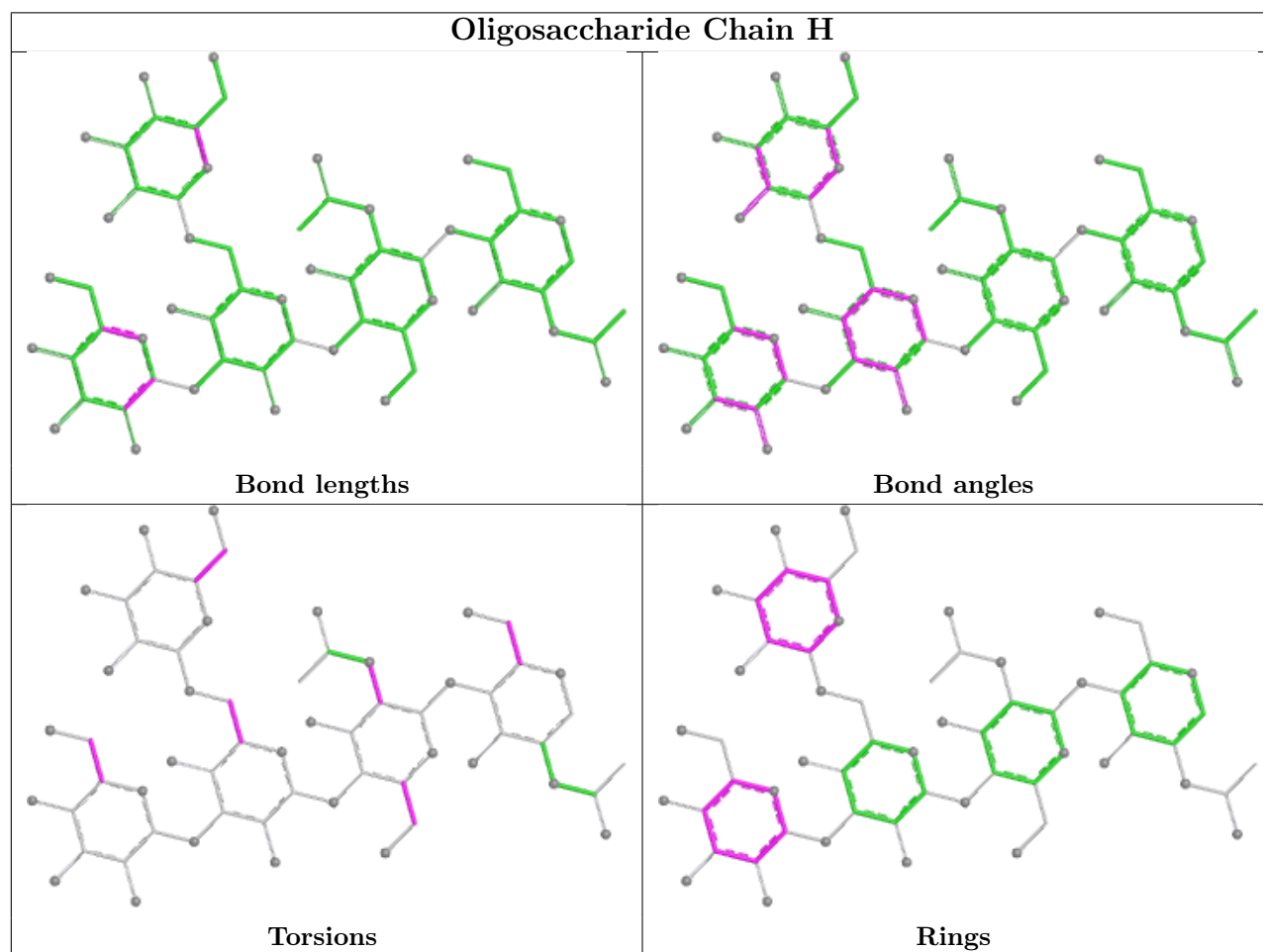
All (2) ring outliers are listed below:

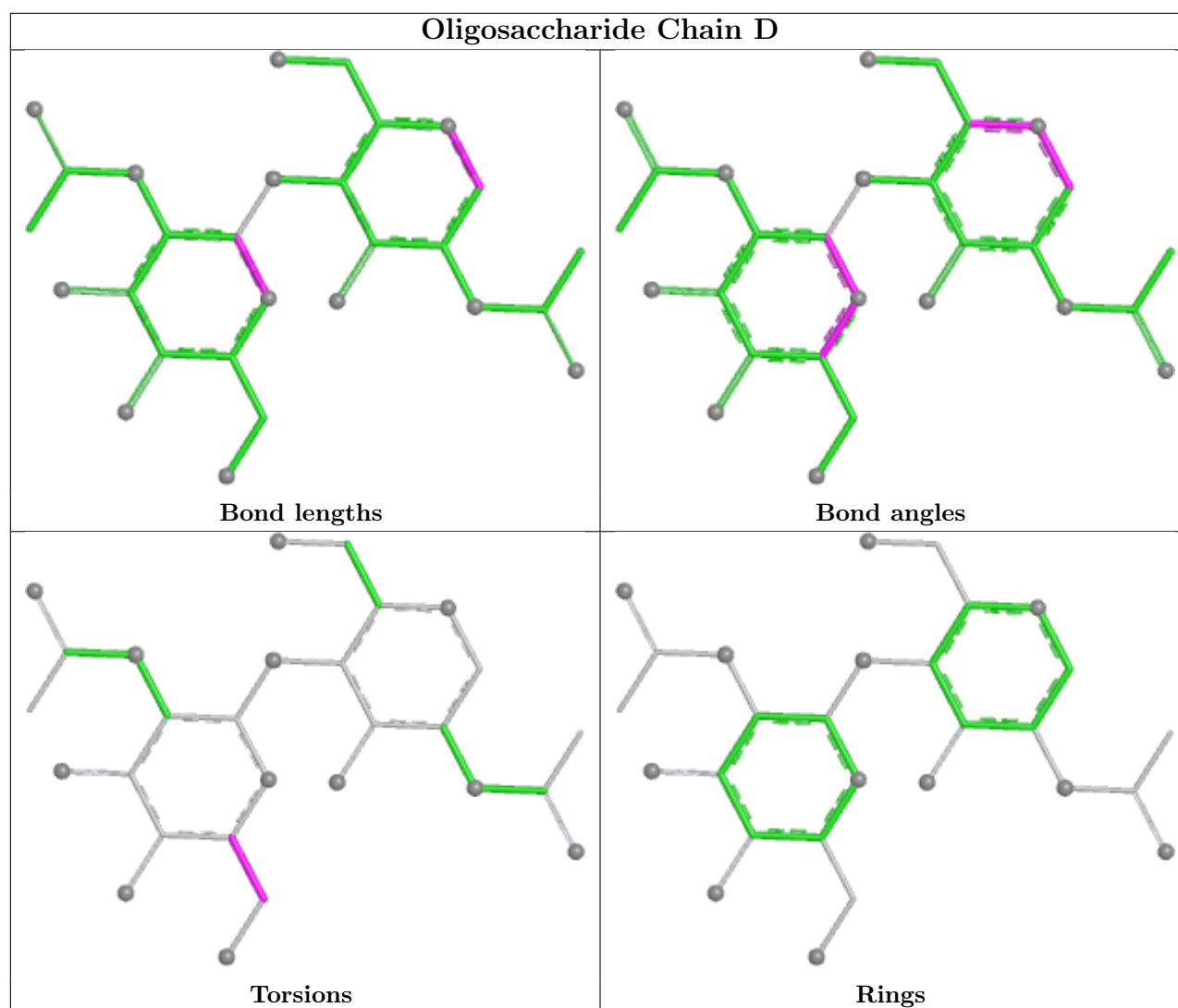
Mol	Chain	Res	Type	Atoms
4	H	5	MAN	C1-C2-C3-C4-C5-O5
4	H	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
4	H	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	2401	1	14,14,15	0.52	0	17,19,21	0.54	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
6	NAG	A	2401	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1265/1467 (86%)	-0.56	0 100 100	73, 137, 194, 330	1 (0%)
2	B	217/223 (97%)	-0.38	3 (1%) 73 53	30, 172, 220, 233	0
3	C	213/213 (100%)	-0.64	0 100 100	99, 156, 232, 243	0
All	All	1695/1903 (89%)	-0.55	3 (0%) 91 81	30, 142, 212, 330	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	THR	4.1
2	B	116	VAL	3.0
2	B	34	MET	2.8

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

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

6.3 Carbohydrates [i](#)

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

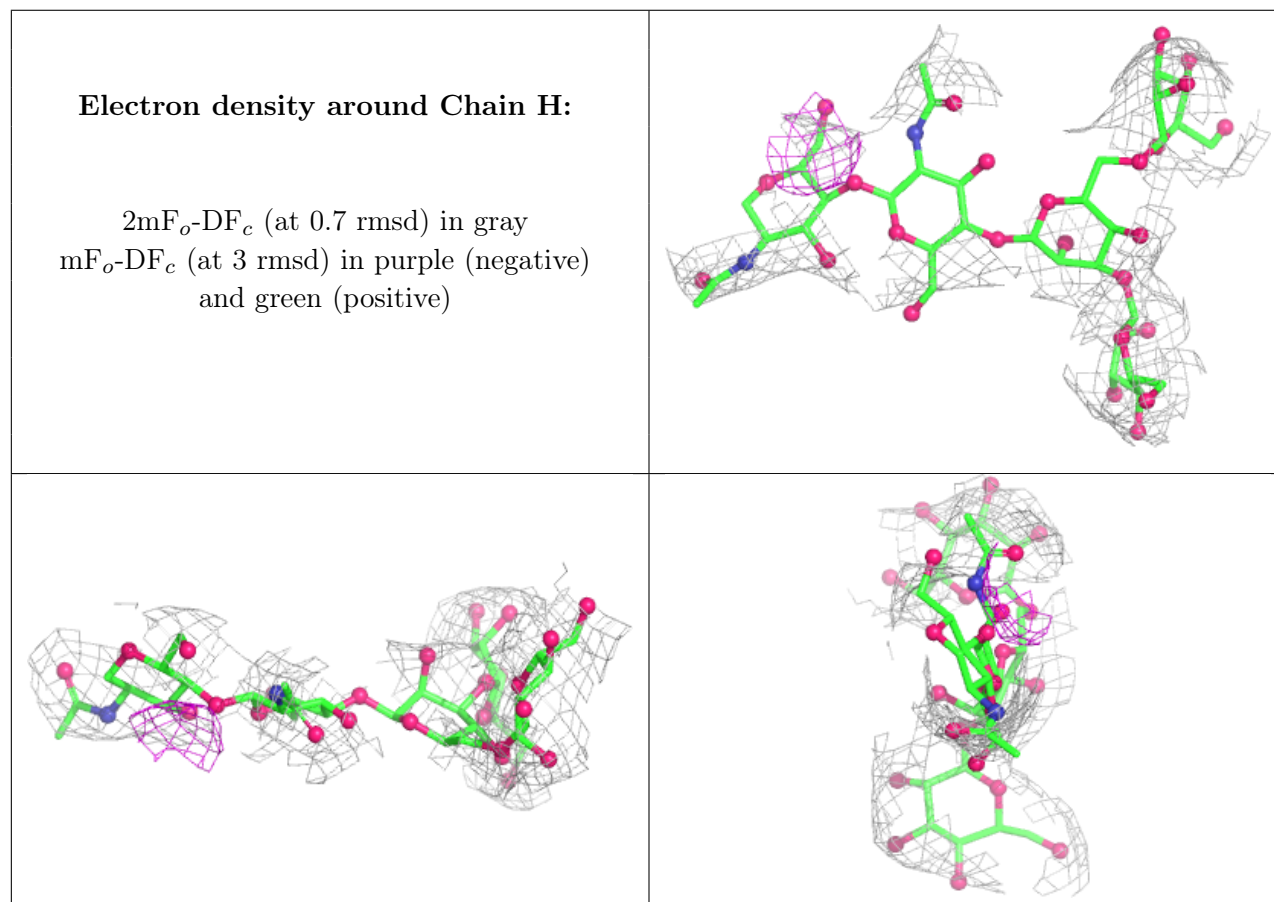
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	1	14/15	-	-	138,150,158,160	0
4	NAG	H	2	14/15	-	-	150,171,185,185	0
4	BMA	H	3	11/12	-	-	179,186,197,202	0
4	MAN	H	4	11/12	-	-	171,188,202,202	0
4	MAN	H	5	11/12	-	-	167,182,186,189	0

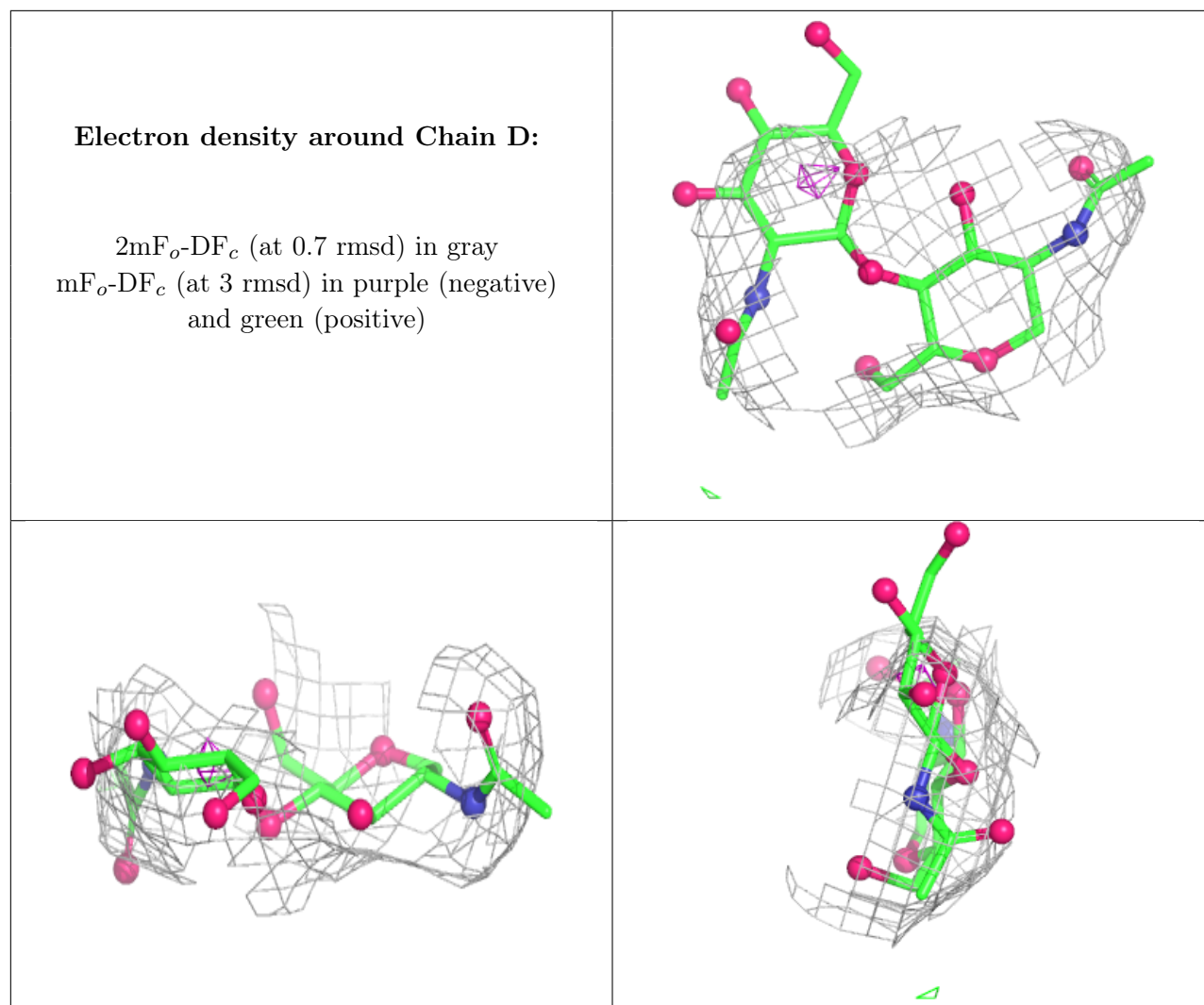
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	D	2	14/15	0.83	0.06	194,209,214,215	0
5	NAG	D	1	14/15	0.87	0.11	164,200,213,214	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	2401	14/15	0.74	0.07	167,182,194,195	0
9	ZN	A	2404	1/1	0.98	0.05	137,137,137,137	0
8	CA	A	2403	1/1	0.99	0.05	141,141,141,141	0
7	CU	A	2402	1/1	0.99	0.05	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.