



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:26 PM UTC

PDB ID : 1IGY / pdb_00001igy
Title : STRUCTURE OF IMMUNOGLOBULIN
Authors : Harris, L.J.; McPherson, A.
Deposited on : 1997-10-09
Resolution : 3.20 Å(reported)

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

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

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

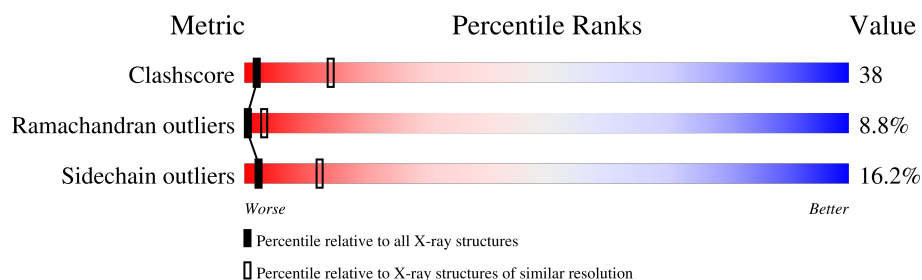
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	213	
1	C	213	
2	B	434	
2	D	434	
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
4	FUC	F	9	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12750 atoms, of which 2498 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 IGG1 INTACT ANTIBODY MAB61.1.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	0	0	0
			2043	1025	393	277	339	9			
1	C	213	Total	C	H	N	O	S	0	0	0
			2043	1025	393	277	339	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	VAL	GLN	conflict	GB 309359
A	?	-	PRO	deletion	GB 309359
C	7	VAL	GLN	conflict	GB 309359
C	?	-	PRO	deletion	GB 309359

- Molecule 2 is a protein called IGG1 INTACT ANTIBODY MAB61.1.3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	434	Total	C	H	N	O	S	33	0	0
			4119	2128	753	565	655	18			
2	D	434	Total	C	H	N	O	S	0	0	0
			4119	2128	753	565	655	18			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LYS	GLN	conflict	GB 194362
B	6	GLU	GLN	conflict	GB 194362
B	9	ALA	PRO	conflict	GB 194362
B	12	ALA	GLU	conflict	GB 194362
B	13	ARG	LYS	conflict	GB 194362
B	20	MET	ILE	conflict	GB 194362
B	27	TYR	PHE	conflict	GB 194362
B	28	THR	SER	conflict	GB 194362

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	PHE	LEU	conflict	GB 194362
B	30	THR	PRO	conflict	GB 194362
B	31	THR	GLY	conflict	GB 194362
B	32	TYR	HIS	conflict	GB 194362
B	33	THR	ASN	conflict	GB 194362
B	35	HIS	ASN	conflict	GB 194362
B	38	LYS	VAL	conflict	GB 194362
B	41	PRO	ASN	conflict	GB 194362
B	43	GLN	LYS	conflict	GB 194362
B	44	GLY	SER	conflict	GB 194362
B	50	TYR	ASN	conflict	GB 194362
B	52	ASN	ASP	conflict	GB 194362
B	53	SER	TYR	conflict	GB 194362
B	54	SER	TYR	conflict	GB 194362
B	55	VAL	GLY	conflict	GB 194362
B	56	TYR	GLY	conflict	GB 194362
B	59	TYR	PHE	conflict	GB 194362
B	61	GLN	PRO	conflict	GB 194362
B	62	ARG	LYS	conflict	GB 194362
B	65	ASP	GLY	conflict	GB 194362
B	71	ARG	VAL	conflict	GB 194362
B	73	ARG	LYS	conflict	GB 194362
B	76	ASN	SER	conflict	GB 194362
B	78	ALA	LEU	conflict	GB 194362
B	79	ASN	TYR	conflict	GB 194362
B	80	ILE	MET	conflict	GB 194362
B	82A	SER	THR	conflict	GB 194362
B	83	THR	GLN	conflict	GB 194362
B	85	ASP	GLU	conflict	GB 194362
B	?	-	ALA	deletion	GB 194362
B	?	-	ARG	deletion	GB 194362
B	93	VAL	ARG	conflict	GB 194362
B	95	GLU	ASP	conflict	GB 194362
B	?	-	ASN	deletion	GB 194362
B	?	-	TYR	deletion	GB 194362
B	97	GLU	GLY	conflict	GB 194362
B	98	VAL	PHE	conflict	GB 194362
B	101	PRO	THR	conflict	GB 194362
B	108	THR	LEU	conflict	GB 194362
B	113	SER	ALA	conflict	GB 194362
B	199	PRO	THR	conflict	GB 194362
B	200	ARG	TRP	conflict	GB 194362

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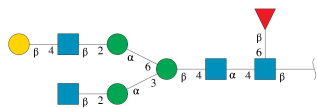
Chain	Residue	Modelled	Actual	Comment	Reference
B	263	THR	VAL	conflict	GB 194362
B	265	LEU	THR	conflict	GB 194362
B	268	VAL	LEU	conflict	GB 194362
B	296	ASN	ASP	conflict	GB 194362
B	321	VAL	SER	conflict	GB 194362
B	324	ALA	GLU	conflict	GB 194362
B	363	LYS	ARG	conflict	GB 194362
B	365	ARG	LYS	conflict	GB 194362
B	408	SER	TRP	conflict	GB 194362
B	410	ASP	ASN	conflict	GB 194362
B	415	ALA	PRO	conflict	GB 194362
B	416	PRO	ALA	conflict	GB 194362
B	427	ASP	ASN	conflict	GB 194362
B	430	ASP	ASN	conflict	GB 194362
D	3	LYS	GLN	conflict	GB 194362
D	6	GLU	GLN	conflict	GB 194362
D	9	ALA	PRO	conflict	GB 194362
D	12	ALA	GLU	conflict	GB 194362
D	13	ARG	LYS	conflict	GB 194362
D	20	MET	ILE	conflict	GB 194362
D	27	TYR	PHE	conflict	GB 194362
D	28	THR	SER	conflict	GB 194362
D	29	PHE	LEU	conflict	GB 194362
D	30	THR	PRO	conflict	GB 194362
D	31	THR	GLY	conflict	GB 194362
D	32	TYR	HIS	conflict	GB 194362
D	33	THR	ASN	conflict	GB 194362
D	35	HIS	ASN	conflict	GB 194362
D	38	LYS	VAL	conflict	GB 194362
D	41	PRO	ASN	conflict	GB 194362
D	43	GLN	LYS	conflict	GB 194362
D	44	GLY	SER	conflict	GB 194362
D	50	TYR	ASN	conflict	GB 194362
D	52	ASN	ASP	conflict	GB 194362
D	53	SER	TYR	conflict	GB 194362
D	54	SER	TYR	conflict	GB 194362
D	55	VAL	GLY	conflict	GB 194362
D	56	TYR	GLY	conflict	GB 194362
D	59	TYR	PHE	conflict	GB 194362
D	61	GLN	PRO	conflict	GB 194362
D	62	ARG	LYS	conflict	GB 194362
D	65	ASP	GLY	conflict	GB 194362

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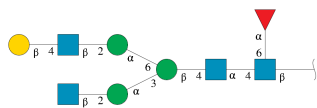
Chain	Residue	Modelled	Actual	Comment	Reference
D	71	ARG	VAL	conflict	GB 194362
D	73	ARG	LYS	conflict	GB 194362
D	76	ASN	SER	conflict	GB 194362
D	78	ALA	LEU	conflict	GB 194362
D	79	ASN	TYR	conflict	GB 194362
D	80	ILE	MET	conflict	GB 194362
D	82A	SER	THR	conflict	GB 194362
D	83	THR	GLN	conflict	GB 194362
D	85	ASP	GLU	conflict	GB 194362
D	?	-	ALA	deletion	GB 194362
D	?	-	ARG	deletion	GB 194362
D	93	VAL	ARG	conflict	GB 194362
D	95	GLU	ASP	conflict	GB 194362
D	?	-	ASN	deletion	GB 194362
D	?	-	TYR	deletion	GB 194362
D	97	GLU	GLY	conflict	GB 194362
D	98	VAL	PHE	conflict	GB 194362
D	101	PRO	THR	conflict	GB 194362
D	108	THR	LEU	conflict	GB 194362
D	113	SER	ALA	conflict	GB 194362
D	199	PRO	THR	conflict	GB 194362
D	200	ARG	TRP	conflict	GB 194362
D	263	THR	VAL	conflict	GB 194362
D	265	LEU	THR	conflict	GB 194362
D	268	VAL	LEU	conflict	GB 194362
D	296	ASN	ASP	conflict	GB 194362
D	321	VAL	SER	conflict	GB 194362
D	324	ALA	GLU	conflict	GB 194362
D	363	LYS	ARG	conflict	GB 194362
D	365	ARG	LYS	conflict	GB 194362
D	408	SER	TRP	conflict	GB 194362
D	410	ASP	ASN	conflict	GB 194362
D	415	ALA	PRO	conflict	GB 194362
D	416	PRO	ALA	conflict	GB 194362
D	427	ASP	ASN	conflict	GB 194362
D	430	ASP	ASN	conflict	GB 194362

- 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-alpha-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	49	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-alpha-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



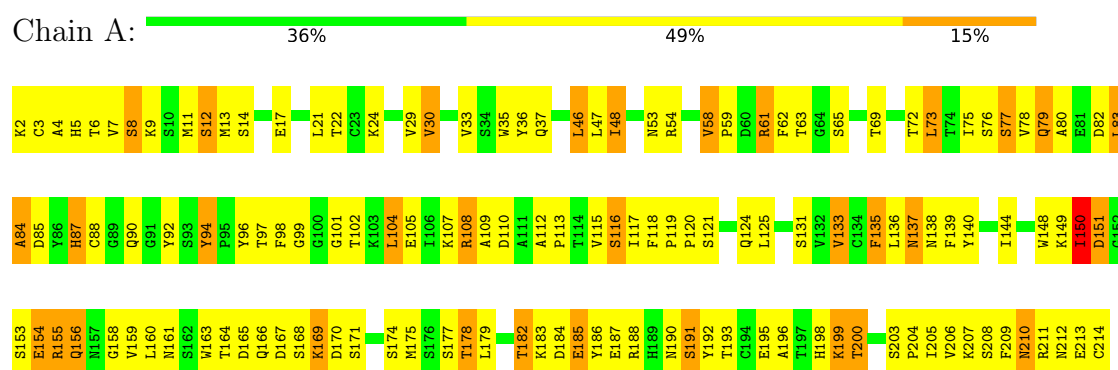
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	9	Total	C	H	N	O	28	0	0
			213	62	103	4	44			

3 Residue-property plots

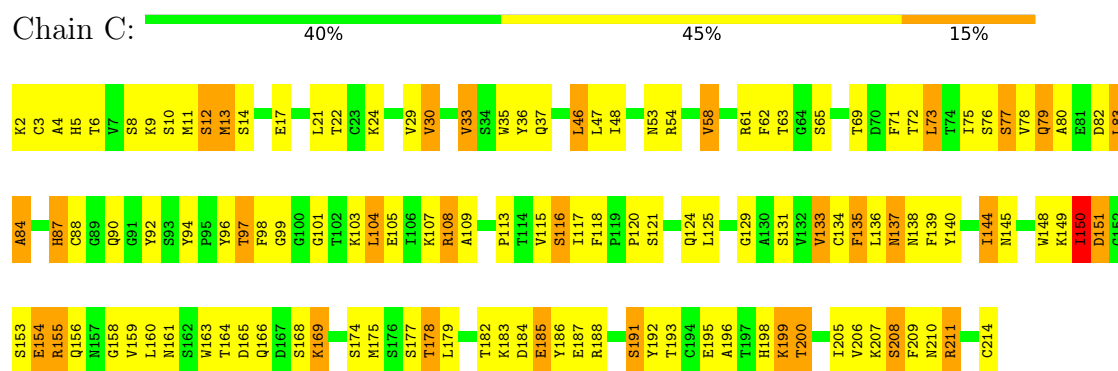
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

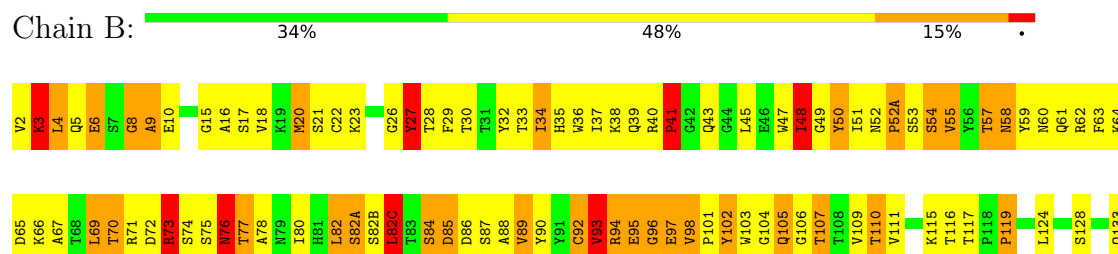
• Molecule 1: IGG1 INTACT ANTIBODY MAB61.1.3

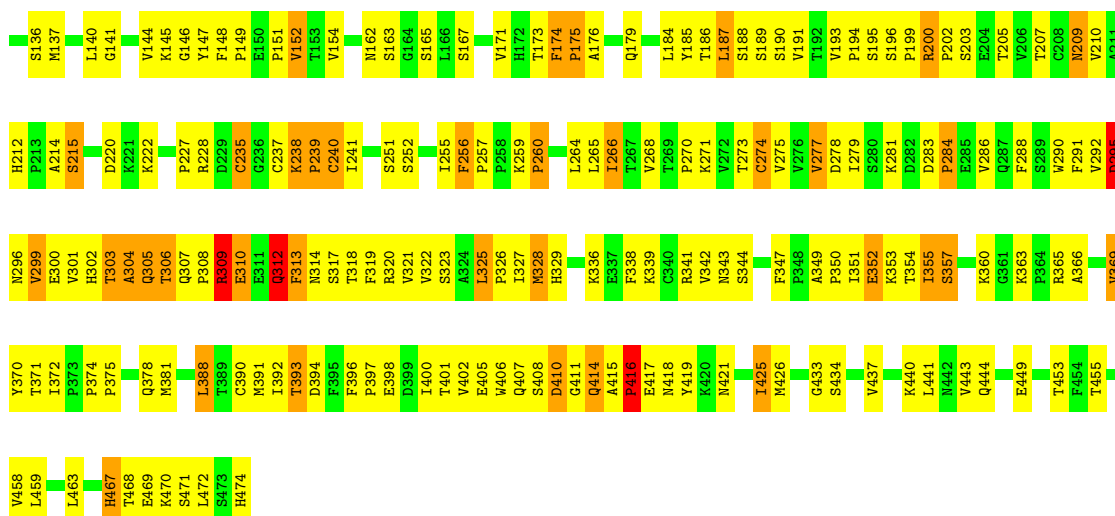


• Molecule 1: IGG1 INTACT ANTIBODY MAB61.1.3



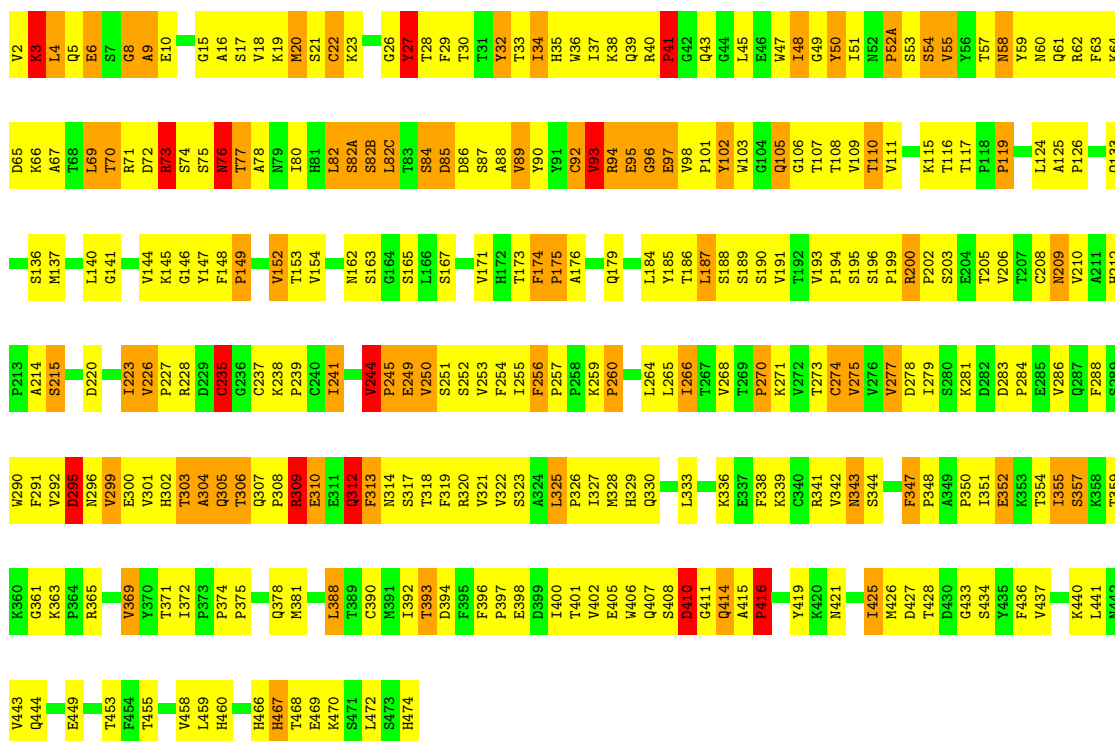
• Molecule 2: IGG1 INTACT ANTIBODY MAB61.1.3





• Molecule 2: IGG1 INTACT ANTIBODY MAB61.1.3

Chain D: 32% 48% 17%



• 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-alpha-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 56% 44%

MAG1	NDG2	BMA3	MAN4	NAG5	GAL6	MAN7	NAG8	FUL9
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- 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-alpha-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  56% 33% 11%

MAG1	NDG2	BMA3	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 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.65Å 190.66Å 73.10Å 90.00° 109.66° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	75.0 (20.00-3.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.211 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: GAL, FUC, NAG, NDG, BMA, FUL, 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	0.55	0/1687	1.07	9/2288 (0.4%)
1	C	0.57	0/1687	1.07	9/2288 (0.4%)
2	B	0.60	1/3458 (0.0%)	1.13	30/4723 (0.6%)
2	D	0.58	0/3458	1.15	31/4723 (0.7%)
All	All	0.58	1/10290 (0.0%)	1.12	79/14022 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	THR	CA-CB	7.86	1.59	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	96	GLY	N-CA-C	-17.23	95.15	113.58
2	B	96	GLY	N-CA-C	-17.03	95.36	113.58
2	B	256	PHE	CA-C-N	9.41	126.43	119.66
2	B	256	PHE	C-N-CA	9.41	126.43	119.66
1	C	58	VAL	CA-C-N	8.71	129.25	119.93
1	C	58	VAL	C-N-CA	8.71	129.25	119.93
2	D	256	PHE	CA-C-N	8.61	125.86	119.66
2	D	256	PHE	C-N-CA	8.61	125.86	119.66
2	B	3	LYS	N-CA-C	8.13	121.83	109.23
1	A	58	VAL	CA-C-N	8.11	128.12	119.76
1	A	58	VAL	C-N-CA	8.11	128.12	119.76
2	D	3	LYS	N-CA-C	8.11	121.80	109.23
1	A	80	ALA	N-CA-C	-7.32	103.00	112.23
1	C	80	ALA	N-CA-C	-7.27	103.07	112.23
1	A	110	ASP	N-CA-C	7.21	119.61	110.24
2	D	250	VAL	N-CA-C	6.95	123.79	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	205	THR	N-CA-C	6.61	119.09	110.43
2	D	402	VAL	N-CA-C	6.51	118.09	108.45
2	D	32	TYR	N-CA-C	6.47	120.05	109.24
2	D	266	ILE	N-CA-C	6.45	117.20	110.62
2	B	240	CYS	N-CA-C	6.39	119.56	110.68
2	B	32	TYR	N-CA-C	6.38	119.58	109.50
2	D	363	LYS	CA-C-N	6.37	126.75	119.93
2	D	363	LYS	C-N-CA	6.37	126.75	119.93
1	A	185	GLU	N-CA-C	-6.30	104.41	111.28
2	B	363	LYS	CA-C-N	6.17	126.53	119.93
2	B	363	LYS	C-N-CA	6.17	126.53	119.93
2	B	266	ILE	N-CA-C	6.09	116.83	110.62
2	B	402	VAL	N-CA-C	6.05	117.41	108.45
1	C	168	SER	N-CA-C	6.04	117.66	111.14
1	A	168	SER	N-CA-C	5.97	117.59	111.14
2	B	78	ALA	N-CA-C	-5.91	101.46	110.14
1	A	161	ASN	N-CA-C	5.81	119.15	107.41
1	C	161	ASN	N-CA-C	5.81	119.14	107.41
1	A	158	GLY	N-CA-C	-5.75	106.58	116.01
2	B	351	ILE	N-CA-C	5.73	117.43	109.80
2	D	174	PHE	N-CA-C	5.71	118.55	109.64
2	B	415	ALA	CA-C-N	5.60	126.84	119.84
2	B	415	ALA	C-N-CA	5.60	126.84	119.84
2	D	351	ILE	N-CA-C	5.55	117.18	109.80
2	D	244	VAL	CA-C-N	5.50	126.71	119.84
2	D	244	VAL	C-N-CA	5.50	126.71	119.84
1	C	158	GLY	N-CA-C	-5.47	107.04	116.01
2	D	415	ALA	CA-C-N	5.45	126.65	119.84
2	D	415	ALA	C-N-CA	5.45	126.65	119.84
2	D	347	PHE	CA-C-N	5.43	125.90	120.04
2	D	347	PHE	C-N-CA	5.43	125.90	120.04
2	B	102	TYR	N-CA-C	5.40	118.33	107.41
1	C	185	GLU	N-CA-C	-5.38	105.42	111.28
2	B	174	PHE	N-CA-C	5.34	117.97	109.64
2	B	357	SER	N-CA-C	5.30	122.09	110.80
2	B	96	GLY	CA-C-N	5.29	131.65	121.54
2	B	96	GLY	C-N-CA	5.29	131.65	121.54
2	B	393	THR	N-CA-C	5.29	117.02	109.14
2	D	357	SER	N-CA-C	5.28	122.05	110.80
2	D	102	TYR	N-CA-C	5.24	118.00	107.41
2	B	277	VAL	N-CA-C	5.24	120.24	109.34
2	D	235	CYS	N-CA-C	5.24	117.58	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	393	THR	N-CA-C	5.23	116.93	109.14
1	C	208	SER	N-CA-C	5.21	114.48	108.49
2	B	471	SER	N-CA-C	5.18	117.26	109.23
2	D	308	PRO	N-CA-C	-5.18	107.11	113.84
2	B	308	PRO	N-CA-C	-5.17	107.12	113.84
1	A	191	SER	N-CA-C	5.17	116.68	108.67
2	D	309	ARG	N-CA-C	5.16	121.78	110.80
2	D	78	ALA	N-CA-C	-5.15	102.16	110.14
2	D	467	HIS	N-CA-C	5.15	116.35	108.52
2	D	275	VAL	N-CA-C	5.14	116.12	108.46
2	B	309	ARG	N-CA-C	5.09	121.64	110.80
2	B	391	MET	N-CA-C	5.08	116.93	107.99
2	D	19	LYS	N-CA-C	5.08	116.68	108.41
2	B	349	ALA	CA-C-N	5.07	126.18	119.84
2	B	349	ALA	C-N-CA	5.07	126.18	119.84
2	B	82(C)	LEU	N-CA-C	5.06	116.90	107.99
2	D	89	VAL	N-CA-C	-5.06	101.20	108.48
1	C	191	SER	N-CA-C	5.05	116.50	108.67
2	D	277	VAL	N-CA-C	5.04	119.82	109.34
2	B	467	HIS	N-CA-C	5.02	116.15	108.42
2	B	89	VAL	N-CA-C	-5.01	101.27	108.53

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	1650	393	1570	120	0
1	C	1650	393	1570	116	0
2	B	3366	753	3284	269	2
2	D	3366	753	3284	286	2
3	E	110	103	93	1	0
4	F	110	103	93	2	0
All	All	10252	2498	9894	759	2

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 38.

All (759) 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:C:29:VAL:HG13	1:C:92:TYR:HB2	1.23	1.14
2:D:194:PRO:HG2	2:D:199:PRO:HG3	1.27	1.14
2:B:194:PRO:HG2	2:B:199:PRO:HG3	1.27	1.11
1:A:29:VAL:HG13	1:A:92:TYR:HB2	1.27	1.08
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.38	1.05
2:D:38:LYS:HE2	2:D:90:TYR:HE1	1.25	1.02
2:D:30:THR:HG22	2:D:73:ARG:HB3	1.42	1.00
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.40	1.00
2:B:38:LYS:HE2	2:B:90:TYR:HE1	1.25	0.98
1:C:214:CYS:HB3	2:D:235:CYS:HA	1.46	0.97
2:B:291:PHE:HB2	2:B:339:LYS:HB2	1.46	0.96
2:D:291:PHE:HB2	2:D:339:LYS:HB2	1.47	0.95
2:B:30:THR:HG22	2:B:73:ARG:HB3	1.48	0.94
2:B:372:ILE:HD11	2:D:375:PRO:HB3	1.49	0.93
2:B:449:GLU:HA	2:B:474:HIS:HD2	1.35	0.92
2:D:449:GLU:HA	2:D:474:HIS:HD2	1.34	0.91
2:B:426:MET:HE3	2:B:433:GLY:HA2	1.54	0.88
2:B:40:ARG:HH21	2:B:86:ASP:HA	1.40	0.86
2:B:372:ILE:HG21	2:D:372:ILE:HG21	1.54	0.86
2:B:200:ARG:HH21	2:B:227:PRO:HB3	1.41	0.85
2:B:375:PRO:HB3	2:D:372:ILE:HD11	1.57	0.84
2:D:40:ARG:HH21	2:D:86:ASP:HA	1.40	0.84
2:D:94:ARG:O	2:D:101:PRO:HD2	1.77	0.83
2:D:95:GLU:HG3	2:D:96:GLY:H	1.42	0.83
2:B:95:GLU:HG3	2:B:96:GLY:H	1.45	0.82
2:B:94:ARG:O	2:B:101:PRO:HD2	1.80	0.81
2:B:200:ARG:HG2	2:B:200:ARG:HH11	1.46	0.81
2:D:426:MET:HE3	2:D:433:GLY:HA2	1.62	0.81
2:D:194:PRO:HG2	2:D:199:PRO:CG	2.10	0.80
2:B:38:LYS:HE2	2:B:90:TYR:CE1	2.15	0.80
2:D:38:LYS:HE2	2:D:90:TYR:CE1	2.15	0.80
2:D:20:MET:SD	2:D:82:LEU:HD11	2.22	0.80
2:B:194:PRO:HG2	2:B:199:PRO:CG	2.10	0.79
2:D:200:ARG:HH22	2:D:227:PRO:HD3	1.46	0.79
2:B:140:LEU:HD11	2:B:200:ARG:HD2	1.64	0.79
2:B:200:ARG:NH2	2:B:227:PRO:HB3	1.97	0.79
1:A:78:VAL:HG12	1:A:79:GLN:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HD13	2:B:71:ARG:HB2	1.65	0.78
2:D:392:ILE:HD11	2:D:437:VAL:HB	1.64	0.77
2:D:140:LEU:HD11	2:D:200:ARG:HD2	1.66	0.77
2:D:60:ASN:HB3	2:D:63:PHE:CZ	2.19	0.77
2:B:60:ASN:HB3	2:B:63:PHE:CZ	2.20	0.77
2:D:40:ARG:HG2	2:D:88:ALA:HB2	1.67	0.77
1:A:190:ASN:OD1	1:A:210:ASN:HB2	1.85	0.76
2:D:51:ILE:HB	2:D:69:LEU:HD21	1.68	0.76
2:D:33:THR:OG1	2:D:95:GLU:HB3	1.86	0.76
1:A:119:PRO:HG2	2:B:228:ARG:HH22	1.50	0.75
2:D:200:ARG:HG2	2:D:200:ARG:HH11	1.51	0.75
2:B:365:ARG:HH21	2:B:394:ASP:HB2	1.51	0.75
2:B:237:CYS:C	2:B:239:PRO:HD3	2.12	0.75
2:B:392:ILE:HD11	2:B:437:VAL:HB	1.69	0.75
2:D:29:PHE:HE1	2:D:34:ILE:HD12	1.52	0.74
2:B:27:TYR:HE2	2:B:94:ARG:HE	1.33	0.74
1:A:115:VAL:HG22	1:A:136:LEU:HG	1.70	0.73
1:A:169:LYS:HD3	1:A:169:LYS:H	1.53	0.73
1:C:117:ILE:HG22	1:C:207:LYS:HD2	1.70	0.73
1:C:169:LYS:H	1:C:169:LYS:HD3	1.52	0.73
2:B:33:THR:OG1	2:B:95:GLU:HB3	1.88	0.73
2:B:259:LYS:HD2	2:B:260:PRO:HD2	1.69	0.73
2:D:84:SER:HA	2:D:111:VAL:HB	1.69	0.73
1:C:78:VAL:HG12	1:C:79:GLN:H	1.53	0.73
1:C:135:PHE:HB3	1:C:137:ASN:HD21	1.54	0.72
2:D:82:LEU:HB3	2:D:82(C):LEU:HD21	1.71	0.72
2:B:82:LEU:HB3	2:B:82(C):LEU:HD21	1.71	0.72
2:B:84:SER:HA	2:B:111:VAL:HB	1.72	0.72
1:A:135:PHE:HB3	1:A:137:ASN:HD21	1.53	0.72
2:B:200:ARG:HG2	2:B:200:ARG:NH1	2.03	0.72
1:A:117:ILE:HG22	1:A:207:LYS:HD2	1.72	0.72
1:A:65:SER:HB3	1:A:72:THR:OG1	1.89	0.72
1:C:29:VAL:HG13	1:C:92:TYR:CB	2.13	0.72
2:B:292:VAL:HG22	2:B:336:LYS:HD3	1.71	0.72
2:D:30:THR:HG22	2:D:73:ARG:CB	2.20	0.72
2:D:365:ARG:HH21	2:D:394:ASP:HB2	1.53	0.72
2:B:29:PHE:HE1	2:B:34:ILE:HD12	1.54	0.71
1:A:148:TRP:HZ2	1:A:177:SER:O	1.74	0.71
2:B:40:ARG:HG2	2:B:88:ALA:HB2	1.71	0.71
2:B:51:ILE:HB	2:B:69:LEU:HD21	1.73	0.71
2:B:128:SER:HB2	2:B:235:CYS:SG	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:LYS:HD2	2:D:260:PRO:HD2	1.71	0.71
2:B:6:GLU:HA	2:B:22:CYS:HA	1.73	0.70
2:D:251:SER:HA	2:D:278:ASP:HB2	1.73	0.70
2:D:449:GLU:HA	2:D:474:HIS:CD2	2.24	0.70
2:D:51:ILE:HD13	2:D:71:ARG:HB2	1.72	0.70
2:D:309:ARG:HB3	2:D:321:VAL:HG13	1.73	0.69
1:C:148:TRP:HZ2	1:C:177:SER:O	1.74	0.69
2:D:48:ILE:HA	2:D:63:PHE:CZ	2.26	0.69
1:A:87:HIS:HB3	1:A:101:GLY:HA2	1.74	0.69
1:C:46:LEU:HD12	2:D:101:PRO:HB3	1.72	0.69
2:B:449:GLU:HA	2:B:474:HIS:CD2	2.24	0.69
2:B:3:LYS:NZ	2:B:3:LYS:HB3	2.07	0.69
2:B:20:MET:SD	2:B:82:LEU:HD11	2.32	0.69
2:D:200:ARG:HG2	2:D:200:ARG:NH1	2.08	0.69
1:C:29:VAL:CG1	1:C:92:TYR:HB2	2.13	0.68
2:B:251:SER:HA	2:B:278:ASP:HB2	1.73	0.68
2:B:309:ARG:HB3	2:B:321:VAL:HG13	1.75	0.68
2:D:3:LYS:NZ	2:D:3:LYS:HB3	2.08	0.68
2:B:48:ILE:HA	2:B:63:PHE:CZ	2.28	0.68
1:A:214:CYS:SG	2:B:128:SER:OG	2.50	0.68
2:D:226:VAL:HG23	2:D:227:PRO:HD2	1.75	0.68
2:D:92:CYS:O	2:D:92:CYS:SG	2.51	0.68
2:B:29:PHE:CD2	2:B:76:ASN:HA	2.29	0.68
2:B:92:CYS:O	2:B:92:CYS:SG	2.52	0.68
2:B:35:HIS:HE1	2:B:95:GLU:HB2	1.59	0.67
1:C:65:SER:HB3	1:C:72:THR:OG1	1.93	0.67
2:D:27:TYR:HE2	2:D:94:ARG:HE	1.40	0.67
1:A:29:VAL:HG12	1:A:29:VAL:O	1.93	0.67
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.74	0.67
2:B:105:GLN:HG3	2:B:106:GLY:H	1.60	0.67
2:D:292:VAL:HG22	2:D:336:LYS:HD3	1.77	0.67
1:A:29:VAL:CG1	1:A:92:TYR:HB2	2.18	0.67
1:A:2:LYS:O	1:A:2:LYS:HG2	1.95	0.67
2:B:260:PRO:O	2:B:264:LEU:HG	1.93	0.67
1:C:2:LYS:O	1:C:2:LYS:HG2	1.95	0.67
1:A:149:LYS:HD3	1:A:153:SER:HA	1.77	0.67
1:C:29:VAL:HG12	1:C:29:VAL:O	1.94	0.67
2:B:279:ILE:HG23	2:B:283:ASP:HB2	1.76	0.66
1:C:87:HIS:HB3	1:C:101:GLY:HA2	1.77	0.66
2:D:6:GLU:HA	2:D:22:CYS:HA	1.78	0.66
2:B:30:THR:HG22	2:B:73:ARG:CB	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LYS:HB3	2:B:90:TYR:CD1	2.31	0.66
1:A:155:ARG:O	1:A:156:GLN:HB2	1.95	0.65
1:C:149:LYS:HB2	1:C:193:THR:HB	1.79	0.65
2:D:313:PHE:HB2	2:D:318:THR:O	1.96	0.65
2:B:154:VAL:HA	2:B:210:VAL:HG12	1.78	0.64
2:D:154:VAL:HA	2:D:210:VAL:HG12	1.79	0.64
2:D:239:PRO:HB2	2:D:241:ILE:HG12	1.79	0.64
2:D:279:ILE:HG23	2:D:283:ASP:HB2	1.79	0.64
2:D:93:VAL:HG12	2:D:94:ARG:H	1.62	0.64
2:D:292:VAL:O	2:D:295:ASP:HB2	1.95	0.64
2:D:29:PHE:CD2	2:D:76:ASN:HA	2.32	0.64
1:C:155:ARG:O	1:C:156:GLN:HB2	1.96	0.64
1:A:35:TRP:HD1	1:A:48:ILE:HD11	1.63	0.64
2:B:26:GLY:O	2:B:27:TYR:HB3	1.98	0.64
2:D:200:ARG:HB3	2:D:202:PRO:HD3	1.78	0.64
2:D:419:TYR:HA	2:D:440:LYS:O	1.97	0.64
2:D:35:HIS:HE1	2:D:95:GLU:HB2	1.63	0.63
2:D:260:PRO:O	2:D:264:LEU:HG	1.99	0.63
1:A:119:PRO:HG2	2:B:228:ARG:NH2	2.13	0.63
2:D:325:LEU:O	2:D:325:LEU:HD23	1.98	0.63
2:B:419:TYR:HA	2:B:440:LYS:O	1.98	0.62
2:D:4:LEU:HD11	2:D:102:TYR:O	1.99	0.62
2:D:136:SER:O	2:D:194:PRO:HA	1.99	0.62
1:A:12:SER:HA	1:A:105:GLU:O	2.00	0.61
2:B:64:LYS:O	2:B:66:LYS:HG2	2.00	0.61
1:C:164:THR:HG22	1:C:174:SER:H	1.64	0.61
2:D:105:GLN:HG3	2:D:106:GLY:H	1.63	0.61
1:A:192:TYR:O	1:A:208:SER:HB2	1.99	0.61
2:B:325:LEU:O	2:B:325:LEU:HD23	2.00	0.61
2:D:390:CYS:HB2	2:D:406:TRP:CZ2	2.34	0.61
2:B:20:MET:HG3	2:B:36:TRP:CZ3	2.35	0.61
2:B:306:THR:HG21	2:B:325:LEU:HA	1.83	0.61
2:B:313:PHE:HB2	2:B:318:THR:O	2.00	0.61
2:D:51:ILE:CB	2:D:69:LEU:HD21	2.29	0.61
2:B:200:ARG:HB3	2:B:202:PRO:HD3	1.83	0.61
1:C:76:SER:O	1:C:77:SER:HB3	2.00	0.61
2:D:193:VAL:HB	2:D:194:PRO:HD2	1.83	0.61
1:A:182:THR:HB	1:A:185:GLU:CB	2.31	0.61
2:B:292:VAL:O	2:B:295:ASP:HB2	2.01	0.60
1:A:149:LYS:HB2	1:A:193:THR:HB	1.83	0.60
2:D:22:CYS:O	2:D:22:CYS:SG	2.59	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:VAL:HG23	2:B:392:ILE:HG22	1.84	0.60
2:D:38:LYS:HB3	2:D:90:TYR:CD1	2.37	0.60
2:D:72:ASP:O	2:D:74:SER:N	2.34	0.60
2:D:406:TRP:O	2:D:407:GLN:HG3	2.02	0.60
2:D:425:ILE:HD13	2:D:425:ILE:H	1.67	0.60
1:C:12:SER:HA	1:C:105:GLU:O	2.02	0.60
2:B:304:ALA:O	2:B:305:GLN:HG2	2.01	0.60
2:D:147:TYR:O	2:D:185:TYR:HB2	2.02	0.59
2:D:341:ARG:HA	2:D:352:GLU:HB3	1.83	0.59
1:A:107:LYS:HG2	1:A:140:TYR:OH	2.01	0.59
2:B:238:LYS:HD2	2:B:238:LYS:O	2.02	0.59
2:D:306:THR:HG21	2:D:325:LEU:HA	1.83	0.59
1:C:149:LYS:HD3	1:C:153:SER:HA	1.83	0.59
2:D:392:ILE:HG12	2:D:437:VAL:O	2.02	0.59
2:B:4:LEU:HD11	2:B:102:TYR:O	2.03	0.59
1:A:164:THR:HG22	1:A:174:SER:H	1.66	0.59
2:B:38:LYS:HZ2	2:B:40:ARG:HH22	1.49	0.59
2:B:193:VAL:HB	2:B:194:PRO:HD2	1.84	0.59
2:B:390:CYS:HB2	2:B:406:TRP:CZ2	2.37	0.59
1:C:135:PHE:CD2	2:D:190:SER:HB3	2.37	0.59
2:D:10:GLU:O	2:D:109:VAL:HA	2.02	0.59
2:D:275:VAL:HG23	2:D:321:VAL:O	2.02	0.59
2:B:406:TRP:O	2:B:407:GLN:HG3	2.02	0.59
2:B:10:GLU:O	2:B:109:VAL:HA	2.03	0.58
2:B:93:VAL:HG12	2:B:94:ARG:H	1.68	0.58
1:C:182:THR:HB	1:C:185:GLU:CB	2.33	0.58
2:B:392:ILE:HG12	2:B:437:VAL:O	2.03	0.58
2:D:93:VAL:HG11	2:D:98:VAL:HG12	1.86	0.58
2:B:75:SER:O	2:B:77:THR:HG22	2.03	0.58
2:D:264:LEU:HD13	2:D:459:LEU:HB3	1.86	0.58
2:B:341:ARG:HA	2:B:352:GLU:HB3	1.84	0.58
2:D:144:VAL:HG23	2:D:187:LEU:HD13	1.84	0.58
1:A:76:SER:O	1:A:77:SER:HB3	2.02	0.58
2:B:338:PHE:O	2:B:354:THR:HA	2.03	0.58
2:D:26:GLY:O	2:D:27:TYR:HB3	2.04	0.58
2:D:266:ILE:HA	2:D:329:HIS:CE1	2.38	0.58
2:D:425:ILE:HD13	2:D:425:ILE:N	2.18	0.58
2:B:136:SER:O	2:B:194:PRO:HA	2.04	0.58
2:D:17:SER:HB3	2:D:82:LEU:O	2.03	0.58
1:A:183:LYS:O	1:A:186:TYR:HB3	2.04	0.57
1:A:206:VAL:HG12	1:A:207:LYS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:CB	2:B:69:LEU:HD21	2.34	0.57
2:B:264:LEU:HD13	2:B:459:LEU:HB3	1.87	0.57
2:B:200:ARG:HH11	2:B:200:ARG:CG	2.16	0.57
2:D:87:SER:OG	2:D:110:THR:HA	2.04	0.57
2:B:425:ILE:HD13	2:B:425:ILE:H	1.69	0.57
2:D:338:PHE:O	2:D:354:THR:HA	2.04	0.56
2:D:270:PRO:HG2	2:D:327:ILE:O	2.05	0.56
1:C:24:LYS:HA	1:C:69:THR:O	2.06	0.56
1:C:192:TYR:O	1:C:208:SER:HB2	2.06	0.56
1:A:148:TRP:CZ2	1:A:177:SER:O	2.58	0.56
1:C:163:TRP:O	2:D:175:PRO:HD2	2.05	0.56
2:D:146:GLY:HA2	2:D:184:LEU:HD22	1.87	0.56
1:A:98:PHE:CD2	2:B:45:LEU:HB3	2.41	0.56
1:A:135:PHE:HD1	1:A:135:PHE:H	1.52	0.56
2:B:72:ASP:O	2:B:74:SER:N	2.39	0.56
2:B:425:ILE:HD13	2:B:425:ILE:N	2.20	0.56
2:B:370:TYR:CZ	2:D:378:GLN:HB2	2.41	0.56
2:D:257:PRO:HG3	2:D:355:ILE:CG1	2.34	0.56
1:A:135:PHE:CD1	1:A:135:PHE:N	2.73	0.56
1:C:135:PHE:C	1:C:136:LEU:HD12	2.31	0.56
2:B:147:TYR:O	2:B:185:TYR:HB2	2.06	0.56
2:D:288:PHE:HA	2:D:342:VAL:HG12	1.88	0.56
2:D:388:LEU:H	2:D:388:LEU:HD12	1.71	0.56
2:B:93:VAL:HG11	2:B:98:VAL:HG12	1.88	0.55
2:B:171:VAL:HG13	2:B:190:SER:O	2.05	0.55
2:B:309:ARG:HA	2:B:321:VAL:HA	1.89	0.55
1:A:184:ASP:O	1:A:188:ARG:HG3	2.07	0.55
2:B:117:THR:O	2:B:147:TYR:HA	2.06	0.55
2:D:103:TRP:N	2:D:103:TRP:CD1	2.74	0.55
2:B:103:TRP:CD1	2:B:103:TRP:N	2.74	0.55
2:D:33:THR:CG2	2:D:52(A):PRO:HD3	2.37	0.55
1:C:78:VAL:HG12	1:C:79:GLN:N	2.20	0.55
1:A:24:LYS:HA	1:A:69:THR:O	2.06	0.55
2:B:57:THR:HG22	2:B:59:TYR:CE1	2.42	0.55
2:D:401:THR:HG22	2:D:459:LEU:HB2	1.89	0.55
1:A:186:TYR:HA	1:A:192:TYR:OH	2.07	0.55
2:B:291:PHE:HD2	2:B:296:ASN:HA	1.71	0.55
1:C:183:LYS:O	1:C:186:TYR:HB3	2.06	0.55
2:B:34:ILE:HA	2:B:94:ARG:HA	1.89	0.55
2:B:398:GLU:O	2:B:400:ILE:HG22	2.06	0.55
1:A:115:VAL:HG12	1:A:116:SER:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:HG13	2:B:49:GLY:H	1.72	0.55
2:D:66:LYS:HE3	2:D:82(B):SER:HG	1.72	0.55
1:A:105:GLU:HG3	1:A:166:GLN:NE2	2.21	0.54
2:D:75:SER:O	2:D:77:THR:HG22	2.07	0.54
1:A:213:GLU:O	1:A:214:CYS:HB3	2.07	0.54
2:B:38:LYS:HZ2	2:B:40:ARG:NH2	2.05	0.54
2:B:275:VAL:HG23	2:B:321:VAL:O	2.08	0.54
2:D:20:MET:HG3	2:D:36:TRP:CZ3	2.42	0.54
2:D:200:ARG:NH2	2:D:227:PRO:HD3	2.21	0.54
2:B:214:ALA:O	2:B:215:SER:HB2	2.07	0.54
1:C:193:THR:HA	1:C:208:SER:HB3	1.89	0.54
2:B:119:PRO:CB	2:B:147:TYR:HB3	2.24	0.54
2:D:51:ILE:CA	2:D:69:LEU:HD21	2.38	0.54
2:D:309:ARG:HA	2:D:321:VAL:HA	1.90	0.54
2:B:141:GLY:HA2	2:B:189:SER:O	2.08	0.54
2:B:29:PHE:CD2	2:B:73:ARG:HA	2.43	0.54
1:A:214:CYS:HB3	2:B:235:CYS:HA	1.89	0.54
2:B:257:PRO:HG3	2:B:355:ILE:CG1	2.38	0.54
2:B:290:TRP:CG	2:B:325:LEU:HD13	2.43	0.54
1:C:105:GLU:HG3	1:C:166:GLN:NE2	2.23	0.54
1:A:206:VAL:HG12	1:A:207:LYS:N	2.23	0.53
1:C:35:TRP:HD1	1:C:48:ILE:HD11	1.71	0.53
1:C:115:VAL:HG12	1:C:116:SER:N	2.23	0.53
1:C:205:ILE:HD12	1:C:205:ILE:N	2.23	0.53
1:A:46:LEU:HD12	2:B:101:PRO:HB3	1.90	0.53
2:B:60:ASN:HB3	2:B:63:PHE:HZ	1.72	0.53
2:D:174:PHE:HD2	2:D:188:SER:HG	1.55	0.53
2:D:271:LYS:HA	2:D:326:PRO:HA	1.90	0.53
2:B:407:GLN:HA	2:B:416:PRO:HD3	1.89	0.53
1:C:120:PRO:HB2	1:C:125:LEU:HD21	1.91	0.53
2:D:214:ALA:O	2:D:215:SER:HB2	2.08	0.53
2:D:265:LEU:HD13	2:D:268:VAL:CG2	2.38	0.53
2:D:468:THR:HG22	2:D:469:GLU:N	2.24	0.53
2:B:3:LYS:HB3	2:B:3:LYS:HZ2	1.71	0.53
1:C:62:PHE:HE1	1:C:75:ILE:HD13	1.74	0.53
2:D:291:PHE:HD2	2:D:296:ASN:HA	1.73	0.53
1:A:120:PRO:HB2	1:A:125:LEU:HD21	1.91	0.53
2:B:51:ILE:CA	2:B:69:LEU:HD21	2.38	0.53
2:D:117:THR:O	2:D:147:TYR:HA	2.08	0.53
2:D:394:ASP:HA	2:D:434:SER:HB2	1.90	0.53
1:A:184:ASP:HA	1:A:187:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLY:HA2	2:B:184:LEU:HD22	1.90	0.53
2:B:468:THR:HG22	2:B:469:GLU:N	2.23	0.53
1:A:182:THR:HB	1:A:185:GLU:HB3	1.91	0.53
2:B:176:ALA:HA	2:B:187:LEU:HB3	1.90	0.53
2:D:304:ALA:O	2:D:305:GLN:HG2	2.08	0.53
1:C:206:VAL:HG12	1:C:207:LYS:N	2.24	0.53
2:B:271:LYS:HA	2:B:326:PRO:HA	1.90	0.53
2:B:371:THR:HB	2:B:472:LEU:HG	1.91	0.53
1:C:184:ASP:HA	1:C:187:GLU:HB2	1.90	0.53
1:C:206:VAL:HG12	1:C:207:LYS:H	1.74	0.53
2:D:171:VAL:HG13	2:D:190:SER:O	2.08	0.53
2:D:400:ILE:HD11	2:D:458:VAL:CG2	2.39	0.53
2:B:87:SER:OG	2:B:110:THR:HA	2.09	0.52
1:A:151:ASP:HA	1:A:191:SER:O	2.09	0.52
2:B:288:PHE:HA	2:B:342:VAL:HG12	1.91	0.52
1:A:83:LEU:O	1:A:84:ALA:HB2	2.09	0.52
2:B:38:LYS:NZ	2:B:40:ARG:NH2	2.57	0.52
2:B:154:VAL:HG22	2:B:210:VAL:HG12	1.91	0.52
1:C:182:THR:HB	1:C:185:GLU:HB3	1.92	0.52
2:D:34:ILE:HG12	2:D:93:VAL:O	2.09	0.52
2:D:38:LYS:HZ2	2:D:40:ARG:HH22	1.56	0.52
1:C:135:PHE:HD1	1:C:135:PHE:H	1.56	0.52
1:C:186:TYR:HA	1:C:192:TYR:OH	2.09	0.52
2:D:119:PRO:CB	2:D:147:TYR:HB3	2.26	0.52
1:A:62:PHE:HE1	1:A:75:ILE:HD13	1.74	0.52
2:D:141:GLY:HA2	2:D:189:SER:O	2.10	0.52
1:A:135:PHE:CD2	2:B:190:SER:HB3	2.45	0.52
2:B:266:ILE:HA	2:B:329:HIS:CE1	2.45	0.52
2:B:375:PRO:HB3	2:D:372:ILE:CD1	2.35	0.52
1:C:98:PHE:CD2	2:D:45:LEU:HB3	2.45	0.52
1:C:113:PRO:HA	1:C:139:PHE:HB3	1.92	0.52
1:A:87:HIS:HB3	1:A:101:GLY:CA	2.40	0.52
2:B:17:SER:HB3	2:B:82:LEU:O	2.10	0.52
1:C:148:TRP:CZ2	1:C:177:SER:O	2.61	0.52
1:A:195:GLU:HG2	1:A:196:ALA:N	2.25	0.52
1:C:151:ASP:HA	1:C:191:SER:O	2.10	0.52
2:B:48:ILE:CG1	2:B:49:GLY:H	2.22	0.51
1:C:90:GLN:NE2	1:C:96:TYR:HD1	2.08	0.51
1:C:135:PHE:N	1:C:135:PHE:CD1	2.77	0.51
2:D:60:ASN:HB3	2:D:63:PHE:HZ	1.70	0.51
2:D:57:THR:HG22	2:D:59:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG22	1:A:179:LEU:H	1.74	0.51
2:B:33:THR:CG2	2:B:52(A):PRO:HD3	2.40	0.51
2:B:144:VAL:HG23	2:B:187:LEU:HD13	1.92	0.51
2:D:20:MET:HE2	2:D:90:TYR:HB2	1.93	0.51
2:D:38:LYS:HE3	2:D:48:ILE:HG21	1.91	0.51
2:D:95:GLU:CG	2:D:96:GLY:H	2.18	0.51
1:C:83:LEU:O	1:C:84:ALA:HB2	2.10	0.51
2:D:64:LYS:O	2:D:66:LYS:HG2	2.09	0.51
1:C:94:TYR:HD1	1:C:94:TYR:H	1.59	0.51
2:D:34:ILE:HA	2:D:94:ARG:HA	1.93	0.51
2:D:200:ARG:HH11	2:D:200:ARG:CG	2.21	0.51
2:D:470:LYS:NZ	2:D:470:LYS:HB3	2.25	0.51
1:C:124:GLN:NE2	1:C:131:SER:H	2.09	0.51
2:D:38:LYS:NZ	2:D:40:ARG:NH2	2.59	0.51
2:D:365:ARG:NH2	2:D:394:ASP:HB2	2.25	0.51
2:B:394:ASP:HA	2:B:434:SER:HB2	1.92	0.51
1:A:78:VAL:HG12	1:A:79:GLN:N	2.20	0.51
1:A:113:PRO:HA	1:A:139:PHE:HB3	1.92	0.51
2:B:401:THR:HG22	2:B:459:LEU:HB2	1.93	0.51
1:C:22:THR:HG22	1:C:72:THR:HG22	1.93	0.51
2:B:470:LYS:NZ	2:B:470:LYS:HB3	2.25	0.50
1:C:169:LYS:HD3	1:C:169:LYS:N	2.23	0.50
2:D:37:ILE:HG12	2:D:47:TRP:HA	1.93	0.50
2:B:205:THR:HG21	2:B:222:LYS:HE3	1.93	0.50
2:B:37:ILE:HG12	2:B:47:TRP:HA	1.93	0.50
2:D:290:TRP:O	2:D:300:GLU:HA	2.11	0.50
2:D:290:TRP:CG	2:D:325:LEU:HD13	2.47	0.50
2:D:355:ILE:HG23	2:D:355:ILE:O	2.12	0.50
2:D:407:GLN:HA	2:D:416:PRO:HD3	1.93	0.50
1:A:124:GLN:NE2	1:A:131:SER:H	2.08	0.50
1:A:169:LYS:HD3	1:A:169:LYS:N	2.24	0.50
2:B:38:LYS:HE3	2:B:48:ILE:HG21	1.91	0.50
2:D:29:PHE:CE1	2:D:34:ILE:HD12	2.41	0.50
1:A:29:VAL:HG13	1:A:92:TYR:CB	2.18	0.50
1:A:87:HIS:ND1	1:A:87:HIS:N	2.59	0.50
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.47	0.50
2:B:406:TRP:HA	2:B:455:THR:O	2.11	0.50
2:D:299:VAL:O	2:D:300:GLU:HB3	2.12	0.50
2:D:48:ILE:CG1	2:D:49:GLY:H	2.25	0.50
2:D:369:VAL:HG23	2:D:392:ILE:HG22	1.92	0.50
1:A:94:TYR:HD1	1:A:94:TYR:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:PRO:HG2	2:B:327:ILE:O	2.12	0.50
1:C:36:TYR:OH	2:D:98:VAL:HB	2.10	0.50
1:C:159:VAL:C	1:C:160:LEU:HD12	2.37	0.50
2:B:290:TRP:O	2:B:300:GLU:HA	2.12	0.50
2:D:265:LEU:HD13	2:D:268:VAL:HG23	1.93	0.50
2:D:371:THR:HB	2:D:472:LEU:HG	1.92	0.50
2:B:90:TYR:HE2	2:B:109:VAL:HG21	1.77	0.49
2:D:29:PHE:CD2	2:D:73:ARG:HA	2.47	0.49
2:D:369:VAL:O	2:D:369:VAL:HG13	2.12	0.49
1:A:163:TRP:CE3	1:A:175:MET:HG3	2.47	0.49
2:D:257:PRO:HG3	2:D:355:ILE:HG12	1.94	0.49
1:A:193:THR:HA	1:A:208:SER:HB3	1.94	0.49
2:B:372:ILE:CD1	2:D:375:PRO:HB3	2.33	0.49
2:B:145:LYS:HG3	2:B:186:THR:HB	1.93	0.49
2:B:154:VAL:HG22	2:B:210:VAL:CG1	2.42	0.49
2:B:174:PHE:HD2	2:B:188:SER:HG	1.59	0.49
1:C:178:THR:HG22	1:C:179:LEU:H	1.77	0.49
1:A:163:TRP:O	2:B:175:PRO:HD2	2.12	0.49
1:A:179:LEU:C	1:A:179:LEU:HD23	2.37	0.49
2:B:238:LYS:NZ	2:B:238:LYS:HB3	2.27	0.49
1:C:107:LYS:HG2	1:C:140:TYR:OH	2.12	0.49
2:D:90:TYR:HE2	2:D:109:VAL:HG21	1.76	0.49
2:D:136:SER:HA	2:D:195:SER:OG	2.12	0.49
2:D:176:ALA:HA	2:D:187:LEU:HB3	1.93	0.49
2:B:299:VAL:O	2:B:300:GLU:HB3	2.13	0.49
1:C:87:HIS:HB3	1:C:101:GLY:CA	2.40	0.49
1:A:125:LEU:O	1:A:183:LYS:HD2	2.13	0.49
1:A:205:ILE:HD12	1:A:205:ILE:N	2.28	0.49
2:B:179:GLN:OE1	2:B:179:GLN:HA	2.13	0.49
1:C:108:ARG:O	1:C:109:ALA:HB3	2.10	0.49
1:C:136:LEU:HD12	1:C:136:LEU:N	2.27	0.49
1:A:22:THR:HG22	1:A:72:THR:HG22	1.93	0.49
1:A:33:VAL:HG11	1:A:88:CYS:HB2	1.94	0.49
1:A:150:ILE:HB	1:A:154:GLU:HG2	1.93	0.49
1:A:108:ARG:O	1:A:109:ALA:HB3	2.12	0.49
2:B:309:ARG:NH1	2:B:310:GLU:HB2	2.28	0.49
2:B:355:ILE:HG23	2:B:355:ILE:O	2.13	0.49
2:B:365:ARG:NH2	2:B:394:ASP:HB2	2.23	0.49
1:C:199:LYS:HD3	1:C:200:THR:N	2.28	0.49
1:A:212:ASN:O	1:A:214:CYS:N	2.46	0.49
2:B:162:ASN:HB3	2:B:165:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:C	1:C:179:LEU:HD23	2.37	0.49
1:C:192:TYR:HB2	1:C:209:PHE:CE1	2.48	0.48
2:D:209:ASN:HB3	2:D:220:ASP:OD1	2.12	0.48
1:C:6:THR:HG21	1:C:87:HIS:HA	1.95	0.48
1:C:62:PHE:HD1	1:C:75:ILE:HG12	1.78	0.48
2:D:40:ARG:HB3	2:D:41:PRO:HD2	1.95	0.48
2:D:48:ILE:HG13	2:D:49:GLY:H	1.77	0.48
2:D:179:GLN:OE1	2:D:179:GLN:HA	2.13	0.48
1:A:135:PHE:C	1:A:136:LEU:HD12	2.39	0.48
1:C:37:GLN:HB2	1:C:47:LEU:HD22	1.94	0.48
2:D:162:ASN:HB3	2:D:165:SER:OG	2.12	0.48
1:A:150:ILE:HD12	1:A:156:GLN:NE2	2.28	0.48
1:A:199:LYS:HD3	1:A:200:THR:N	2.28	0.48
2:B:238:LYS:N	2:B:239:PRO:HD3	2.28	0.48
1:C:87:HIS:ND1	1:C:87:HIS:N	2.61	0.48
1:C:184:ASP:O	1:C:188:ARG:HG3	2.12	0.48
2:D:41:PRO:O	2:D:43:GLN:HG2	2.13	0.48
2:D:103:TRP:CD1	2:D:103:TRP:H	2.31	0.48
2:D:303:THR:O	2:D:304:ALA:HB2	2.14	0.48
1:A:11:MET:O	1:A:104:LEU:HD23	2.13	0.48
2:B:48:ILE:HG13	2:B:49:GLY:N	2.28	0.48
2:B:400:ILE:HD11	2:B:458:VAL:CG2	2.43	0.48
2:B:444:GLN:H	2:B:444:GLN:NE2	2.11	0.48
1:C:4:ALA:O	1:C:99:GLY:HA2	2.13	0.48
2:D:444:GLN:H	2:D:444:GLN:NE2	2.11	0.48
1:A:62:PHE:HD1	1:A:75:ILE:HG12	1.79	0.48
2:B:209:ASN:HB3	2:B:220:ASP:OD1	2.14	0.48
1:C:6:THR:HG23	1:C:88:CYS:SG	2.53	0.48
2:D:145:LYS:HG3	2:D:186:THR:HB	1.94	0.48
1:A:33:VAL:CG1	1:A:88:CYS:HB2	2.42	0.48
2:B:40:ARG:HB3	2:B:41:PRO:HD2	1.96	0.48
2:B:388:LEU:HD12	2:B:388:LEU:H	1.78	0.48
1:C:54:ARG:HD2	1:C:58:VAL:HG12	1.96	0.48
2:D:343:ASN:ND2	2:D:350:PRO:HB3	2.28	0.48
2:D:347:PHE:HA	2:D:348:PRO:HD3	1.70	0.48
2:D:371:THR:HB	2:D:472:LEU:CG	2.44	0.48
2:D:406:TRP:HA	2:D:455:THR:O	2.13	0.48
2:B:406:TRP:CD1	2:B:419:TYR:HB2	2.49	0.48
2:B:200:ARG:HH22	2:B:227:PRO:HD3	1.78	0.48
2:B:290:TRP:HA	2:B:339:LYS:O	2.14	0.48
2:D:37:ILE:HG22	2:D:38:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLN:O	2:D:88:ALA:HB1	2.13	0.48
2:D:51:ILE:HD12	2:D:69:LEU:O	2.13	0.48
2:B:95:GLU:CG	2:B:96:GLY:H	2.23	0.48
1:A:159:VAL:C	1:A:160:LEU:HD12	2.39	0.47
2:B:103:TRP:CD1	2:B:103:TRP:H	2.32	0.47
2:B:371:THR:HB	2:B:472:LEU:CG	2.44	0.47
2:B:6:GLU:OE1	2:B:104:GLY:HA3	2.14	0.47
2:B:265:LEU:HD13	2:B:268:VAL:CG2	2.43	0.47
1:A:90:GLN:NE2	1:A:96:TYR:HD1	2.12	0.47
2:B:115:LYS:HD2	2:B:116:THR:N	2.29	0.47
2:B:116:THR:HA	2:B:148:PHE:O	2.14	0.47
1:C:61:ARG:HH12	1:C:82:ASP:CG	2.21	0.47
2:D:256:PHE:HA	2:D:257:PRO:HD3	1.77	0.47
1:C:33:VAL:HG11	1:C:88:CYS:HB2	1.95	0.47
2:D:3:LYS:HB3	2:D:3:LYS:HZ3	1.78	0.47
2:D:48:ILE:HG13	2:D:49:GLY:N	2.30	0.47
2:D:50:TYR:CE1	2:D:51:ILE:O	2.68	0.47
2:B:89:VAL:HA	2:B:107:THR:O	2.14	0.47
2:D:27:TYR:N	2:D:27:TYR:CD1	2.82	0.47
2:D:51:ILE:HB	2:D:69:LEU:CD2	2.42	0.47
2:D:105:GLN:HG3	2:D:106:GLY:N	2.29	0.47
2:D:406:TRP:CD1	2:D:419:TYR:HB2	2.49	0.47
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.50	0.47
2:D:115:LYS:HD2	2:D:116:THR:N	2.30	0.47
2:D:252:SER:O	2:D:277:VAL:HG12	2.15	0.47
4:F:5:NAG:O3	4:F:6:GAL:C1	2.62	0.47
1:C:195:GLU:HG2	1:C:196:ALA:N	2.29	0.47
2:D:388:LEU:HD12	2:D:388:LEU:N	2.29	0.47
1:A:63:THR:O	1:A:73:LEU:HA	2.15	0.47
2:B:37:ILE:HG22	2:B:38:LYS:N	2.29	0.47
1:C:63:THR:O	1:C:73:LEU:HA	2.13	0.47
1:C:125:LEU:O	1:C:183:LYS:HD2	2.14	0.47
2:D:144:VAL:HG23	2:D:144:VAL:O	2.14	0.47
2:D:425:ILE:HG12	2:D:436:PHE:CE1	2.50	0.47
1:A:6:THR:HG21	1:A:87:HIS:HA	1.96	0.46
1:A:182:THR:HB	1:A:185:GLU:HB2	1.95	0.46
2:B:329:HIS:H	2:B:329:HIS:CD2	2.33	0.46
1:C:133:VAL:HG21	2:D:124:LEU:HD13	1.97	0.46
2:D:53:SER:OG	2:D:55:VAL:HG23	2.15	0.46
2:D:89:VAL:HA	2:D:107:THR:O	2.15	0.46
3:E:5:NAG:O3	3:E:6:GAL:C1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:HE22	1:C:96:TYR:HD1	1.64	0.46
2:D:344:SER:HB3	2:D:347:PHE:CD1	2.50	0.46
2:D:398:GLU:O	2:D:400:ILE:HG22	2.15	0.46
1:A:185:GLU:HA	1:A:188:ARG:CZ	2.45	0.46
2:B:256:PHE:HB2	2:B:273:THR:CG2	2.45	0.46
2:D:241:ILE:HD13	2:D:241:ILE:H	1.81	0.46
2:D:309:ARG:NH1	2:D:310:GLU:HB2	2.30	0.46
2:D:322:VAL:HG12	2:D:323:SER:N	2.31	0.46
2:B:343:ASN:ND2	2:B:350:PRO:HB3	2.30	0.46
1:C:185:GLU:HA	1:C:188:ARG:CZ	2.46	0.46
2:D:33:THR:HG23	2:D:52(A):PRO:HD3	1.96	0.46
2:D:126:PRO:O	2:D:228:ARG:HG2	2.15	0.46
2:D:329:HIS:H	2:D:329:HIS:CD2	2.34	0.46
2:B:369:VAL:HA	2:B:392:ILE:HA	1.98	0.46
1:C:210:ASN:O	1:C:211:ARG:CB	2.63	0.46
2:D:8:GLY:O	2:D:9:ALA:HB2	2.16	0.46
2:B:27:TYR:HE2	2:B:94:ARG:NE	2.09	0.46
2:B:27:TYR:N	2:B:27:TYR:CD1	2.84	0.46
2:B:303:THR:O	2:B:304:ALA:HB2	2.16	0.46
2:D:125:ALA:O	2:D:228:ARG:HD3	2.16	0.46
2:B:29:PHE:CE1	2:B:34:ILE:HD12	2.42	0.46
2:B:265:LEU:HD13	2:B:268:VAL:HG23	1.98	0.46
1:C:149:LYS:HA	1:C:154:GLU:O	2.16	0.46
1:C:182:THR:HB	1:C:185:GLU:HB2	1.98	0.46
1:C:33:VAL:CG1	1:C:88:CYS:HB2	2.46	0.46
2:D:154:VAL:HG22	2:D:210:VAL:HG12	1.97	0.46
1:A:136:LEU:HD12	1:A:136:LEU:N	2.31	0.46
2:D:50:TYR:N	2:D:69:LEU:HD13	2.31	0.46
2:D:200:ARG:HH21	2:D:227:PRO:HB3	1.81	0.46
2:D:17:SER:OG	2:D:82(A):SER:HA	2.15	0.46
2:B:105:GLN:HG3	2:B:106:GLY:N	2.28	0.45
1:C:191:SER:HA	1:C:209:PHE:O	2.15	0.45
2:D:40:ARG:CG	2:D:88:ALA:HB2	2.43	0.45
1:A:124:GLN:HE22	1:A:131:SER:H	1.63	0.45
2:B:84:SER:HA	2:B:111:VAL:CB	2.45	0.45
2:D:38:LYS:HB3	2:D:90:TYR:CE1	2.51	0.45
2:D:58:ASN:OD1	2:D:58:ASN:N	2.49	0.45
1:A:133:VAL:HG21	2:B:124:LEU:HD13	1.98	0.45
1:A:214:CYS:SG	2:B:128:SER:CB	3.04	0.45
1:C:90:GLN:OE1	1:C:97:THR:N	2.50	0.45
2:B:8:GLY:O	2:B:9:ALA:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:THR:HG22	2:D:57:THR:O	2.16	0.45
2:D:244:VAL:HG12	2:D:245:PRO:HD2	1.98	0.45
2:D:343:ASN:CG	2:D:350:PRO:HB3	2.41	0.45
1:A:54:ARG:HD2	1:A:58:VAL:HG12	1.99	0.45
2:B:38:LYS:HB3	2:B:90:TYR:CE1	2.51	0.45
1:C:150:ILE:HB	1:C:154:GLU:HG2	1.98	0.45
2:D:33:THR:HG1	2:D:95:GLU:HB3	1.80	0.45
2:D:38:LYS:HZ2	2:D:40:ARG:NH2	2.14	0.45
1:A:9:LYS:HB2	1:A:9:LYS:HE3	1.74	0.45
1:A:98:PHE:CD2	2:B:45:LEU:CB	2.99	0.45
2:B:39:GLN:O	2:B:88:ALA:HB1	2.17	0.45
2:B:252:SER:O	2:B:277:VAL:HG12	2.15	0.45
2:B:264:LEU:CD1	2:B:459:LEU:HB3	2.46	0.45
2:B:343:ASN:CG	2:B:350:PRO:HB3	2.42	0.45
2:D:27:TYR:N	2:D:27:TYR:HD1	2.14	0.45
1:A:149:LYS:HA	1:A:154:GLU:O	2.16	0.45
2:B:388:LEU:HD12	2:B:388:LEU:N	2.32	0.45
1:C:98:PHE:CZ	2:D:37:ILE:HD13	2.52	0.45
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.78	0.45
2:B:274:CYS:HB3	2:B:290:TRP:CH2	2.52	0.45
2:D:407:GLN:HG2	2:D:414:GLN:C	2.42	0.45
1:A:150:ILE:HD12	1:A:156:GLN:CD	2.42	0.45
2:B:274:CYS:HB3	2:B:290:TRP:CZ2	2.52	0.44
2:B:327:ILE:CD1	2:B:328:MET:HE3	2.46	0.44
1:A:6:THR:HG23	1:A:88:CYS:SG	2.57	0.44
2:B:136:SER:HA	2:B:195:SER:OG	2.16	0.44
1:C:11:MET:O	1:C:104:LEU:HD23	2.16	0.44
1:A:62:PHE:CE1	1:A:75:ILE:HD13	2.52	0.44
2:B:4:LEU:HD22	2:B:92:CYS:SG	2.56	0.44
1:C:62:PHE:CE1	1:C:75:ILE:HD13	2.52	0.44
2:D:15:GLY:N	2:D:82(C):LEU:O	2.51	0.44
2:D:59:TYR:CE2	2:D:67:ALA:O	2.70	0.44
2:D:93:VAL:HG12	2:D:94:ARG:N	2.31	0.44
2:B:34:ILE:HG12	2:B:94:ARG:CB	2.48	0.44
2:D:33:THR:HG22	2:D:52(A):PRO:HD3	2.00	0.44
2:D:196:SER:N	2:D:199:PRO:HD2	2.33	0.44
2:D:313:PHE:CE2	2:D:320:ARG:HD3	2.52	0.44
2:D:313:PHE:HB3	2:D:314:ASN:H	1.57	0.44
1:A:98:PHE:CZ	2:B:37:ILE:HD13	2.52	0.44
2:B:256:PHE:HA	2:B:257:PRO:HD3	1.78	0.44
2:D:40:ARG:NE	2:D:85:ASP:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:MET:HE2	2:B:90:TYR:HB2	1.98	0.44
2:B:58:ASN:N	2:B:58:ASN:OD1	2.50	0.44
2:B:344:SER:HB3	2:B:347:PHE:CD1	2.53	0.44
2:D:200:ARG:HH22	2:D:227:PRO:CD	2.23	0.44
2:B:171:VAL:HG22	2:B:191:VAL:HG23	2.00	0.44
1:A:7:VAL:HG12	1:A:8:SER:OG	2.18	0.44
1:A:163:TRP:HA	1:A:175:MET:HB2	1.99	0.44
2:D:89:VAL:HA	2:D:108:THR:HA	2.00	0.44
1:C:94:TYR:HD2	2:D:47:TRP:CH2	2.35	0.44
2:B:17:SER:OG	2:B:82(A):SER:HA	2.17	0.43
2:D:152:VAL:HG12	2:D:212:HIS:HA	1.99	0.43
2:D:163:SER:H	2:D:209:ASN:ND2	2.16	0.43
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.76	0.43
2:B:191:VAL:HG13	2:B:191:VAL:O	2.19	0.43
2:D:6:GLU:N	2:D:6:GLU:OE1	2.51	0.43
2:D:36:TRP:C	2:D:37:ILE:HG13	2.43	0.43
2:D:84:SER:HA	2:D:111:VAL:CB	2.43	0.43
2:D:468:THR:HG22	2:D:469:GLU:H	1.83	0.43
2:B:15:GLY:N	2:B:82(C):LEU:O	2.51	0.43
2:B:50:TYR:CZ	2:B:51:ILE:O	2.71	0.43
2:D:408:SER:O	2:D:411:GLY:N	2.51	0.43
1:A:22:THR:HG22	1:A:72:THR:HA	2.00	0.43
2:B:407:GLN:HG2	2:B:414:GLN:C	2.43	0.43
2:D:401:THR:CG2	2:D:459:LEU:HB2	2.48	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD22	2.01	0.43
2:B:20:MET:HG3	2:B:36:TRP:CH2	2.54	0.43
1:C:14:SER:OG	1:C:107:LYS:HB2	2.17	0.43
2:D:63:PHE:CD1	2:D:63:PHE:N	2.86	0.43
2:D:208:CYS:HB2	2:D:223:ILE:HD11	2.00	0.43
2:D:4:LEU:HD22	2:D:92:CYS:SG	2.59	0.43
2:D:70:THR:OG1	2:D:71:ARG:N	2.50	0.43
2:D:93:VAL:CG1	2:D:94:ARG:H	2.24	0.43
2:D:125:ALA:HB1	2:D:227:PRO:HA	1.99	0.43
2:D:184:LEU:HD23	2:D:184:LEU:HA	1.76	0.43
2:D:410:ASP:HB2	2:D:411:GLY:H	1.73	0.43
2:B:27:TYR:N	2:B:27:TYR:HD1	2.15	0.43
2:B:70:THR:OG1	2:B:71:ARG:N	2.52	0.43
2:B:196:SER:N	2:B:199:PRO:HD2	2.33	0.43
2:B:59:TYR:CE2	2:B:67:ALA:O	2.72	0.43
2:B:137:MET:HA	2:B:193:VAL:O	2.18	0.43
2:B:313:PHE:HB3	2:B:314:ASN:H	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:SER:HA	1:C:103:LYS:H	1.83	0.43
1:A:85:ASP:HA	1:A:102:THR:O	2.19	0.43
2:B:51:ILE:HD13	2:B:71:ARG:CB	2.44	0.43
2:B:140:LEU:HB2	2:B:191:VAL:CG1	2.49	0.43
2:B:144:VAL:HG23	2:B:144:VAL:O	2.19	0.43
2:B:309:ARG:CZ	2:B:310:GLU:HB2	2.49	0.43
2:B:322:VAL:HG12	2:B:323:SER:N	2.34	0.43
2:D:374:PRO:HD3	2:D:388:LEU:HG	2.00	0.43
2:D:392:ILE:HD12	2:D:400:ILE:HD13	2.01	0.43
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.18	0.43
2:B:33:THR:HG22	2:B:52(A):PRO:HD3	2.00	0.43
2:B:50:TYR:CE1	2:B:51:ILE:O	2.71	0.43
2:B:207:THR:HG22	2:B:222:LYS:HG3	2.01	0.43
2:D:90:TYR:HE2	2:D:109:VAL:CG2	2.31	0.43
2:B:33:THR:HG23	2:B:52(A):PRO:HD3	2.00	0.42
2:B:255:ILE:HG13	2:B:273:THR:O	2.17	0.42
1:C:124:GLN:HE22	1:C:131:SER:H	1.65	0.42
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.53	0.42
2:B:95:GLU:HG3	2:B:96:GLY:N	2.24	0.42
2:B:147:TYR:CE1	2:B:185:TYR:HB3	2.54	0.42
2:B:257:PRO:HG3	2:B:355:ILE:HG12	2.00	0.42
2:D:116:THR:HA	2:D:148:PHE:O	2.19	0.42
2:D:226:VAL:HG22	2:D:227:PRO:O	2.20	0.42
2:D:277:VAL:HG13	2:D:278:ASP:H	1.84	0.42
1:A:14:SER:OG	1:A:107:LYS:HB2	2.18	0.42
1:A:121:SER:O	1:A:125:LEU:HG	2.18	0.42
2:B:26:GLY:O	2:B:27:TYR:CB	2.64	0.42
2:B:52:ASN:O	2:B:52(A):PRO:O	2.37	0.42
2:B:152:VAL:HG12	2:B:212:HIS:HA	2.01	0.42
2:B:200:ARG:NH2	2:B:227:PRO:CB	2.77	0.42
2:D:174:PHE:CD2	2:D:188:SER:O	2.73	0.42
2:D:206:VAL:O	2:D:223:ILE:HG12	2.19	0.42
1:A:115:VAL:HA	1:A:135:PHE:O	2.19	0.42
1:A:174:SER:O	2:B:174:PHE:HE1	2.01	0.42
2:B:93:VAL:CG1	2:B:94:ARG:H	2.29	0.42
2:B:301:VAL:HG22	2:B:302:HIS:H	1.84	0.42
1:C:121:SER:O	1:C:125:LEU:HG	2.19	0.42
2:D:50:TYR:CZ	2:D:51:ILE:O	2.72	0.42
2:B:40:ARG:NE	2:B:85:ASP:O	2.53	0.42
2:B:259:LYS:CD	2:B:260:PRO:HD2	2.45	0.42
2:B:408:SER:O	2:B:411:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:HG22	1:C:72:THR:HA	2.00	0.42
2:D:32:TYR:O	2:D:71:ARG:NH2	2.50	0.42
2:D:256:PHE:HB2	2:D:273:THR:CG2	2.49	0.42
2:B:291:PHE:CD2	2:B:296:ASN:HA	2.53	0.42
2:D:365:ARG:O	2:D:460:HIS:NE2	2.52	0.42
2:B:396:PHE:HA	2:B:397:PRO:HA	1.81	0.42
1:C:150:ILE:HD12	1:C:156:GLN:NE2	2.34	0.42
2:D:274:CYS:HB3	2:D:290:TRP:CZ2	2.55	0.42
2:D:427:ASP:CG	2:D:428:THR:H	2.28	0.42
2:B:50:TYR:N	2:B:69:LEU:HD13	2.34	0.42
2:D:53:SER:O	2:D:54:SER:CB	2.68	0.42
2:D:310:GLU:H	2:D:321:VAL:HG22	1.84	0.42
2:B:343:ASN:OD1	2:B:350:PRO:HB3	2.20	0.42
2:D:301:VAL:HG22	2:D:302:HIS:H	1.85	0.42
1:A:13:MET:HG3	1:A:17:GLU:OE1	2.20	0.42
1:A:65:SER:O	1:A:72:THR:N	2.53	0.42
2:B:53:SER:O	2:B:54:SER:CB	2.67	0.42
1:C:150:ILE:HD12	1:C:156:GLN:CD	2.45	0.42
2:D:147:TYR:CE1	2:D:185:TYR:HB3	2.55	0.42
2:D:274:CYS:HB3	2:D:290:TRP:CH2	2.55	0.42
2:B:406:TRP:CE3	2:B:441:LEU:HD22	2.54	0.41
1:C:118:PHE:CE2	2:D:124:LEU:O	2.73	0.41
1:C:144:ILE:HD12	1:C:145:ASN:H	1.85	0.41
1:C:164:THR:CG2	1:C:174:SER:H	2.29	0.41
1:C:174:SER:O	2:D:174:PHE:HE1	2.03	0.41
2:D:140:LEU:HB2	2:D:191:VAL:CG1	2.50	0.41
2:D:191:VAL:O	2:D:191:VAL:HG13	2.20	0.41
2:D:396:PHE:HA	2:D:397:PRO:HA	1.82	0.41
2:B:283:ASP:HA	2:B:284:PRO:HD2	1.95	0.41
2:B:374:PRO:HD3	2:B:388:LEU:HG	2.01	0.41
2:D:154:VAL:HG22	2:D:210:VAL:CG1	2.49	0.41
1:A:118:PHE:CE2	2:B:124:LEU:O	2.73	0.41
2:B:312:GLN:HG2	2:B:319:PHE:CE1	2.54	0.41
2:B:468:THR:HG22	2:B:469:GLU:H	1.84	0.41
1:C:163:TRP:HA	1:C:175:MET:HB2	2.00	0.41
1:A:61:ARG:HH12	1:A:82:ASP:CG	2.27	0.41
2:B:369:VAL:CG2	2:B:392:ILE:HG22	2.50	0.41
2:D:245:PRO:HB2	2:D:249:GLU:H	1.72	0.41
2:D:255:ILE:HG13	2:D:273:THR:O	2.19	0.41
2:D:327:ILE:CD1	2:D:328:MET:HE3	2.50	0.41
1:A:90:GLN:HE22	1:A:96:TYR:HD1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:ARG:O	2:B:202:PRO:C	2.64	0.41
2:B:360:LYS:O	2:B:396:PHE:HE1	2.04	0.41
2:D:153:THR:O	2:D:210:VAL:HA	2.21	0.41
2:B:163:SER:H	2:B:209:ASN:ND2	2.19	0.41
2:B:353:LYS:HE2	2:B:353:LYS:HB3	1.89	0.41
2:B:417:GLU:O	2:B:418:ASN:HB2	2.20	0.41
1:C:9:LYS:HB2	1:C:9:LYS:HE3	1.80	0.41
1:C:13:MET:HG3	1:C:17:GLU:OE1	2.21	0.41
2:D:312:GLN:HG2	2:D:319:PHE:CE1	2.55	0.41
2:D:444:GLN:H	2:D:444:GLN:CD	2.29	0.41
1:C:90:GLN:HE22	1:C:96:TYR:HA	1.86	0.41
1:C:136:LEU:N	1:C:136:LEU:CD1	2.83	0.41
1:C:214:CYS:CB	2:D:235:CYS:HA	2.33	0.41
2:D:148:PHE:HA	2:D:149:PRO:HA	1.83	0.41
2:D:290:TRP:HA	2:D:339:LYS:O	2.20	0.41
2:B:53:SER:OG	2:B:55:VAL:HG23	2.20	0.41
2:B:338:PHE:HB2	2:B:355:ILE:HG22	2.03	0.41
2:B:369:VAL:O	2:B:369:VAL:HG13	2.21	0.41
2:D:137:MET:HA	2:D:193:VAL:O	2.20	0.41
2:D:333:LEU:HD13	2:D:466:HIS:HE1	1.86	0.41
1:A:36:TYR:OH	2:B:98:VAL:HB	2.21	0.41
2:B:63:PHE:CD1	2:B:63:PHE:N	2.89	0.41
2:D:9:ALA:HB2	2:D:20:MET:HB3	2.03	0.41
2:D:195:SER:C	2:D:199:PRO:HD2	2.45	0.41
2:D:277:VAL:HG21	4:F:2:NDG:C1	2.51	0.41
2:D:327:ILE:HG13	2:D:328:MET:N	2.35	0.41
2:D:375:PRO:HG2	2:D:378:GLN:HB3	2.03	0.41
2:D:392:ILE:CD1	2:D:437:VAL:HB	2.42	0.41
1:A:4:ALA:O	1:A:99:GLY:HA2	2.21	0.41
1:A:112:ALA:N	1:A:200:THR:HG21	2.35	0.41
2:B:76:ASN:ND2	2:B:76:ASN:N	2.69	0.41
2:D:266:ILE:HA	2:D:329:HIS:HE1	1.84	0.41
2:D:309:ARG:CZ	2:D:310:GLU:HB2	2.51	0.41
1:A:167:ASP:O	1:A:171:SER:HA	2.21	0.40
1:A:191:SER:HA	1:A:209:PHE:O	2.20	0.40
1:A:203:SER:HB2	1:A:204:PRO:HD2	2.03	0.40
2:B:51:ILE:HG23	2:B:71:ARG:HH11	1.86	0.40
2:B:366:ALA:HB1	2:B:463:LEU:HD23	2.04	0.40
2:B:392:ILE:HD12	2:B:400:ILE:HD13	2.03	0.40
1:C:33:VAL:HG21	1:C:71:PHE:CD2	2.56	0.40
2:D:359:THR:HG22	2:D:359:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:TRP:CE3	2:D:441:LEU:HD22	2.56	0.40
2:B:313:PHE:CE2	2:B:320:ARG:HD3	2.56	0.40
1:C:105:GLU:HG3	1:C:166:GLN:HE22	1.85	0.40
1:C:129:GLY:H	1:C:183:LYS:HB2	1.86	0.40
1:C:163:TRP:HB3	1:C:164:THR:H	1.72	0.40
1:C:198:HIS:CG	1:C:199:LYS:H	2.39	0.40
2:D:144:VAL:CG2	2:D:187:LEU:HD13	2.51	0.40
2:D:253:VAL:HG22	2:D:254:PHE:N	2.36	0.40
2:B:41:PRO:O	2:B:43:GLN:HG2	2.21	0.40
2:B:375:PRO:HG2	2:B:378:GLN:HB3	2.03	0.40
2:B:444:GLN:H	2:B:444:GLN:CD	2.29	0.40
1:C:65:SER:O	1:C:72:THR:N	2.54	0.40
1:A:29:VAL:O	1:A:30:VAL:C	2.63	0.40
1:A:198:HIS:CG	1:A:199:LYS:H	2.40	0.40
2:B:52(A):PRO:HB2	2:B:53:SER:H	1.75	0.40
2:B:372:ILE:HG21	2:D:372:ILE:CG2	2.38	0.40
2:D:163:SER:H	2:D:209:ASN:HD21	1.70	0.40
2:D:238:LYS:HD3	2:D:238:LYS:HA	1.89	0.40
2:D:309:ARG:CB	2:D:321:VAL:HG13	2.48	0.40
1:A:167:ASP:CG	1:A:170:ASP:HB3	2.46	0.40
1:C:29:VAL:O	1:C:30:VAL:C	2.64	0.40
1:C:134:CYS:O	1:C:136:LEU:CD1	2.70	0.40
2:D:94:ARG:HG2	2:D:94:ARG:HH11	1.86	0.40
2:D:103:TRP:H	2:D:103:TRP:HD1	1.69	0.40
2:D:259:LYS:CD	2:D:260:PRO:HD2	2.46	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:SER:H	2:D:23:LYS:HZ3[1_554]	1.25	0.35
2:B:23:LYS:HZ3	2:D:196:SER:H[1_554]	1.33	0.27

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	211/213 (99%)	168 (80%)	32 (15%)	11 (5%)	1	12
1	C	211/213 (99%)	169 (80%)	32 (15%)	10 (5%)	2	14
2	B	432/434 (100%)	301 (70%)	89 (21%)	42 (10%)	0	3
2	D	432/434 (100%)	302 (70%)	80 (18%)	50 (12%)	0	1
All	All	1286/1294 (99%)	940 (73%)	233 (18%)	113 (9%)	0	3

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	138	ASN
2	B	9	ALA
2	B	27	TYR
2	B	54	SER
2	B	55	VAL
2	B	61	GLN
2	B	73	ARG
2	B	97	GLU
2	B	215	SER
2	B	304	ALA
2	B	309	ARG
2	B	369	VAL
1	C	30	VAL
1	C	138	ASN
2	D	9	ALA
2	D	54	SER
2	D	55	VAL
2	D	73	ARG
2	D	97	GLU
2	D	215	SER
2	D	250	VAL
2	D	295	ASP
2	D	304	ALA
2	D	309	ARG
2	D	369	VAL
1	A	151	ASP
1	A	211	ARG
2	B	8	GLY
2	B	16	ALA

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Mol	Chain	Res	Type
2	B	50	TYR
2	B	52(A)	PRO
2	B	62	ARG
2	B	65	ASP
2	B	76	ASN
2	B	203	SER
2	B	295	ASP
2	B	306	THR
2	B	310	GLU
2	B	312	GLN
2	B	317	SER
2	B	355	ILE
2	B	453	THR
1	C	151	ASP
1	C	211	ARG
2	D	8	GLY
2	D	16	ALA
2	D	27	TYR
2	D	50	TYR
2	D	52(A)	PRO
2	D	61	GLN
2	D	62	ARG
2	D	76	ASN
2	D	203	SER
2	D	237	CYS
2	D	306	THR
2	D	310	GLU
2	D	312	GLN
2	D	317	SER
2	D	355	ILE
2	D	361	GLY
2	D	453	THR
1	A	53	ASN
1	A	150	ILE
2	B	48	ILE
2	B	95	GLU
2	B	167	SER
2	B	284	PRO
1	C	53	ASN
1	C	150	ILE
2	D	48	ILE
2	D	65	ASP

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Mol	Chain	Res	Type
2	D	84	SER
2	D	95	GLU
2	D	167	SER
2	D	249	GLU
2	D	284	PRO
2	D	357	SER
2	B	286	VAL
2	B	303	THR
2	B	357	SER
2	B	410	ASP
2	B	416	PRO
1	C	8	SER
1	C	200	THR
2	D	245	PRO
2	D	286	VAL
2	D	303	THR
2	D	330	GLN
2	D	416	PRO
1	A	8	SER
1	A	77	SER
1	A	84	ALA
1	A	156	GLN
1	A	200	THR
2	B	84	SER
2	B	239	PRO
2	B	313	PHE
1	C	77	SER
1	C	84	ALA
2	D	313	PHE
2	D	410	ASP
2	D	119	PRO
2	B	41	PRO
2	B	93	VAL
2	B	119	PRO
2	D	41	PRO
2	D	93	VAL
2	D	223	ILE
2	D	241	ILE
2	D	270	PRO
2	B	149	PRO
2	D	149	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	188/188 (100%)	159 (85%)	29 (15%)	2	14
1	C	188/188 (100%)	162 (86%)	26 (14%)	3	18
2	B	390/390 (100%)	322 (83%)	68 (17%)	2	10
2	D	390/390 (100%)	326 (84%)	64 (16%)	2	12
All	All	1156/1156 (100%)	969 (84%)	187 (16%)	2	12

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	5	HIS
1	A	12	SER
1	A	21	LEU
1	A	46	LEU
1	A	48	ILE
1	A	61	ARG
1	A	73	LEU
1	A	79	GLN
1	A	83	LEU
1	A	87	HIS
1	A	94	TYR
1	A	97	THR
1	A	104	LEU
1	A	108	ARG
1	A	116	SER
1	A	133	VAL
1	A	135	PHE
1	A	137	ASN
1	A	144	ILE
1	A	150	ILE
1	A	154	GLU
1	A	155	ARG
1	A	165	ASP

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Mol	Chain	Res	Type
1	A	169	LYS
1	A	178	THR
1	A	182	THR
1	A	199	LYS
1	A	210	ASN
2	B	2	VAL
2	B	3	LYS
2	B	4	LEU
2	B	5	GLN
2	B	6	GLU
2	B	18	VAL
2	B	20	MET
2	B	21	SER
2	B	27	TYR
2	B	28	THR
2	B	34	ILE
2	B	41	PRO
2	B	48	ILE
2	B	58	ASN
2	B	69	LEU
2	B	70	THR
2	B	73	ARG
2	B	76	ASN
2	B	77	THR
2	B	80	ILE
2	B	82	LEU
2	B	82(A)	SER
2	B	82(B)	SER
2	B	82(C)	LEU
2	B	85	ASP
2	B	92	CYS
2	B	93	VAL
2	B	94	ARG
2	B	97	GLU
2	B	98	VAL
2	B	105	GLN
2	B	107	THR
2	B	110	THR
2	B	133	GLN
2	B	151	PRO
2	B	152	VAL
2	B	173	THR

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Mol	Chain	Res	Type
2	B	175	PRO
2	B	187	LEU
2	B	200	ARG
2	B	209	ASN
2	B	235	CYS
2	B	238	LYS
2	B	240	CYS
2	B	241	ILE
2	B	260	PRO
2	B	274	CYS
2	B	281	LYS
2	B	295	ASP
2	B	299	VAL
2	B	305	GLN
2	B	307	GLN
2	B	309	ARG
2	B	312	GLN
2	B	325	LEU
2	B	328	MET
2	B	352	GLU
2	B	381	MET
2	B	388	LEU
2	B	393	THR
2	B	405	GLU
2	B	410	ASP
2	B	414	GLN
2	B	416	PRO
2	B	421	ASN
2	B	425	ILE
2	B	443	VAL
2	B	467	HIS
1	C	3	CYS
1	C	5	HIS
1	C	12	SER
1	C	13	MET
1	C	21	LEU
1	C	33	VAL
1	C	46	LEU
1	C	73	LEU
1	C	79	GLN
1	C	83	LEU
1	C	87	HIS

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Mol	Chain	Res	Type
1	C	97	THR
1	C	104	LEU
1	C	108	ARG
1	C	116	SER
1	C	133	VAL
1	C	135	PHE
1	C	137	ASN
1	C	144	ILE
1	C	150	ILE
1	C	154	GLU
1	C	155	ARG
1	C	165	ASP
1	C	169	LYS
1	C	178	THR
1	C	199	LYS
2	D	2	VAL
2	D	3	LYS
2	D	4	LEU
2	D	5	GLN
2	D	6	GLU
2	D	18	VAL
2	D	20	MET
2	D	21	SER
2	D	22	CYS
2	D	27	TYR
2	D	28	THR
2	D	34	ILE
2	D	41	PRO
2	D	58	ASN
2	D	69	LEU
2	D	70	THR
2	D	73	ARG
2	D	76	ASN
2	D	77	THR
2	D	80	ILE
2	D	82	LEU
2	D	82(A)	SER
2	D	82(B)	SER
2	D	82(C)	LEU
2	D	85	ASP
2	D	92	CYS
2	D	93	VAL

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Mol	Chain	Res	Type
2	D	94	ARG
2	D	97	GLU
2	D	105	GLN
2	D	110	THR
2	D	133	GLN
2	D	152	VAL
2	D	173	THR
2	D	175	PRO
2	D	187	LEU
2	D	200	ARG
2	D	209	ASN
2	D	226	VAL
2	D	235	CYS
2	D	244	VAL
2	D	260	PRO
2	D	274	CYS
2	D	281	LYS
2	D	295	ASP
2	D	299	VAL
2	D	305	GLN
2	D	307	GLN
2	D	309	ARG
2	D	312	GLN
2	D	325	LEU
2	D	343	ASN
2	D	352	GLU
2	D	381	MET
2	D	388	LEU
2	D	393	THR
2	D	405	GLU
2	D	410	ASP
2	D	414	GLN
2	D	416	PRO
2	D	421	ASN
2	D	425	ILE
2	D	443	VAL
2	D	467	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	137	ASN
2	B	5	GLN
2	B	43	GLN
2	B	133	GLN
2	B	135	ASN
2	B	305	GLN
2	B	307	GLN
2	B	312	GLN
2	B	329	HIS
2	B	334	ASN
2	B	407	GLN
2	B	414	GLN
2	B	423	GLN
2	B	444	GLN
2	B	465	ASN
2	B	474	HIS
1	C	124	GLN
1	C	137	ASN
1	C	210	ASN
2	D	5	GLN
2	D	35	HIS
2	D	43	GLN
2	D	135	ASN
2	D	305	GLN
2	D	307	GLN
2	D	312	GLN
2	D	329	HIS
2	D	334	ASN
2	D	407	GLN
2	D	414	GLN
2	D	444	GLN
2	D	465	ASN
2	D	466	HIS
2	D	474	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	1.17	2 (14%)	17,19,21	1.13	1 (5%)
3	NDG	E	2	3	14,14,15	0.72	0	17,19,21	1.11	2 (11%)
3	BMA	E	3	3	11,11,12	0.72	0	15,15,17	0.50	0
3	MAN	E	4	3	11,11,12	0.53	0	15,15,17	0.59	0
3	NAG	E	5	3	14,14,15	0.56	0	17,19,21	0.70	0
3	GAL	E	6	3	11,11,12	0.70	0	15,15,17	0.49	0
3	MAN	E	7	3	11,11,12	0.68	0	15,15,17	0.57	0
3	NAG	E	8	3	14,14,15	0.41	0	17,19,21	0.61	0
3	FUL	E	9	3	10,10,11	0.36	0	14,14,16	0.38	0
4	NAG	F	1	4,2	14,14,15	0.84	0	17,19,21	1.18	1 (5%)
4	NDG	F	2	4	14,14,15	0.66	0	17,19,21	1.16	2 (11%)
4	BMA	F	3	4	11,11,12	0.81	0	15,15,17	0.44	0
4	MAN	F	4	4	11,11,12	0.41	0	15,15,17	0.57	0
4	NAG	F	5	4	14,14,15	0.55	0	17,19,21	0.68	0
4	GAL	F	6	4	11,11,12	0.64	0	15,15,17	0.45	0
4	MAN	F	7	4	11,11,12	0.68	0	15,15,17	0.56	0
4	NAG	F	8	4	14,14,15	0.44	0	17,19,21	0.61	0
4	FUC	F	9	4	10,10,11	0.41	0	14,14,16	0.44	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	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	E	2	3	-	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	-	2/6/23/26	0/1/1/1
3	GAL	E	6	3	-	0/2/19/22	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	4,2	-	0/6/23/26	0/1/1/1
4	NDG	F	2	4	-	1/6/23/26	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	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
4	NAG	F	8	4	-	2/6/23/26	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	2.57	1.55	1.52
3	E	1	NAG	O5-C5	2.09	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	3.51	116.89	112.19
3	E	1	NAG	C1-O5-C5	3.23	116.52	112.19
4	F	2	NDG	O5-C1-C2	3.14	116.14	111.29
3	E	2	NDG	O5-C1-C2	3.08	116.05	111.29
3	E	2	NDG	C1-O5-C5	2.40	115.40	112.19
4	F	2	NDG	C1-O5-C5	2.37	115.37	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	9	FUC	C1

All (10) torsion outliers are listed below:

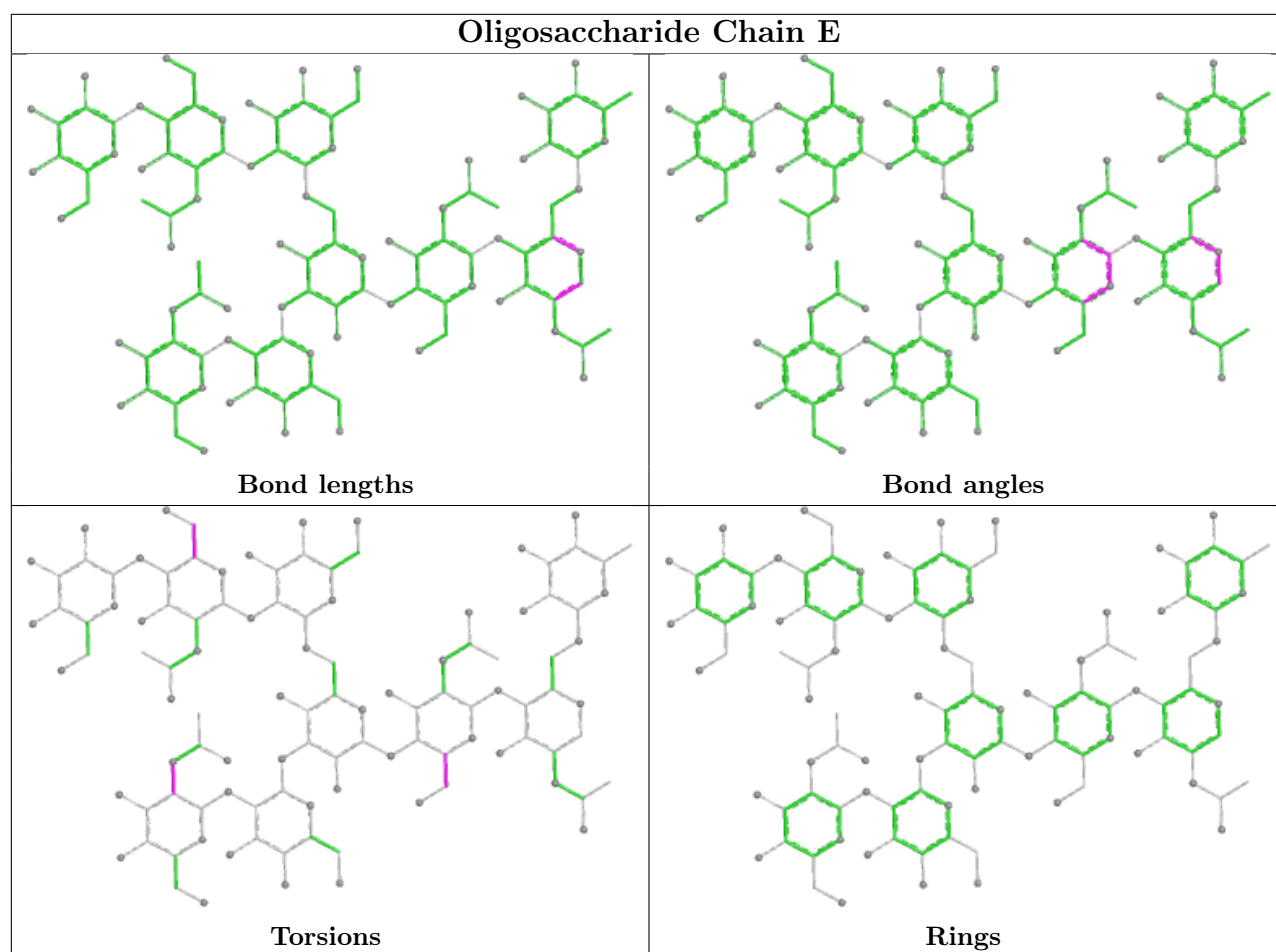
Mol	Chain	Res	Type	Atoms
3	E	5	NAG	O5-C5-C6-O6
4	F	5	NAG	O5-C5-C6-O6
3	E	2	NDG	O5-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6
3	E	8	NAG	C1-C2-N2-C7
4	F	8	NAG	C1-C2-N2-C7
3	E	5	NAG	C4-C5-C6-O6
3	E	8	NAG	C3-C2-N2-C7
4	F	8	NAG	C3-C2-N2-C7
4	F	5	NAG	C4-C5-C6-O6

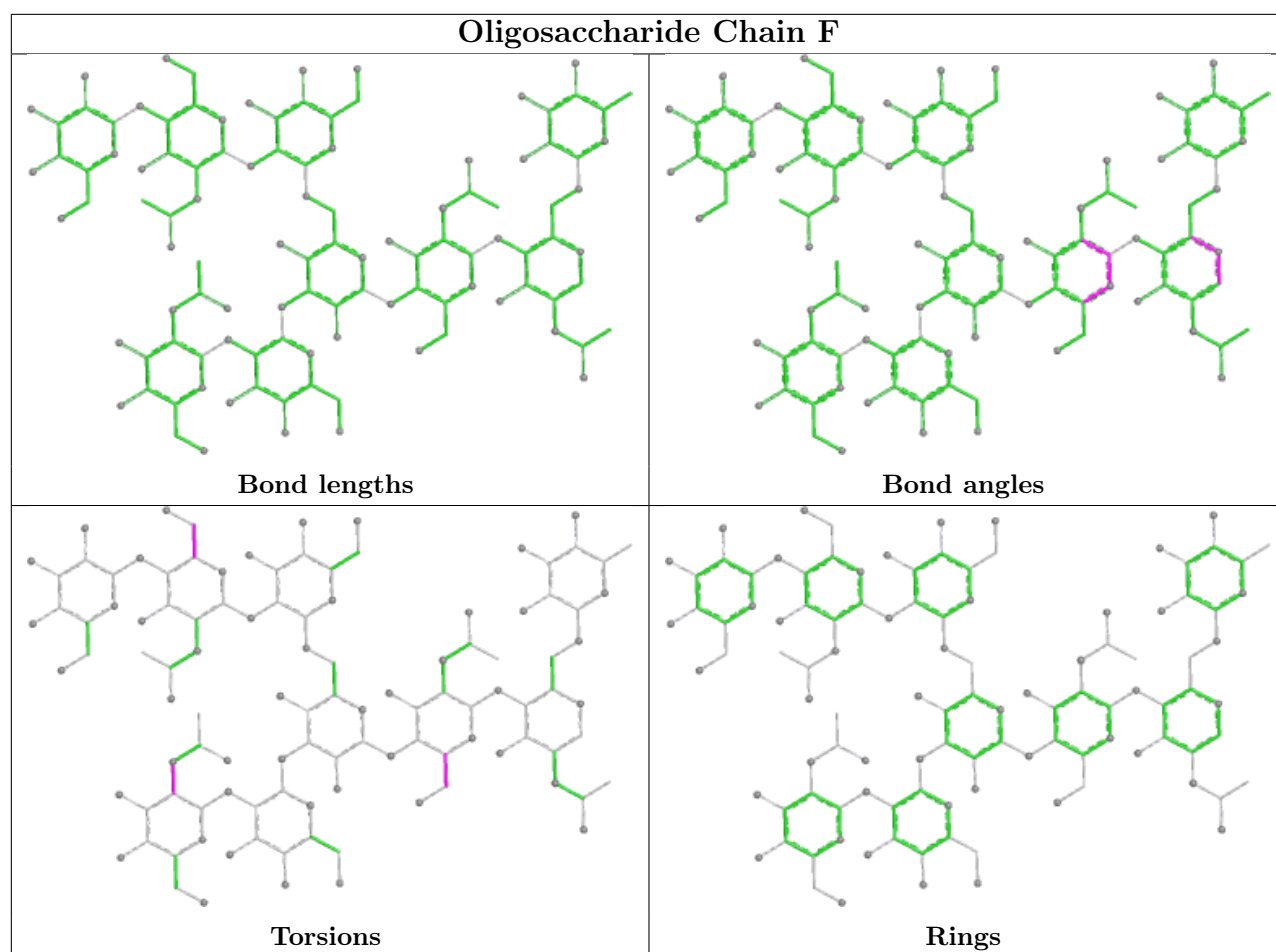
There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	NAG	1	0
4	F	5	NAG	1	0
4	F	6	GAL	1	0
3	E	6	GAL	1	0
4	F	2	NDG	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](#)

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.