



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 1IGT / pdb_00001igt
Title : STRUCTURE OF IMMUNOGLOBULIN
Authors : Harris, L.J.; Larson, S.B.; Hasel, K.W.; McPherson, A.
Deposited on : 1996-10-25
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

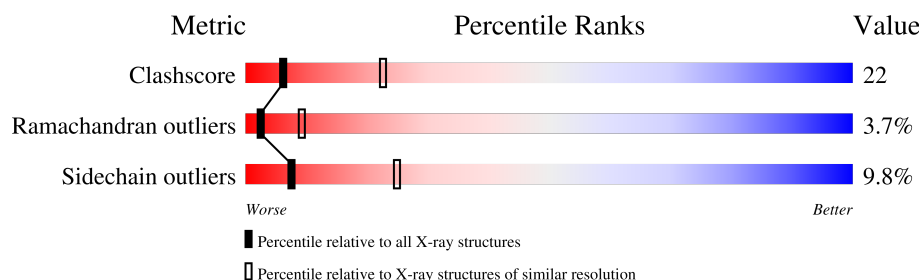
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	C	214	
2	B	444	
2	D	444	
3	E	9	
4	F	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	2	X	-	-	-
4	NAG	F	2	X	-	-	-
4	FUC	F	9	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12956 atoms, of which 2522 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.

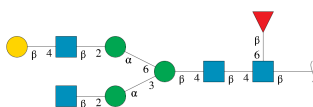
- Molecule 1 is a protein called IGG2A INTACT ANTIBODY - MAB231.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	H	N	O	S	0	0	0
			2033	1029	386	276	336	6			
1	C	214	Total	C	H	N	O	S	0	0	0
			2033	1029	386	276	336	6			

- Molecule 2 is a protein called IGG2A INTACT ANTIBODY - MAB231.

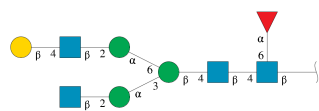
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	444	Total	C	H	N	O	S	9	0	0
			4232	2191	772	576	671	22			
2	D	444	Total	C	H	N	O	S	9	0	0
			4232	2191	772	576	671	22			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	9	Total	C	H	N	O	0	0	0
			213	62	103	4	44			

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



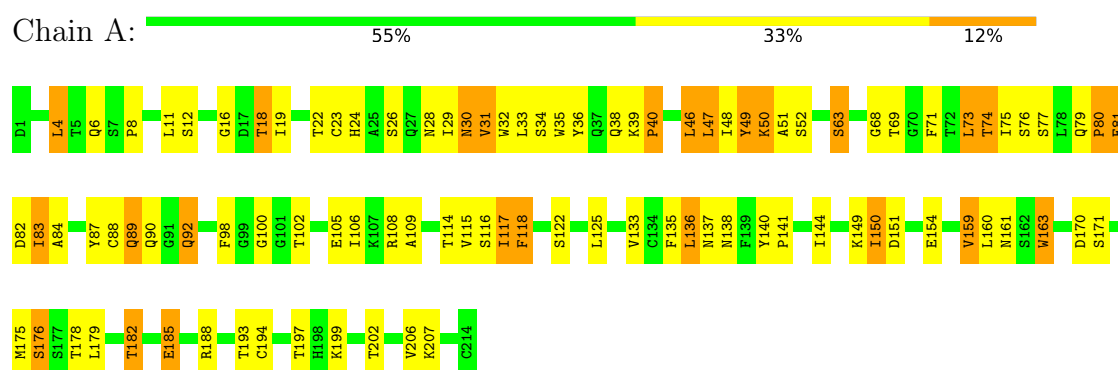
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	9	Total	C	H	N	O	0	0	0
			213	62	103	4	44			

3 Residue-property plots [i](#)

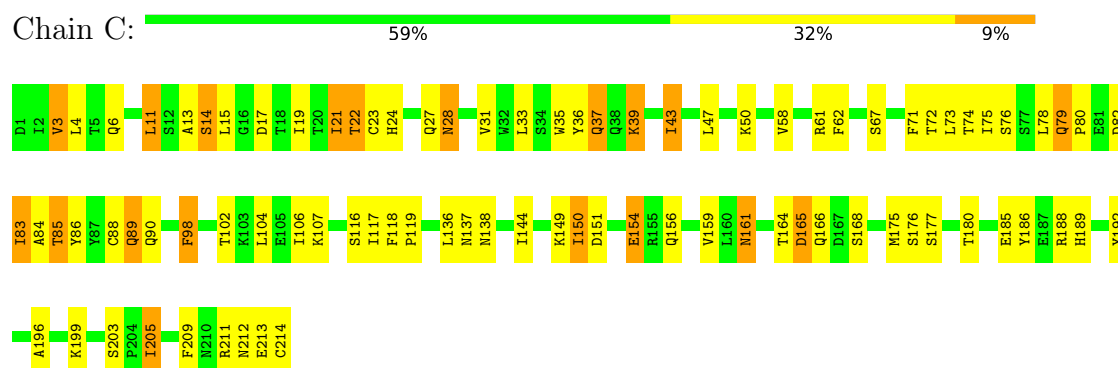
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

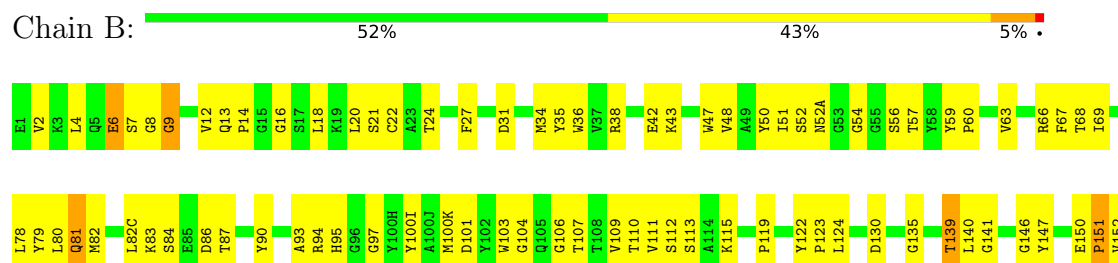
• Molecule 1: IGG2A INTACT ANTIBODY - MAB231

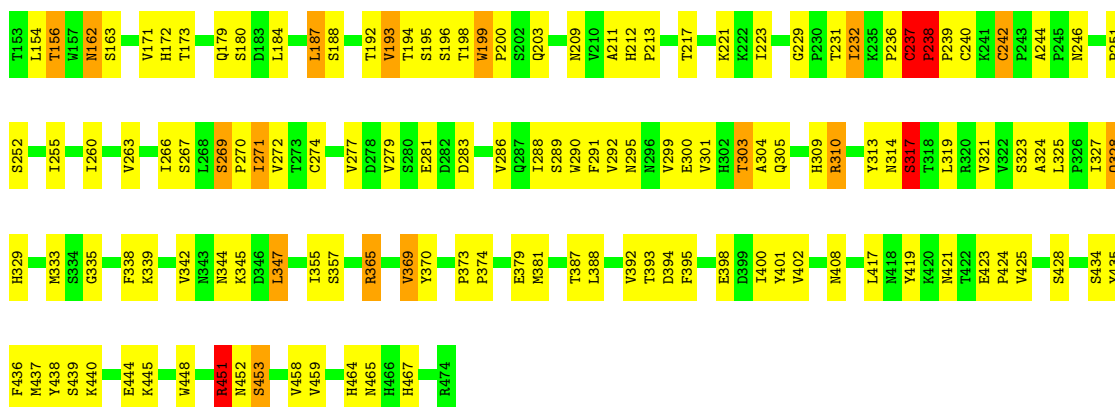


• Molecule 1: IGG2A INTACT ANTIBODY - MAB231



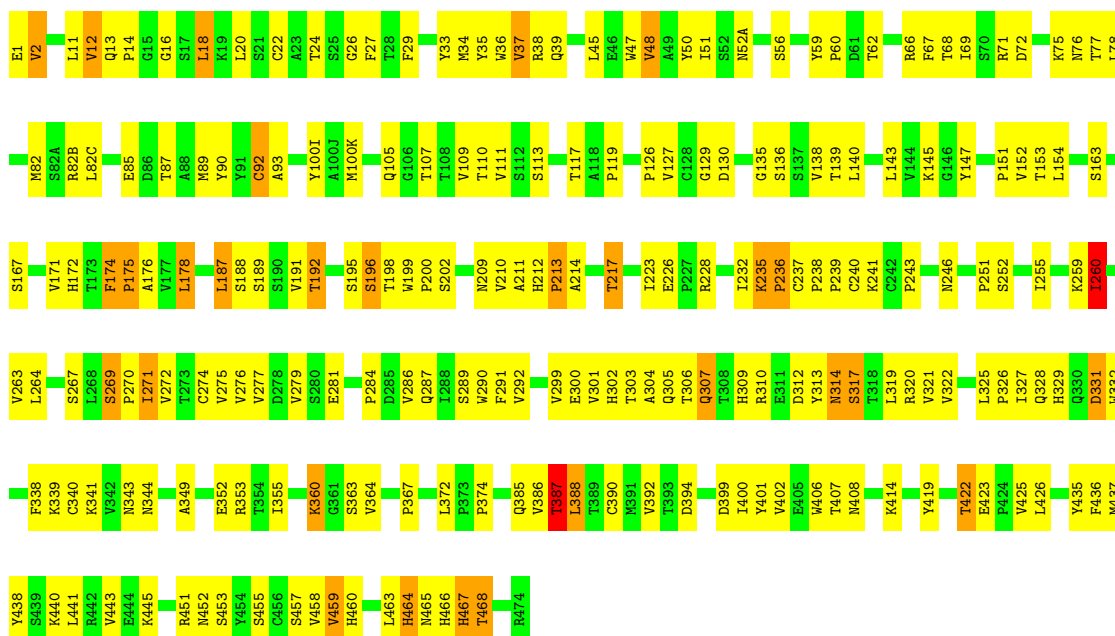
• Molecule 2: IGG2A INTACT ANTIBODY - MAB231





• Molecule 2: IGG2A INTACT ANTIBODY - MAB231

Chain D: 50% 43% 7%

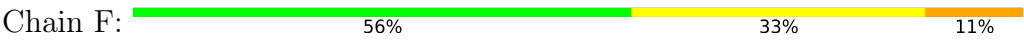


• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 67% 11% 22%



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



NAG1	NAG2	BGL3	MAN4	NAG5	GAL6	MAN7	NAG8	FUC9
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.82Å 76.77Å 100.64Å 88.05° 92.35° 97.23°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	86.2 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.209 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12956	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, FUL, GAL, BMA, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/1685	1.01	6/2292 (0.3%)
1	C	0.51	0/1685	1.05	11/2292 (0.5%)
2	B	0.58	0/3554	1.05	20/4847 (0.4%)
2	D	0.56	0/3554	1.00	17/4847 (0.4%)
All	All	0.57	0/10478	1.03	54/14278 (0.4%)

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
2	D	0	1

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	LYS	N-CA-C	-7.60	100.49	110.07
1	C	58	VAL	CA-C-N	7.47	127.47	119.78
1	C	58	VAL	C-N-CA	7.47	127.47	119.78
2	B	423	GLU	N-CA-C	-7.07	99.92	110.24
1	A	118	PHE	CA-C-N	6.89	124.62	119.66
1	A	118	PHE	C-N-CA	6.89	124.62	119.66
2	B	238	PRO	N-CA-C	6.88	119.09	110.70
2	D	269	SER	CA-C-N	6.85	126.83	119.78
2	D	269	SER	C-N-CA	6.85	126.83	119.78
2	D	423	GLU	N-CA-C	-6.79	100.21	110.39
2	B	199	TRP	N-CA-C	6.71	121.30	112.17
2	D	174	PHE	N-CA-C	6.54	117.90	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	N-CA-C	-6.29	106.15	113.88
2	B	229	GLY	CA-C-N	6.21	127.60	119.84
2	B	229	GLY	C-N-CA	6.21	127.60	119.84
1	C	85	THR	N-CA-C	-6.15	99.69	109.59
2	B	369	VAL	N-CA-C	6.14	116.46	107.37
2	D	468	THR	N-CA-C	-6.11	101.15	110.14
1	C	137	ASN	N-CA-C	6.09	117.90	110.41
1	C	203	SER	CA-C-N	5.89	126.23	119.93
1	C	203	SER	C-N-CA	5.89	126.23	119.93
2	B	310	ARG	N-CA-C	5.85	119.08	110.59
2	B	263	VAL	N-CA-C	5.76	116.50	110.62
2	B	82(C)	LEU	N-CA-C	5.75	118.17	110.35
2	B	269	SER	CA-C-N	5.65	125.55	119.85
2	B	269	SER	C-N-CA	5.65	125.55	119.85
2	D	226	GLU	CA-C-N	5.64	125.93	119.83
2	D	226	GLU	C-N-CA	5.64	125.93	119.83
2	D	387	THR	N-CA-C	5.57	117.77	108.02
2	B	237	CYS	N-CA-C	5.50	121.97	109.81
2	D	92	CYS	N-CA-C	-5.47	100.37	109.46
1	C	159	VAL	N-CA-C	5.44	117.14	108.87
1	A	137	ASN	N-CA-C	5.41	117.50	110.53
2	D	178	LEU	N-CA-C	5.36	118.13	109.40
1	A	182	THR	N-CA-C	-5.34	101.47	109.95
2	B	387	THR	N-CA-C	5.33	117.35	108.02
2	B	236	PRO	N-CA-C	5.30	122.13	111.69
2	B	193	VAL	N-CA-C	5.27	115.79	110.05
1	C	83	ILE	N-CA-C	-5.26	101.89	108.84
1	C	72	THR	N-CA-C	5.26	116.99	108.26
2	B	345	LYS	N-CA-C	5.25	117.69	111.33
2	B	8	GLY	N-CA-C	-5.24	104.99	111.70
1	A	18	THR	N-CA-C	-5.23	100.65	109.07
2	B	393	THR	N-CA-C	5.21	117.33	109.41
2	D	48	VAL	N-CA-C	5.20	116.11	111.90
2	D	467	HIS	N-CA-C	5.20	116.89	108.26
2	D	281	GLU	N-CA-C	5.13	119.00	112.34
2	D	267	SER	N-CA-C	5.11	117.24	111.11
2	D	33	TYR	N-CA-C	-5.09	101.41	109.96
2	D	394	ASP	N-CA-C	5.08	118.22	111.30
2	B	467	HIS	N-CA-C	5.05	116.28	107.49
1	C	165	ASP	N-CA-C	-5.01	103.78	110.55
2	B	419	TYR	N-CA-C	-5.01	101.58	109.50
2	D	314	ASN	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	35	TYR	Sidechain

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	1647	386	1588	74	0
1	C	1647	386	1588	72	0
2	B	3460	772	3377	154	0
2	D	3460	772	3377	162	0
3	E	110	103	94	6	0
4	F	110	103	94	3	0
All	All	10434	2522	10118	460	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (460) 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:118:PHE:HB3	2:B:124:LEU:HD12	1.38	1.06
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.44	0.99
2:D:136:SER:HA	2:D:195:SER:HB3	1.48	0.95
2:D:37:VAL:HG12	2:D:47:TRP:HA	1.55	0.88
2:D:367:PRO:HD3	2:D:460:HIS:HD2	1.42	0.85
1:A:36:TYR:HE2	1:A:89:GLN:HG2	1.43	0.84
2:B:52:SER:HB2	2:B:56:SER:HB2	1.64	0.80
1:A:29:ILE:HA	1:A:92:GLN:HG3	1.65	0.79
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.66	0.78
2:B:374:PRO:HD3	2:B:388:LEU:HD23	1.66	0.77
2:B:238:PRO:HB2	2:B:239:PRO:HD3	1.65	0.76
1:A:63:SER:HB2	1:A:74:THR:HG23	1.67	0.76
1:A:6:GLN:HE22	1:A:87:TYR:HA	1.51	0.75
1:A:32:TRP:HD1	1:A:92:GLN:HG2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:ILE:HD13	2:D:260:ILE:H	1.49	0.74
1:C:19:ILE:HG12	1:C:78:LEU:HD21	1.70	0.74
1:C:37:GLN:HG3	1:C:86:TYR:CE2	2.22	0.74
2:B:87:THR:HG23	2:B:110:THR:HA	1.68	0.74
2:B:6:GLU:HA	2:B:22:CYS:HA	1.69	0.73
2:B:301:VAL:HB	2:B:304:ALA:HB2	1.70	0.73
2:D:290:TRP:NE1	2:D:306:THR:HG21	2.04	0.73
2:B:48:VAL:O	2:B:60:PRO:HD2	1.89	0.73
2:B:9:GLY:HA2	2:B:18:LEU:HD21	1.71	0.72
1:A:188:ARG:HB3	1:A:188:ARG:HH11	1.54	0.72
2:D:276:VAL:HB	2:D:321:VAL:HG12	1.72	0.72
1:C:37:GLN:HG3	1:C:86:TYR:CZ	2.25	0.71
2:B:51:ILE:HG13	2:B:57:THR:HG22	1.73	0.71
2:B:152:VAL:HG12	2:B:212:HIS:HD2	1.55	0.70
1:C:83:ILE:HD12	1:C:168:SER:HA	1.73	0.70
2:B:47:TRP:HZ2	2:B:50:TYR:HB3	1.57	0.70
1:A:118:PHE:CB	2:B:124:LEU:HD12	2.19	0.69
2:B:266:ILE:HG13	2:B:267:SER:H	1.58	0.68
2:B:63:VAL:HB	2:B:67:PHE:CD2	2.29	0.67
1:A:39:LYS:HG2	1:A:83:ILE:O	1.94	0.67
2:D:291:PHE:CD1	2:D:300:GLU:HA	2.28	0.67
1:A:108:ARG:HG2	1:A:109:ALA:N	2.09	0.67
2:B:20:LEU:HD12	2:B:80:LEU:HD23	1.77	0.67
2:B:156:THR:HG23	2:B:209:ASN:HB2	1.77	0.67
1:A:12:SER:HA	1:A:105:GLU:O	1.95	0.66
1:A:115:VAL:HG13	1:A:207:LYS:HG3	1.76	0.66
2:D:390:CYS:HB2	2:D:406:TRP:CZ2	2.30	0.66
2:D:18:LEU:HB3	2:D:82:MET:HE3	1.78	0.66
2:D:66:ARG:HD2	2:D:82(B):ARG:HB2	1.77	0.66
1:A:8:PRO:HG3	1:A:11:LEU:HG	1.76	0.66
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.77	0.65
1:C:62:PHE:CD1	1:C:75:ILE:HG13	2.31	0.65
2:B:301:VAL:HB	2:B:304:ALA:CB	2.26	0.65
1:C:4:LEU:HD21	1:C:90:GLN:HG2	1.79	0.65
2:B:83:LYS:O	2:B:111:VAL:HG21	1.97	0.64
1:A:182:THR:OG1	1:A:185:GLU:HB2	1.99	0.63
2:D:163:SER:H	2:D:209:ASN:ND2	1.96	0.63
2:D:272:VAL:HG23	2:D:327:ILE:HG13	1.80	0.63
1:C:106:ILE:H	1:C:166:GLN:HE22	1.46	0.63
2:B:252:SER:HB2	2:B:277:VAL:HG22	1.80	0.63
1:C:136:LEU:HD12	1:C:136:LEU:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLY:HA2	1:A:77:SER:HA	1.79	0.62
1:A:32:TRP:CD1	1:A:92:GLN:HG2	2.32	0.62
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.80	0.62
2:B:95:HIS:NE2	2:B:97:GLY:O	2.31	0.62
4:F:6:GAL:H2	4:F:6:GAL:C6	2.30	0.62
2:B:4:LEU:HD22	2:B:24:THR:HG22	1.82	0.62
1:C:22:THR:HG22	1:C:23:CYS:H	1.64	0.62
2:B:7:SER:HA	2:B:107:THR:HG21	1.81	0.62
2:B:140:LEU:HD13	2:B:223:ILE:HG21	1.82	0.61
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.35	0.61
1:A:11:LEU:CD1	1:A:19:ILE:HD11	2.30	0.61
1:C:84:ALA:HB3	1:C:86:TYR:CE1	2.35	0.61
1:C:36:TYR:HE1	1:C:89:GLN:HB3	1.66	0.61
1:C:119:PRO:HD2	2:D:228:ARG:HH12	1.65	0.61
2:D:465:ASN:O	2:D:466:HIS:HB2	1.99	0.61
2:B:292:VAL:O	2:B:299:VAL:HG12	2.00	0.61
2:B:327:ILE:HG22	2:B:328:GLN:N	2.16	0.61
2:D:87:THR:HG23	2:D:110:THR:HA	1.82	0.61
1:A:11:LEU:HD12	1:A:19:ILE:HD11	1.82	0.61
2:D:292:VAL:O	2:D:299:VAL:HG22	2.01	0.61
2:D:36:TRP:HD1	2:D:69:ILE:HD12	1.66	0.61
2:B:266:ILE:HG13	2:B:267:SER:N	2.16	0.60
3:E:1:NAG:H61	3:E:2:NAG:HN2	1.65	0.60
2:D:139:THR:HB	2:D:192:THR:HG23	1.83	0.60
2:D:275:VAL:HG12	2:D:322:VAL:HG12	1.82	0.60
2:B:84:SER:HA	2:B:111:VAL:HG23	1.83	0.60
1:A:92:GLN:HE21	1:A:92:GLN:C	2.10	0.60
2:D:69:ILE:HD11	2:D:78:LEU:HD11	1.84	0.60
1:C:13:ALA:HA	1:C:107:LYS:HE2	1.82	0.60
2:D:290:TRP:HE1	2:D:306:THR:HG21	1.65	0.60
2:B:325:LEU:HD23	2:B:327:ILE:HD11	1.83	0.59
2:D:327:ILE:HD12	2:D:338:PHE:CE1	2.38	0.59
1:C:196:ALA:HB3	1:C:205:ILE:HG23	1.85	0.59
2:D:22:CYS:SG	2:D:22:CYS:O	2.61	0.59
1:C:161:ASN:HA	1:C:177:SER:HA	1.84	0.59
2:D:255:ILE:HG22	2:D:353:ARG:CZ	2.33	0.58
2:D:176:ALA:HB2	2:D:187:LEU:HB2	1.85	0.58
1:C:61:ARG:HH11	1:C:79:GLN:HG3	1.68	0.58
2:B:279:VAL:HG21	2:B:321:VAL:HG23	1.85	0.58
2:B:310:ARG:HG3	2:B:321:VAL:HG22	1.85	0.58
2:D:38:ARG:HA	2:D:89:MET:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ILE:CD1	2:B:324:ALA:HB1	2.33	0.57
1:A:87:TYR:HD2	1:A:100:GLY:O	1.87	0.57
2:B:438:TYR:OH	2:D:440:LYS:HB2	2.04	0.57
1:C:19:ILE:O	1:C:74:THR:HA	2.04	0.57
2:B:20:LEU:HB2	2:B:80:LEU:HB3	1.86	0.57
1:C:106:ILE:N	1:C:166:GLN:HE22	2.02	0.57
3:E:6:GAL:C6	3:E:6:GAL:H2	2.35	0.57
1:C:33:LEU:HD13	1:C:71:PHE:CD1	2.40	0.56
1:C:35:TRP:CH2	1:C:88:CYS:HB3	2.39	0.56
1:A:73:LEU:HD12	1:A:74:THR:N	2.19	0.56
2:D:289:SER:HB2	2:D:341:LYS:HB3	1.86	0.56
2:D:211:ALA:HA	2:D:217:THR:O	2.05	0.56
2:B:238:PRO:HB2	2:B:239:PRO:CD	2.35	0.56
2:D:138:VAL:HG22	2:D:140:LEU:HD21	1.87	0.56
2:D:246:ASN:HA	2:D:349:ALA:CB	2.36	0.55
2:D:20:LEU:HD22	2:D:107:THR:HG21	1.87	0.55
1:A:8:PRO:HG3	1:A:11:LEU:CG	2.37	0.55
2:D:274:CYS:HB2	2:D:290:TRP:CH2	2.42	0.55
2:B:67:PHE:CD1	2:B:82:MET:HA	2.42	0.55
2:B:291:PHE:HB2	2:B:339:LYS:HB3	1.88	0.55
1:C:214:CYS:HB2	2:D:228:ARG:HD3	1.89	0.55
1:A:193:THR:HG23	1:A:206:VAL:HG23	1.90	0.54
2:B:303:THR:HG22	2:B:305:GLN:H	1.72	0.54
2:D:213:PRO:HG2	2:D:214:ALA:H	1.73	0.54
1:C:21:ILE:HG23	1:C:73:LEU:HB3	1.88	0.54
1:C:106:ILE:H	1:C:166:GLN:NE2	2.04	0.54
2:D:374:PRO:HD3	2:D:388:LEU:HD12	1.90	0.54
2:B:152:VAL:HG12	2:B:212:HIS:CD2	2.41	0.54
2:B:272:VAL:HG23	2:B:327:ILE:HG13	1.90	0.54
2:B:123:PRO:HD3	2:B:221:LYS:HG2	1.90	0.54
2:B:452:ASN:ND2	2:B:453:SER:H	2.05	0.54
1:C:80:PRO:O	1:C:83:ILE:HG13	2.08	0.53
2:B:425:VAL:HB	2:B:436:PHE:CE1	2.43	0.53
2:B:408:ASN:HA	2:B:453:SER:O	2.08	0.53
1:C:149:LYS:HA	1:C:154:GLU:O	2.09	0.53
2:D:13:GLN:H	2:D:13:GLN:CD	2.16	0.53
1:A:81:GLU:CD	1:A:81:GLU:H	2.15	0.53
1:C:6:GLN:NE2	1:C:21:ILE:HD11	2.24	0.53
2:B:242:CYS:O	2:B:244:ALA:N	2.42	0.53
1:A:50:LYS:O	1:A:52:SER:N	2.40	0.52
2:B:313:TYR:HE2	3:E:1:NAG:O6	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:CYS:HB2	2:B:290:TRP:CZ2	2.44	0.52
2:D:307:GLN:H	2:D:307:GLN:NE2	2.05	0.52
1:C:35:TRP:O	1:C:47:LEU:HB2	2.09	0.52
2:B:211:ALA:HA	2:B:217:THR:O	2.10	0.52
1:A:73:LEU:HD12	1:A:74:THR:H	1.74	0.52
2:B:52:SER:HB3	2:B:54:GLY:O	2.10	0.52
1:C:119:PRO:HD2	2:D:228:ARG:NH1	2.24	0.52
1:A:115:VAL:HG22	1:A:116:SER:N	2.24	0.52
2:B:21:SER:HA	2:B:79:TYR:HD1	1.73	0.52
2:B:187:LEU:HD23	2:B:188:SER:N	2.24	0.52
1:C:175:MET:HG2	1:C:176:SER:N	2.24	0.52
2:B:12:VAL:O	2:B:111:VAL:HA	2.10	0.52
2:D:126:PRO:HD3	2:D:140:LEU:HD22	1.92	0.52
2:D:386:VAL:HG23	2:D:443:VAL:HG23	1.92	0.52
2:D:400:ILE:HG12	2:D:401:TYR:N	2.25	0.52
2:D:463:LEU:O	2:D:464:HIS:C	2.52	0.52
2:D:400:ILE:HG12	2:D:401:TYR:H	1.75	0.51
2:D:93:ALA:CB	2:D:100(K):MET:HG2	2.40	0.51
2:D:291:PHE:HD1	2:D:300:GLU:HA	1.74	0.51
2:B:179:GLN:HG3	2:B:184:LEU:O	2.10	0.51
2:B:327:ILE:HD12	2:B:338:PHE:CE2	2.45	0.51
1:C:189:HIS:O	1:C:211:ARG:HD3	2.10	0.51
1:A:87:TYR:CD2	1:A:100:GLY:O	2.63	0.51
2:B:163:SER:H	2:B:209:ASN:ND2	2.08	0.51
1:C:4:LEU:HA	1:C:24:HIS:O	2.11	0.51
2:B:4:LEU:HB2	2:B:104:GLY:HA2	1.92	0.51
2:D:39:GLN:HG3	2:D:45:LEU:HG	1.91	0.51
2:D:48:VAL:O	2:D:60:PRO:HD3	2.11	0.51
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.45	0.51
2:B:195:SER:O	2:B:198:THR:N	2.43	0.51
2:D:401:TYR:CD1	2:D:401:TYR:C	2.89	0.51
3:E:6:GAL:H2	3:E:6:GAL:H61	1.92	0.51
1:A:8:PRO:CG	1:A:11:LEU:HG	2.41	0.51
1:A:33:LEU:HD22	1:A:71:PHE:CB	2.41	0.50
2:D:47:TRP:HZ2	2:D:50:TYR:HB2	1.75	0.50
1:A:36:TYR:CE2	1:A:89:GLN:HG2	2.35	0.50
2:B:303:THR:C	2:B:305:GLN:N	2.69	0.50
2:B:47:TRP:O	2:B:60:PRO:HG3	2.11	0.50
2:D:47:TRP:O	2:D:60:PRO:HG2	2.12	0.50
2:D:11:LEU:HA	2:D:110:THR:O	2.12	0.50
1:A:133:VAL:HG22	1:A:178:THR:OG1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG23	1:C:50:LYS:HG3	1.93	0.50
2:D:67:PHE:CD1	2:D:67:PHE:N	2.79	0.50
2:B:171:VAL:HG12	2:B:172:HIS:N	2.27	0.50
1:C:88:CYS:SG	1:C:88:CYS:O	2.69	0.50
2:B:124:LEU:HB2	2:B:141:GLY:O	2.12	0.50
2:B:271:ILE:HD12	2:B:324:ALA:HB1	1.93	0.50
1:C:98:PHE:CD1	1:C:98:PHE:N	2.79	0.50
2:D:309:HIS:HB2	2:D:322:VAL:CG2	2.41	0.50
4:F:6:GAL:C6	4:F:6:GAL:C2	2.87	0.50
2:B:458:VAL:HG12	2:B:459:VAL:N	2.26	0.49
2:D:24:THR:HG21	2:D:27:PHE:CZ	2.47	0.49
2:B:223:ILE:HG22	2:B:223:ILE:O	2.12	0.49
2:D:260:ILE:CG2	2:D:399:ASP:HB3	2.42	0.49
2:D:463:LEU:CD1	2:D:468:THR:HG22	2.42	0.49
1:A:24:HIS:HA	1:A:69:THR:O	2.13	0.49
2:B:2:VAL:HG23	2:B:27:PHE:CE2	2.48	0.49
2:B:84:SER:HA	2:B:111:VAL:CG2	2.42	0.49
2:B:374:PRO:HD3	2:B:388:LEU:CD2	2.40	0.49
1:C:150:ILE:HD12	1:C:192:TYR:HE1	1.78	0.49
2:D:119:PRO:HB3	2:D:147:TYR:CB	2.29	0.49
2:D:252:SER:HB2	2:D:277:VAL:CG2	2.42	0.49
2:D:408:ASN:HA	2:D:453:SER:O	2.11	0.49
2:B:47:TRP:CZ3	2:B:60:PRO:HD3	2.48	0.49
2:D:246:ASN:HA	2:D:349:ALA:HB3	1.93	0.49
1:C:185:GLU:O	1:C:189:HIS:HD2	1.94	0.49
2:D:260:ILE:HG21	2:D:399:ASP:HB3	1.95	0.49
2:D:286:VAL:HG13	2:D:344:ASN:HB2	1.94	0.49
3:E:1:NAG:C6	3:E:2:NAG:HN2	2.26	0.49
1:A:108:ARG:HG2	1:A:109:ALA:H	1.74	0.49
2:B:193:VAL:HG12	2:B:194:THR:N	2.27	0.49
1:C:27:GLN:HG2	1:C:28:ASN:N	2.27	0.49
1:C:186:TYR:CE1	1:C:192:TYR:CE2	3.00	0.49
2:D:327:ILE:HG22	2:D:328:GLN:N	2.27	0.49
3:E:6:GAL:C6	3:E:6:GAL:C2	2.90	0.49
2:B:290:TRP:CE3	2:B:325:LEU:HD22	2.48	0.49
2:B:59:TYR:HB3	2:B:63:VAL:HG23	1.95	0.49
2:D:152:VAL:HG12	2:D:212:HIS:CD2	2.48	0.49
2:B:59:TYR:OH	2:B:69:ILE:HG22	2.13	0.49
2:B:421:ASN:ND2	2:B:439:SER:CB	2.76	0.49
2:D:291:PHE:HA	2:D:301:VAL:HG22	1.95	0.49
2:B:400:ILE:HG12	2:B:401:TYR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:339:LYS:HG2	2:D:340:CYS:N	2.27	0.48
2:D:152:VAL:HG12	2:D:212:HIS:HD2	1.78	0.48
1:A:83:ILE:HG13	1:A:106:ILE:HD11	1.95	0.48
1:A:188:ARG:HB3	1:A:188:ARG:NH1	2.26	0.48
2:D:235:LYS:HB2	2:D:236:PRO:HD3	1.94	0.48
1:C:192:TYR:HB2	1:C:209:PHE:CE1	2.48	0.48
2:B:281:GLU:HG2	2:B:319:LEU:HD13	1.94	0.48
2:B:400:ILE:HG12	2:B:401:TYR:N	2.28	0.48
2:D:291:PHE:CE1	2:D:300:GLU:HA	2.49	0.48
2:D:463:LEU:HD13	2:D:468:THR:HG22	1.95	0.48
2:B:36:TRP:NE1	2:B:80:LEU:HB2	2.29	0.48
2:B:47:TRP:HZ2	2:B:50:TYR:CB	2.26	0.48
2:B:244:ALA:C	2:B:246:ASN:H	2.21	0.48
2:D:332:TRP:HH2	2:D:355:ILE:HG13	1.78	0.48
1:A:150:ILE:HG22	1:A:151:ASP:N	2.28	0.48
1:C:61:ARG:NH1	1:C:79:GLN:HG3	2.28	0.48
2:B:139:THR:HB	2:B:192:THR:HG23	1.96	0.47
1:A:161:ASN:HB3	1:A:175:MET:HE3	1.96	0.47
1:C:3:VAL:C	1:C:4:LEU:HD22	2.40	0.47
1:C:27:GLN:HG2	1:C:28:ASN:H	1.78	0.47
2:D:52(A):ASN:HA	2:D:71:ARG:NH1	2.29	0.47
2:D:303:THR:O	2:D:305:GLN:N	2.47	0.47
1:C:150:ILE:HD12	1:C:192:TYR:CE1	2.50	0.47
2:D:93:ALA:HB3	2:D:100(K):MET:HG2	1.97	0.47
2:D:310:ARG:HG3	2:D:321:VAL:HG23	1.96	0.47
2:B:146:GLY:C	2:B:184:LEU:HD12	2.40	0.47
2:B:451:ARG:HD3	2:B:451:ARG:C	2.39	0.47
1:C:78:LEU:C	1:C:79:GLN:HG2	2.39	0.47
1:C:117:ILE:HG13	1:C:118:PHE:N	2.30	0.47
2:D:459:VAL:HA	2:D:466:HIS:O	2.14	0.47
2:D:154:LEU:HD23	2:D:187:LEU:HD21	1.97	0.47
2:D:38:ARG:HD3	2:D:90:TYR:CE1	2.50	0.47
2:D:279:VAL:HG23	2:D:319:LEU:HB3	1.97	0.47
2:D:290:TRP:CD1	2:D:306:THR:HG21	2.50	0.47
1:C:188:ARG:NH1	1:C:189:HIS:NE2	2.63	0.46
2:D:59:TYR:OH	2:D:68:THR:HA	2.15	0.46
2:D:140:LEU:HD13	2:D:223:ILE:HG21	1.97	0.46
2:D:419:TYR:HB3	2:D:441:LEU:HD13	1.98	0.46
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.50	0.46
1:A:79:GLN:HB3	1:A:81:GLU:OE2	2.15	0.46
2:D:270:PRO:O	2:D:271:ILE:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:PRO:HA	2:B:277:VAL:O	2.16	0.46
1:C:71:PHE:CD1	1:C:71:PHE:N	2.84	0.46
2:D:38:ARG:HB3	2:D:90:TYR:CD1	2.51	0.46
1:A:31:VAL:O	1:A:31:VAL:HG22	2.15	0.46
2:B:38:ARG:HB3	2:B:90:TYR:CE2	2.51	0.46
2:B:314:ASN:OD1	2:B:317:SER:N	2.49	0.46
2:B:398:GLU:HG2	2:B:435:TYR:CZ	2.51	0.46
2:D:263:VAL:O	2:D:329:HIS:HD2	1.98	0.46
1:A:38:GLN:C	1:A:84:ALA:HB1	2.41	0.46
2:D:314:ASN:O	2:D:317:SER:HB2	2.15	0.46
1:C:161:ASN:HA	1:C:176:SER:O	2.15	0.46
1:A:30:ASN:ND2	1:A:92:GLN:OE1	2.47	0.46
1:A:46:LEU:HD23	1:A:47:LEU:N	2.31	0.46
2:D:191:VAL:O	2:D:191:VAL:HG13	2.16	0.46
1:A:159:VAL:HG12	1:A:160:LEU:H	1.81	0.45
1:A:149:LYS:HA	1:A:154:GLU:O	2.16	0.45
2:B:173:THR:HG23	2:B:187:LEU:HD21	1.97	0.45
2:B:392:VAL:HG12	2:B:395:PHE:CE1	2.52	0.45
1:C:17:ASP:O	1:C:78:LEU:HD23	2.16	0.45
1:C:136:LEU:HD23	1:C:144:ILE:HD11	1.97	0.45
2:D:171:VAL:HG22	2:D:172:HIS:N	2.31	0.45
2:B:344:ASN:HD21	2:B:347:LEU:HD13	1.80	0.45
2:B:424:PRO:HA	2:B:437:MET:HB3	1.97	0.45
2:D:51:ILE:O	2:D:51:ILE:HG23	2.17	0.45
2:D:374:PRO:HD3	2:D:388:LEU:CD1	2.47	0.45
1:A:115:VAL:HA	1:A:135:PHE:O	2.17	0.45
2:B:328:GLN:O	2:B:329:HIS:C	2.60	0.45
2:D:407:THR:CG2	2:D:455:SER:HB2	2.47	0.45
1:A:4:LEU:HD21	1:A:90:GLN:HB3	1.98	0.45
1:C:150:ILE:HG22	1:C:151:ASP:N	2.32	0.45
1:A:12:SER:HB3	1:A:105:GLU:CD	2.42	0.45
2:D:328:GLN:O	2:D:331:ASP:HB2	2.16	0.45
2:D:367:PRO:HD3	2:D:460:HIS:CD2	2.34	0.45
2:B:150:GLU:OE1	2:B:151:PRO:HA	2.17	0.45
1:C:22:THR:HG22	1:C:23:CYS:N	2.30	0.45
1:C:78:LEU:HA	1:C:78:LEU:HD13	1.84	0.45
2:D:426:LEU:HD12	2:D:435:TYR:CZ	2.52	0.45
1:A:46:LEU:HD12	2:B:101:ASP:HA	1.98	0.44
1:C:37:GLN:HE22	1:C:39:LYS:HE3	1.81	0.44
2:D:239:PRO:O	2:D:241:LYS:N	2.51	0.44
1:C:136:LEU:N	1:C:136:LEU:CD1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:LYS:HE3	2:D:360:LYS:HA	1.99	0.44
2:D:392:VAL:HB	2:D:437:MET:HG3	1.99	0.44
2:B:4:LEU:HB2	2:B:104:GLY:CA	2.48	0.44
2:B:154:LEU:HD23	2:B:156:THR:N	2.32	0.44
1:C:78:LEU:O	1:C:79:GLN:HG2	2.17	0.44
1:A:170:ASP:O	1:A:171:SER:HB2	2.18	0.44
2:B:42:GLU:O	2:B:43:LYS:HB2	2.17	0.44
2:D:299:VAL:HG23	2:D:301:VAL:HG13	1.97	0.44
2:D:372:LEU:N	2:D:372:LEU:HD12	2.33	0.44
1:A:4:LEU:HD12	1:A:88:CYS:SG	2.58	0.44
1:A:49:TYR:O	1:A:50:LYS:C	2.61	0.44
2:B:20:LEU:HD11	2:B:82:MET:SD	2.58	0.44
2:B:35:TYR:HE1	2:B:50:TYR:CD1	2.34	0.44
2:B:333:MET:C	2:B:335:GLY:H	2.26	0.44
1:A:29:ILE:HD11	1:A:71:PHE:CE1	2.52	0.44
1:A:34:SER:HA	1:A:48:ILE:O	2.18	0.44
1:A:163:TRP:N	1:A:163:TRP:CE3	2.86	0.44
2:B:425:VAL:HG21	2:D:422:THR:HA	1.99	0.44
1:C:164:THR:HG22	1:C:165:ASP:O	2.18	0.44
2:D:387:THR:HG22	2:D:440:LYS:HG3	1.99	0.44
1:C:43:ILE:HD13	1:C:43:ILE:H	1.81	0.44
1:A:136:LEU:N	1:A:136:LEU:HD22	2.32	0.44
2:D:67:PHE:N	2:D:67:PHE:HD1	2.14	0.44
2:D:85:GLU:C	2:D:87:THR:H	2.26	0.44
2:D:322:VAL:HG23	2:D:322:VAL:O	2.18	0.44
2:B:162:ASN:HD22	2:B:162:ASN:HA	1.62	0.43
2:B:421:ASN:HD22	2:B:439:SER:HA	1.83	0.43
2:D:72:ASP:OD1	2:D:75:LYS:HB2	2.18	0.43
2:D:82(C):LEU:HB3	2:D:111:VAL:HG21	2.00	0.43
2:B:13:GLN:HA	2:B:112:SER:O	2.18	0.43
2:B:93:ALA:HB1	2:B:100(K):MET:HB3	2.00	0.43
2:D:29:PHE:HE1	2:D:34:MET:HE2	1.83	0.43
2:D:167:SER:O	2:D:171:VAL:HG12	2.18	0.43
2:D:340:CYS:O	2:D:352:GLU:HA	2.19	0.43
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.99	0.43
2:B:47:TRP:CZ2	2:B:50:TYR:HB3	2.46	0.43
2:D:1:GLU:HG2	2:D:2:VAL:H	1.83	0.43
2:D:154:LEU:HD13	2:D:210:VAL:CG2	2.47	0.43
1:A:16:GLY:CA	1:A:77:SER:HA	2.46	0.43
1:A:28:ASN:OD1	1:A:68:GLY:HA2	2.18	0.43
1:A:89:GLN:O	1:A:89:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:SER:HA	2:B:270:PRO:HD2	1.89	0.43
2:B:365:ARG:HB2	2:B:395:PHE:HA	2.01	0.43
2:B:240:CYS:C	2:B:242:CYS:H	2.27	0.43
2:B:310:ARG:CG	2:B:321:VAL:HG22	2.48	0.43
2:D:100(I):TYR:N	2:D:100(I):TYR:CD1	2.87	0.43
2:B:95:HIS:NE2	2:B:100(I):TYR:N	2.66	0.43
2:B:436:PHE:O	2:B:437:MET:HB3	2.19	0.43
1:C:6:GLN:HE22	1:C:21:ILE:HD11	1.84	0.43
1:C:188:ARG:O	1:C:188:ARG:HG3	2.19	0.43
2:D:419:TYR:HB3	2:D:441:LEU:CD1	2.49	0.43
2:D:136:SER:CA	2:D:195:SER:HB3	2.34	0.43
2:B:154:LEU:HD23	2:B:154:LEU:C	2.44	0.43
1:C:36:TYR:OH	1:C:89:GLN:NE2	2.52	0.43
1:A:33:LEU:HD23	1:A:35:TRP:NE1	2.34	0.42
2:B:194:THR:O	2:B:195:SER:HB3	2.19	0.42
2:D:251:PRO:HA	2:D:277:VAL:O	2.19	0.42
2:D:78:LEU:HD23	2:D:92:CYS:HB2	2.00	0.42
2:D:388:LEU:HD23	2:D:441:LEU:HD23	2.00	0.42
2:D:66:ARG:C	2:D:67:PHE:HD1	2.27	0.42
1:C:80:PRO:C	1:C:82:ASP:H	2.26	0.42
2:D:12:VAL:HG23	2:D:111:VAL:HG22	2.01	0.42
2:D:163:SER:H	2:D:209:ASN:HD21	1.65	0.42
2:D:199:TRP:HB3	2:D:200:PRO:HD3	2.01	0.42
2:B:103:TRP:CD1	2:B:103:TRP:N	2.88	0.42
1:C:11:LEU:HD22	1:C:11:LEU:HA	1.82	0.42
1:C:82:ASP:O	1:C:104:LEU:HD23	2.20	0.42
2:D:138:VAL:HG22	2:D:138:VAL:O	2.18	0.42
1:A:18:THR:HG23	1:A:76:SER:HA	2.02	0.42
2:D:153:THR:O	2:D:210:VAL:HA	2.19	0.42
2:D:238:PRO:HB3	2:D:239:PRO:HD2	2.01	0.42
2:B:68:THR:HB	2:B:81:GLN:CB	2.49	0.42
2:D:252:SER:O	2:D:276:VAL:HA	2.19	0.42
2:D:401:TYR:HB3	2:D:459:VAL:HG22	2.01	0.42
2:D:259:LYS:N	2:D:259:LYS:HD2	2.34	0.42
2:D:260:ILE:H	2:D:260:ILE:CD1	2.17	0.42
1:A:118:PHE:CD2	2:B:124:LEU:HB3	2.55	0.42
1:A:144:ILE:HG13	1:A:197:THR:O	2.20	0.42
2:B:87:THR:OG1	2:B:111:VAL:HG22	2.20	0.42
1:A:135:PHE:CE1	1:A:176:SER:HB2	2.55	0.41
2:B:68:THR:HB	2:B:81:GLN:HB2	2.02	0.41
2:B:231:THR:O	2:B:232:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:SER:HB2	2:B:277:VAL:CG2	2.48	0.41
2:D:154:LEU:HD21	2:D:189:SER:HB2	2.03	0.41
2:D:195:SER:O	2:D:196:SER:C	2.63	0.41
2:D:198:THR:HB	2:D:202:SER:OG	2.20	0.41
2:D:386:VAL:CG2	2:D:443:VAL:HG23	2.50	0.41
2:B:421:ASN:ND2	2:B:439:SER:HB2	2.35	0.41
1:C:67:SER:HA	1:C:71:PHE:CE2	2.55	0.41
2:D:127:VAL:HG23	2:D:129:GLY:O	2.20	0.41
1:A:163:TRP:HE3	1:A:163:TRP:H	1.69	0.41
2:B:244:ALA:C	2:B:246:ASN:N	2.79	0.41
2:B:272:VAL:HG12	2:B:290:TRP:HH2	1.85	0.41
2:B:401:TYR:CD1	2:B:401:TYR:C	2.97	0.41
2:D:139:THR:HA	2:D:192:THR:HA	2.02	0.41
1:A:98:PHE:CD1	1:A:98:PHE:N	2.87	0.41
2:B:286:VAL:CG2	2:B:321:VAL:HG21	2.50	0.41
2:B:452:ASN:HD22	2:B:453:SER:H	1.67	0.41
2:D:154:LEU:CD2	2:D:189:SER:HB2	2.51	0.41
2:B:14:PRO:HD3	2:B:112:SER:C	2.45	0.41
2:B:327:ILE:CG2	2:B:328:GLN:N	2.82	0.41
2:D:36:TRP:CD1	2:D:69:ILE:HD12	2.50	0.41
2:D:408:ASN:O	2:D:414:LYS:HG2	2.20	0.41
2:B:150:GLU:HA	2:B:151:PRO:HA	1.86	0.41
2:B:400:ILE:CG1	2:B:401:TYR:H	2.33	0.41
2:D:75:LYS:O	2:D:76:ASN:HB2	2.20	0.41
1:A:117:ILE:HD12	1:A:194:CYS:HB2	2.02	0.41
2:B:94:ARG:NH2	2:B:101:ASP:OD2	2.54	0.41
2:B:122:TYR:HA	2:B:123:PRO:HD2	1.87	0.41
2:B:374:PRO:HD2	2:B:448:TRP:CZ2	2.54	0.41
2:D:287:GLN:HB3	2:D:343:ASN:HB3	2.03	0.41
1:A:49:TYR:N	1:A:49:TYR:CD1	2.89	0.41
1:A:122:SER:HA	1:A:125:LEU:HD12	2.03	0.41
2:B:394:ASP:HA	2:B:434:SER:OG	2.21	0.41
2:D:310:ARG:HB3	2:D:319:LEU:HD21	2.02	0.41
4:F:6:GAL:H2	4:F:6:GAL:H61	2.03	0.41
1:A:18:THR:HA	1:A:75:ILE:O	2.21	0.41
1:A:39:LYS:CG	1:A:84:ALA:HB2	2.51	0.41
2:B:31:ASP:HA	2:B:52(A):ASN:OD1	2.21	0.41
2:B:260:ILE:HD12	2:B:260:ILE:HA	1.81	0.41
2:B:288:ILE:HD12	2:B:323:SER:HB2	2.02	0.41
2:B:400:ILE:CG1	2:B:401:TYR:N	2.84	0.41
1:C:80:PRO:C	1:C:82:ASP:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:H	1:C:166:GLN:CD	2.28	0.41
2:D:195:SER:O	2:D:198:THR:N	2.54	0.41
2:D:264:LEU:O	2:D:466:HIS:HD2	2.03	0.41
2:D:320:ARG:O	2:D:320:ARG:HG3	2.21	0.41
2:D:325:LEU:HA	2:D:326:PRO:HD2	1.96	0.41
2:B:66:ARG:HH21	2:B:86:ASP:CG	2.29	0.41
2:B:344:ASN:ND2	2:B:347:LEU:HD13	2.36	0.41
2:B:379:GLU:O	2:B:379:GLU:HG2	2.21	0.41
2:D:269:SER:HA	2:D:270:PRO:HD3	1.81	0.41
2:D:392:VAL:O	2:D:436:PHE:HA	2.20	0.41
2:D:467:HIS:CD2	2:D:467:HIS:C	2.98	0.41
2:B:14:PRO:C	2:B:16:GLY:H	2.29	0.40
2:B:199:TRP:O	2:B:200:PRO:C	2.63	0.40
2:B:303:THR:C	2:B:305:GLN:H	2.28	0.40
2:B:451:ARG:HD3	2:B:452:ASN:N	2.36	0.40
1:C:180:THR:HG21	2:D:145:LYS:HE3	2.02	0.40
2:D:1:GLU:HG2	2:D:2:VAL:N	2.35	0.40
2:D:174:PHE:HD2	2:D:188:SER:O	2.03	0.40
2:D:176:ALA:CB	2:D:187:LEU:HB2	2.51	0.40
2:D:400:ILE:CG1	2:D:401:TYR:N	2.84	0.40
2:D:400:ILE:CG1	2:D:401:TYR:H	2.33	0.40
2:B:59:TYR:CE1	2:B:69:ILE:HG22	2.56	0.40
2:D:199:TRP:CD1	2:D:199:TRP:C	2.99	0.40
2:D:422:THR:OG1	2:D:438:TYR:O	2.39	0.40
1:A:185:GLU:HA	1:A:188:ARG:HG3	2.03	0.40
2:D:87:THR:HG23	2:D:109:VAL:O	2.21	0.40
2:B:35:TYR:CE1	2:B:50:TYR:HB2	2.56	0.40
2:B:90:TYR:O	2:B:106:GLY:HA2	2.22	0.40
2:B:291:PHE:CD1	2:B:300:GLU:HA	2.56	0.40
2:B:464:HIS:O	2:B:465:ASN:HB2	2.21	0.40
1:C:14:SER:O	1:C:15:LEU:C	2.65	0.40
2:D:66:ARG:HD2	2:D:82(B):ARG:CB	2.50	0.40
2:B:327:ILE:HG22	2:B:328:GLN:H	1.84	0.40
1:C:85:THR:HA	1:C:102:THR:O	2.22	0.40
2:D:16:GLY:O	2:D:82(C):LEU:HD12	2.22	0.40
2:D:237:CYS:HA	2:D:238:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	179 (84%)	24 (11%)	9 (4%)	2	7
1	C	212/214 (99%)	186 (88%)	22 (10%)	4 (2%)	6	22
2	B	442/444 (100%)	365 (83%)	63 (14%)	14 (3%)	3	11
2	D	442/444 (100%)	365 (83%)	56 (13%)	21 (5%)	2	6
All	All	1308/1316 (99%)	1095 (84%)	165 (13%)	48 (4%)	2	9

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
1	A	150	ILE
2	B	130	ASP
2	B	317	SER
1	C	138	ASN
1	C	150	ILE
2	D	130	ASP
2	D	284	PRO
2	D	304	ALA
2	D	317	SER
2	D	464	HIS
1	A	138	ASN
2	B	196	SER
2	B	238	PRO
2	B	303	THR
2	D	236	PRO
2	D	240	CYS
2	D	302	HIS
1	A	30	ASN
1	A	199	LYS
2	B	445	LYS
1	C	199	LYS

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Mol	Chain	Res	Type
2	D	196	SER
2	D	235	LYS
2	D	445	LYS
1	A	40	PRO
1	A	80	PRO
2	B	9	GLY
2	B	451	ARG
1	C	76	SER
2	D	26	GLY
2	D	313	TYR
2	B	180	SER
2	B	242	CYS
2	D	243	PRO
2	B	237	CYS
2	D	175	PRO
2	D	232	ILE
2	D	451	ARG
1	A	31	VAL
2	D	260	ILE
1	A	83	ILE
2	D	151	PRO
2	D	213	PRO
2	B	135	GLY
2	B	213	PRO
2	D	135	GLY
2	B	151	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	190/190 (100%)	164 (86%)	26 (14%)	3	13
1	C	190/190 (100%)	172 (90%)	18 (10%)	8	26
2	B	399/399 (100%)	363 (91%)	36 (9%)	9	28
2	D	399/399 (100%)	364 (91%)	35 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1178/1178 (100%)	1063 (90%)	115 (10%)	7 25

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	22	THR
1	A	23	CYS
1	A	26	SER
1	A	40	PRO
1	A	46	LEU
1	A	47	LEU
1	A	49	TYR
1	A	50	LYS
1	A	63	SER
1	A	73	LEU
1	A	74	THR
1	A	80	PRO
1	A	81	GLU
1	A	89	GLN
1	A	92	GLN
1	A	102	THR
1	A	114	THR
1	A	117	ILE
1	A	136	LEU
1	A	159	VAL
1	A	163	TRP
1	A	176	SER
1	A	179	LEU
1	A	185	GLU
1	A	202	THR
2	B	6	GLU
2	B	81	GLN
2	B	109	VAL
2	B	113	SER
2	B	115	LYS
2	B	139	THR
2	B	156	THR
2	B	162	ASN
2	B	187	LEU
2	B	203	GLN
2	B	232	ILE

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Mol	Chain	Res	Type
2	B	237	CYS
2	B	255	ILE
2	B	271	ILE
2	B	283	ASP
2	B	289	SER
2	B	295	ASN
2	B	309	HIS
2	B	317	SER
2	B	328	GLN
2	B	342	VAL
2	B	347	LEU
2	B	355	ILE
2	B	357	SER
2	B	365	ARG
2	B	369	VAL
2	B	370	TYR
2	B	373	PRO
2	B	381	MET
2	B	402	VAL
2	B	417	LEU
2	B	428	SER
2	B	440	LYS
2	B	444	GLU
2	B	451	ARG
2	B	453	SER
1	C	3	VAL
1	C	11	LEU
1	C	14	SER
1	C	21	ILE
1	C	22	THR
1	C	28	ASN
1	C	37	GLN
1	C	43	ILE
1	C	79	GLN
1	C	89	GLN
1	C	98	PHE
1	C	116	SER
1	C	154	GLU
1	C	156	GLN
1	C	161	ASN
1	C	205	ILE
1	C	212	ASN

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Mol	Chain	Res	Type
1	C	213	GLU
2	D	2	VAL
2	D	12	VAL
2	D	14	PRO
2	D	18	LEU
2	D	37	VAL
2	D	56	SER
2	D	62	THR
2	D	77	THR
2	D	105	GLN
2	D	113	SER
2	D	117	THR
2	D	143	LEU
2	D	175	PRO
2	D	178	LEU
2	D	187	LEU
2	D	192	THR
2	D	217	THR
2	D	260	ILE
2	D	271	ILE
2	D	307	GLN
2	D	312	ASP
2	D	331	ASP
2	D	360	LYS
2	D	363	SER
2	D	364	VAL
2	D	385	GLN
2	D	387	THR
2	D	388	LEU
2	D	402	VAL
2	D	422	THR
2	D	425	VAL
2	D	452	ASN
2	D	457	SER
2	D	458	VAL
2	D	459	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	38	GLN
1	A	89	GLN
1	A	92	GLN
1	A	124	GLN
1	A	137	ASN
1	A	210	ASN
2	B	39	GLN
2	B	162	ASN
2	B	179	GLN
2	B	203	GLN
2	B	209	ASN
2	B	295	ASN
2	B	328	GLN
2	B	330	GLN
2	B	421	ASN
2	B	465	ASN
1	C	6	GLN
1	C	37	GLN
1	C	89	GLN
1	C	92	GLN
1	C	138	ASN
1	C	190	ASN
1	C	198	HIS
1	C	210	ASN
2	D	52(A)	ASN
2	D	209	ASN
2	D	307	GLN
2	D	343	ASN
2	D	368	GLN
2	D	385	GLN
2	D	460	HIS
2	D	465	ASN
2	D	466	HIS

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 ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	E	1	3,2	14,14,15	0.92	1 (7%)	17,19,21	1.58	3 (17%)
3	NAG	E	2	3	14,14,15	0.70	0	17,19,21	1.12	2 (11%)
3	BMA	E	3	3	11,11,12	0.47	0	15,15,17	0.76	0
3	MAN	E	4	3	11,11,12	0.59	0	15,15,17	0.51	0
3	NAG	E	5	3	14,14,15	0.50	0	17,19,21	0.50	0
3	GAL	E	6	3	11,11,12	0.57	0	15,15,17	0.58	0
3	MAN	E	7	3	11,11,12	0.37	0	15,15,17	0.53	0
3	NAG	E	8	3	14,14,15	0.47	0	17,19,21	0.57	0
3	FUL	E	9	3	10,10,11	0.53	0	14,14,16	0.45	0
4	NAG	F	1	2,4	14,14,15	0.84	1 (7%)	17,19,21	0.62	0
4	NAG	F	2	4	14,14,15	0.88	0	17,19,21	0.92	2 (11%)
4	BMA	F	3	4	11,11,12	0.51	0	15,15,17	0.56	0
4	MAN	F	4	4	11,11,12	0.66	0	15,15,17	0.66	0
4	NAG	F	5	4	14,14,15	0.63	0	17,19,21	0.76	1 (5%)
4	GAL	F	6	4	11,11,12	0.54	0	15,15,17	0.74	1 (6%)
4	MAN	F	7	4	11,11,12	0.47	0	15,15,17	0.50	0
4	NAG	F	8	4	14,14,15	0.50	0	17,19,21	0.62	0
4	FUC	F	9	4	10,10,11	0.43	0	14,14,16	0.45	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
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	1/1/7/7	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	E	6	3	-	2/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
3	NAG	E	8	3	-	2/6/23/26	0/1/1/1
3	FUL	E	9	3	-	-	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	1/1/7/7	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	NAG	F	5	4	-	2/6/23/26	0/1/1/1
4	GAL	F	6	4	-	2/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
4	NAG	F	8	4	-	1/6/23/26	0/1/1/1
4	FUC	F	9	4	1/1/5/5	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	2.55	1.55	1.52
4	F	1	NAG	C1-C2	2.08	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C4-C3-C2	-4.16	104.93	111.02
3	E	2	NAG	C3-C4-C5	-3.04	104.73	110.23
3	E	1	NAG	C2-N2-C7	-2.67	119.32	122.90
3	E	1	NAG	C3-C4-C5	-2.37	105.94	110.23
3	E	2	NAG	C1-O5-C5	2.32	115.29	112.19
4	F	2	NAG	O5-C1-C2	2.28	114.82	111.29
4	F	2	NAG	C1-O5-C5	2.25	115.20	112.19
4	F	6	GAL	C1-O5-C5	2.15	115.07	112.19
4	F	5	NAG	C2-N2-C7	-2.05	120.16	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	NAG	C1
4	F	2	NAG	C1
4	F	9	FUC	C1

All (14) torsion outliers are listed below:

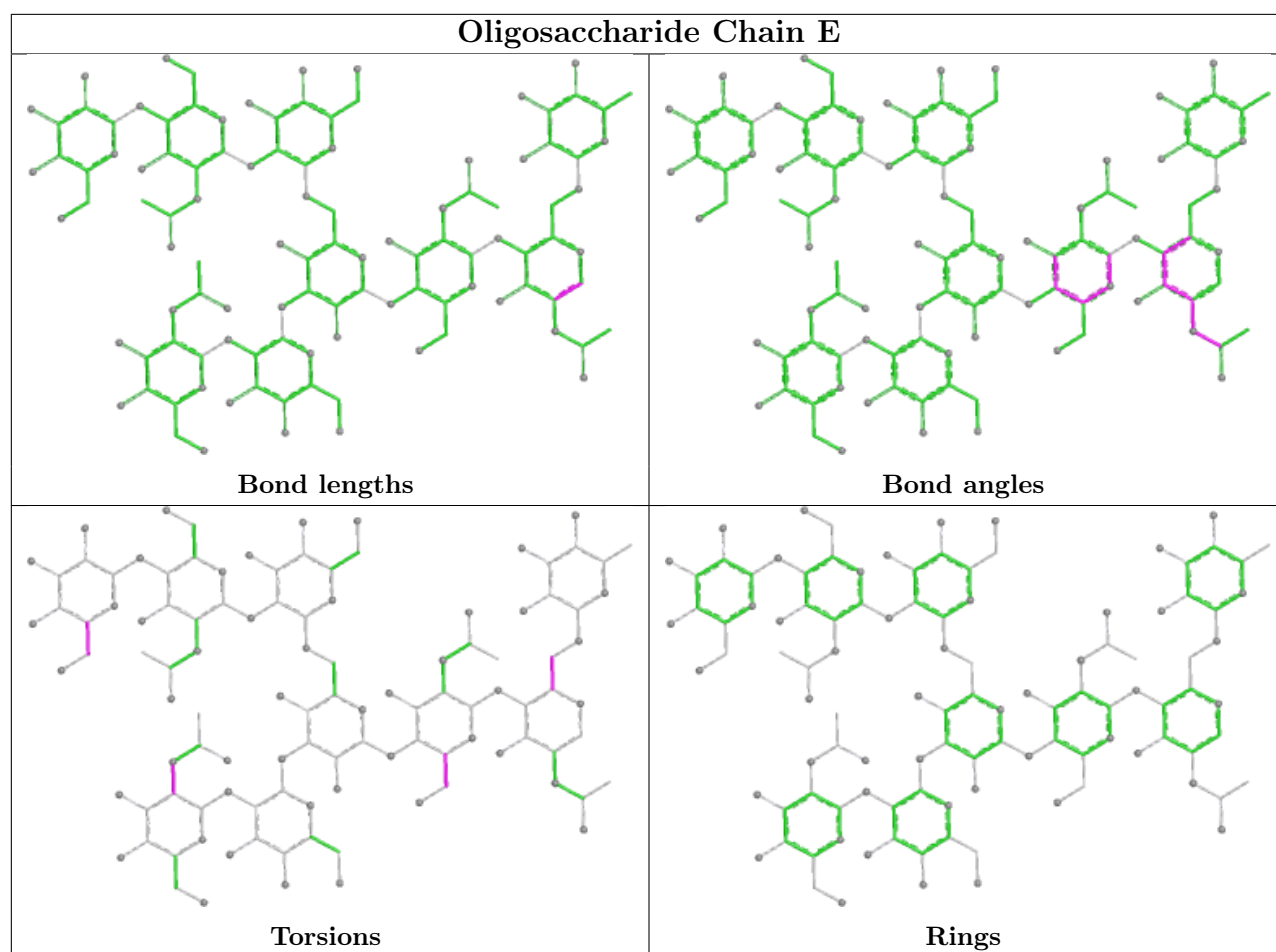
Mol	Chain	Res	Type	Atoms
4	F	8	NAG	C1-C2-N2-C7
4	F	6	GAL	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	6	GAL	O5-C5-C6-O6
4	F	6	GAL	C4-C5-C6-O6
3	E	6	GAL	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	F	5	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	8	NAG	C3-C2-N2-C7
3	E	8	NAG	C1-C2-N2-C7
4	F	5	NAG	C1-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6

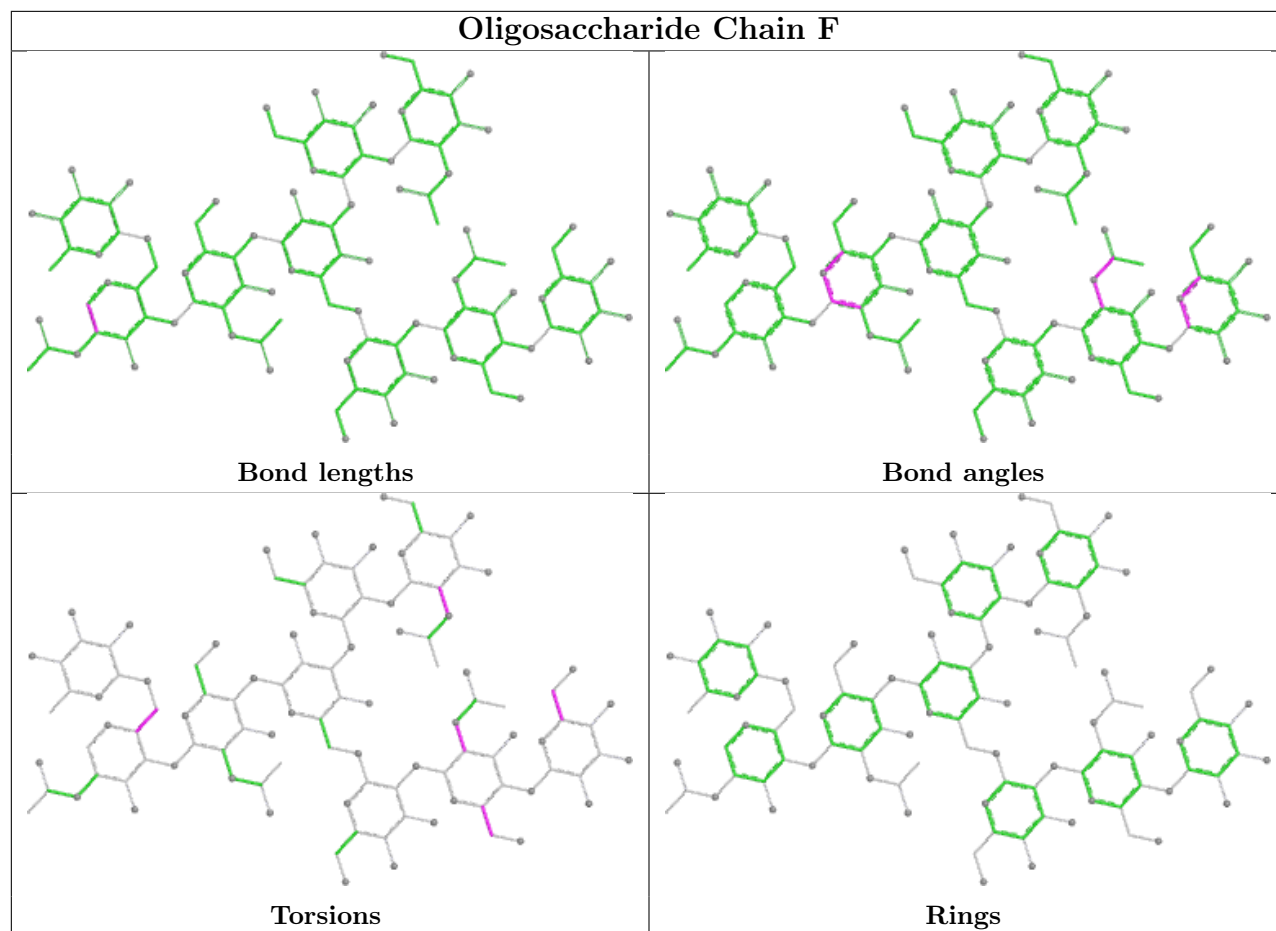
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	GAL	3	0
3	E	6	GAL	3	0
3	E	1	NAG	3	0
3	E	2	NAG	2	0

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.