



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3J0A
EMDB ID: : EMD-5287
Title : Homology model of human Toll-like receptor 5 fitted into an electron microscopy single particle reconstruction
Authors : Modis, Y.; Zhou, K.; Kanai, R.; Lee, P.; Wang, H.W.
Deposited on : 2011-06-02
Resolution : 26.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

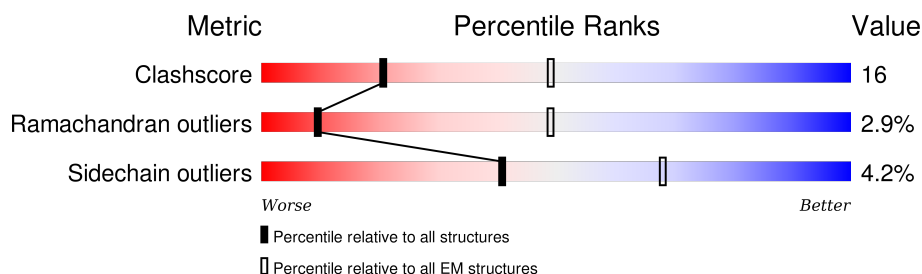
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 26.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	844	 60% 31% • 6%
1	B	844	 46% 26% • 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11828 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Toll-like receptor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			6437	4155	1081	1176	25		
1	B	632	Total	C	N	O	S	0	0
			5055	3272	839	927	17		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	859	GLY	-	EXPRESSION TAG	UNP O60602
A	860	SER	-	EXPRESSION TAG	UNP O60602
A	861	HIS	-	EXPRESSION TAG	UNP O60602
A	862	HIS	-	EXPRESSION TAG	UNP O60602
A	863	HIS	-	EXPRESSION TAG	UNP O60602
A	864	HIS	-	EXPRESSION TAG	UNP O60602
A	865	HIS	-	EXPRESSION TAG	UNP O60602
A	866	HIS	-	EXPRESSION TAG	UNP O60602
B	859	GLY	-	EXPRESSION TAG	UNP O60602
B	860	SER	-	EXPRESSION TAG	UNP O60602
B	861	HIS	-	EXPRESSION TAG	UNP O60602
B	862	HIS	-	EXPRESSION TAG	UNP O60602
B	863	HIS	-	EXPRESSION TAG	UNP O60602
B	864	HIS	-	EXPRESSION TAG	UNP O60602
B	865	HIS	-	EXPRESSION TAG	UNP O60602
B	866	HIS	-	EXPRESSION TAG	UNP O60602

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			168	98	7	63	
2	A	2	Total	C	N	O	0
			168	98	7	63	

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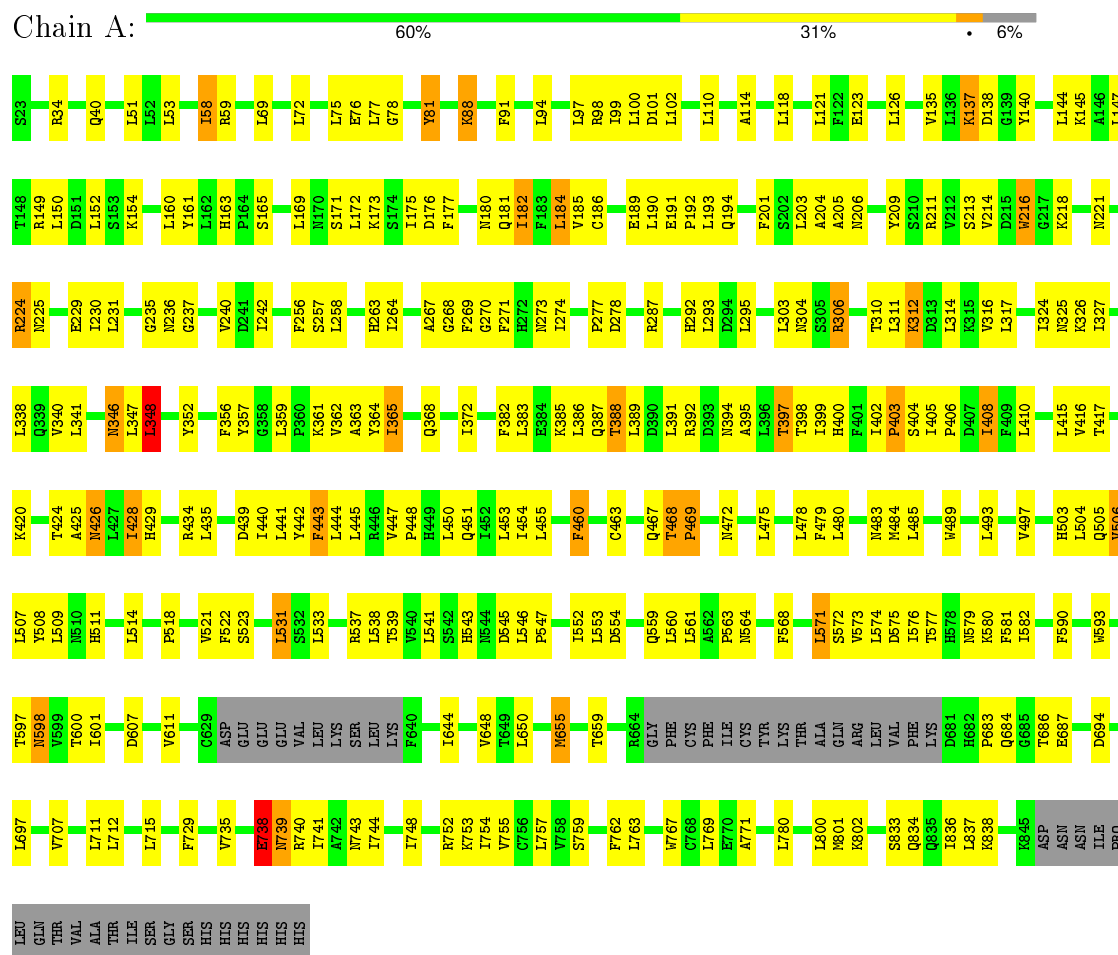
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Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0

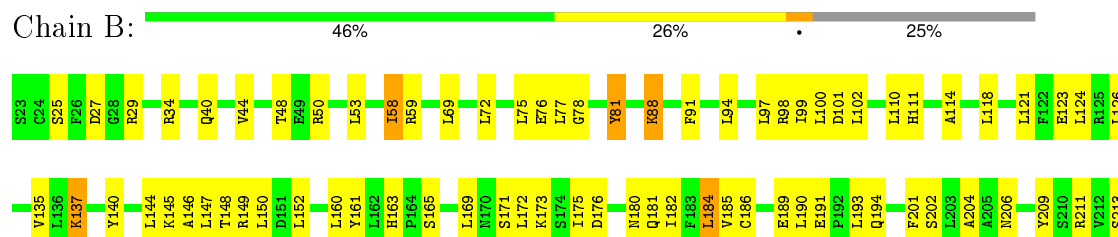
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Molecule 1: Toll-like receptor 5



- Molecule 1: Toll-like receptor 5



PHE	TRP	ASP	P605	HE03	S404	N318	W216
VAL	ASN	MET	I608	L504	I405	N325	N221
GLN	SER	TYR		Q505	P406		P222
GLN	ARG	LYS	V611	V506	I408	A331	F223
GLN	ILE	TYR		L507	F409	L335	R224
TYR	VAL	ALA	P616	Y608	L410		N225
LEU	CYS	TYR		L509		L338	
ARG	LEU	LEU	C629	N510	L415	Q339	E229
VAL	VAL	CYS	GLU	H511	Y416	V340	I230
PRO	SER	PHE	GLU		T417	L341	
GLU	ARG	SER	GLU	L514	K420	N342	G235
ASP	HIS	SER		P518			N236
PHE	PHE	LYS	VAL			N346	G237
GLN	LEU	ASP	LEU	V521	T424	L347	
ASP	ARG	PHE	LYS	F522	A425		
VAL	ASP	THR	SER	S523	N426	L348	V240
GLY	GLY	THR	LEU		L427	G349	G241
TRP	TRP	VAL	LYS		I428	E350	I242
PHE	CYS	GLN	F640	L531	H429		
LEU	ASN	ASN		S532		F356	F246
HIS	GLU	ALA	I644	L533	R434	Y357	
LEU	ALA	LEU	V645		L435	G358	I250
PHE	PHE	LEU		L538		L359	
SER	SER	LYS	V648	T539	D439	P360	F256
GLN	TYR	HIS		Y540	I440	K361	S257
GLN	ALA	LEU	F653	L541	L441	V362	
ILE	GLN	ASP	L654		Y442	A363	H263
LEU	GLY	THR	V655	L546	F443	Y364	I264
LYS	ARG	GLN	V656	P547	L444	I365	
LYS	CYS	TYR	I657				G268
GLU	LEU	SER		D554	V447	K369	F269
LYS	SER	ASP	V660	I555	P448	N370	G270
GLU	GLN	GLN			H449	H371	
LYS	LEU	ASN	F663	Q559	L450	I372	I273
LYS	ASN	ARG	B664	L560	Q451		I274
LYS	SER	PHE		L561	I452	I375	K275
ASP	ALA	ASN	PHE	A562	L453		D276
ASN	LEU	LEU	GLY	P563	I454	F380	F277
ASN	ILE	CYS	PHE		L455	K381	D278
ILE	MET	PHE	PHE	F568		F382	
PRO	VAL	GLU	CYS		F460	L383	R287
LEU	VAL	GLU	TYR	L571		E384	
GLN	VAL	ARG	LYS		Q467	K385	H292
THR	GLY	ASP	THR	L574	T468	L386	
VAL	SER	PHE	ALA	D575	P469	Q387	L295
ALA	LEU	VAL	GLN	I576		T388	
THR	SER	PRO	ARG		L475	L389	L303
ILE	GLN	GLY	LEU	K580		D390	N304
SER	TYR	GLU	VAL	F581	L478	L391	S305
GLN	GLN	ASN	PHE	I582	F479		R306
SER	GLN	LYS	LYS		L480	A395	V307
HIS	MET	ILE	ASP	F590	E481	L396	
HIS	LYS	ALA	ALA		N482	T397	T310
HIS	ASN	PRO	PRO	HIS	N483	T398	L311
HIS	ILE	GLN	GLN	T597	N484	I399	K312
HIS	SER	GLN	GLY	N598		H400	B313
HIS	ASP	ASP	THR	Y599	W489	F401	L314
	ALA	ALA	GLU	I601		I402	L317
	GLY	ILE	PRO			P403	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	4241	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	52000	Depositor
Image detector	Gatan Ultra4000	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.87	7/6589 (0.1%)	0.61	1/8938 (0.0%)
1	B	0.75	2/5172 (0.0%)	0.59	3/7029 (0.0%)
All	All	0.82	9/11761 (0.1%)	0.61	4/15967 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	GLU	CD-OE1	-28.34	0.94	1.25
1	A	738	GLU	CD-OE2	9.38	1.35	1.25
1	A	582	ILE	C-O	7.25	1.37	1.23
1	A	738	GLU	CA-C	7.20	1.71	1.52
1	B	616	PHE	CE2-CZ	6.46	1.49	1.37
1	A	739	ASN	CB-CG	-5.80	1.37	1.51
1	B	582	ILE	C-O	5.66	1.34	1.23
1	A	738	GLU	CG-CD	-5.36	1.44	1.51
1	A	738	GLU	C-O	5.08	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	GLU	OE1-CD-OE2	-11.45	109.56	123.30
1	B	664	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	B	664	ARG	NH1-CZ-NH2	5.22	125.15	119.40
1	B	660	VAL	CG1-CB-CG2	-5.15	102.66	110.90

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	6437	0	6385	214	0
1	B	5055	0	5041	160	0
2	A	168	0	154	2	0
2	B	168	0	154	2	0
All	All	11828	0	11734	372	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 16.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:LEU:HD13	1:B:538:LEU:HG	1.55	0.87
1:A:748:ILE:HG23	1:A:754:ILE:HD11	1.58	0.86
1:A:123:GLU:HG2	1:A:149:ARG:HB3	1.58	0.85
1:B:123:GLU:HG2	1:B:149:ARG:HB3	1.58	0.85
1:A:707:VAL:HG13	1:A:711:LEU:HD23	1.64	0.78
1:A:389:LEU:HB3	1:A:408:ILE:HG22	1.63	0.78
1:B:389:LEU:HB3	1:B:408:ILE:HG22	1.65	0.77
1:B:600:THR:HG23	1:B:601:ILE:HG13	1.66	0.75
1:A:398:THR:HG23	1:A:417:THR:HG21	1.67	0.75
1:A:365:ILE:HD12	1:A:386:LEU:HD11	1.67	0.74
1:A:600:THR:HG23	1:A:601:ILE:HG13	1.67	0.74
1:B:98:ARG:HG2	1:B:99:ILE:HG23	1.70	0.74
1:A:317:LEU:HD23	1:A:338:LEU:HD13	1.70	0.73
1:A:400:HIS:HA	1:A:420:LYS:HD2	1.69	0.73
1:A:738:GLU:HA	1:A:738:GLU:OE2	1.89	0.72
1:B:400:HIS:HA	1:B:420:LYS:HD2	1.72	0.72
1:B:257:SER:HA	1:B:292:HIS:HB3	1.70	0.72
1:B:347:LEU:HG	1:B:372:ILE:HD11	1.71	0.72
1:B:340:VAL:HG11	2:B:1342:NAG:H83	1.71	0.72
1:B:356:PHE:HB3	1:B:359:LEU:HD12	1.72	0.71
1:A:340:VAL:HG11	2:A:1342:NAG:H83	1.70	0.71
1:B:335:LEU:HD13	1:B:338:LEU:HD22	1.70	0.70
1:A:257:SER:HA	1:A:292:HIS:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LYS:HD3	1:A:611:VAL:HG21	1.73	0.69
1:B:365:ILE:HD12	1:B:386:LEU:HD11	1.73	0.69
1:A:98:ARG:HG2	1:A:99:ILE:HG23	1.75	0.68
1:B:398:THR:HG23	1:B:417:THR:HG21	1.75	0.68
1:B:523:SER:HA	1:B:546:LEU:HD23	1.76	0.67
1:A:347:LEU:HG	1:A:372:ILE:HD11	1.77	0.67
1:A:507:LEU:HB2	1:A:509:LEU:HG	1.78	0.66
1:A:468:THR:HB	1:A:469:PRO:HD3	1.78	0.66
1:B:511:HIS:HA	1:B:514:LEU:HD12	1.77	0.66
1:B:386:LEU:HD23	1:B:405:ILE:HD11	1.77	0.66
1:B:147:LEU:HD11	1:B:150:LEU:HD23	1.78	0.66
1:A:426:ASN:HD22	1:A:426:ASN:H	1.44	0.65
1:B:426:ASN:HD22	1:B:426:ASN:H	1.44	0.65
1:B:563:PRO:HD3	1:B:590:PHE:HB2	1.79	0.65
1:B:531:LEU:HD12	1:B:533:LEU:HG	1.79	0.65
1:A:221:ASN:HB2	1:A:224:ARG:HB2	1.79	0.64
1:B:468:THR:HB	1:B:469:PRO:HD3	1.80	0.64
1:B:88:LYS:H	1:B:88:LYS:HD3	1.62	0.64
1:A:161:TYR:HD1	1:A:189:GLU:HA	1.63	0.64
1:B:475:LEU:HD11	1:B:478:LEU:HB2	1.80	0.64
1:B:541:LEU:HB2	1:B:560:LEU:HD13	1.79	0.64
1:B:597:THR:HA	2:B:2598:NAG:H83	1.78	0.63
1:A:147:LEU:HD11	1:A:150:LEU:HD23	1.80	0.63
1:B:363:ALA:HA	1:B:386:LEU:HA	1.81	0.63
1:A:554:ASP:HA	1:A:575:ASP:HB3	1.80	0.63
1:A:514:LEU:HD13	1:A:538:LEU:HG	1.79	0.63
1:B:221:ASN:HB2	1:B:224:ARG:HB2	1.81	0.63
1:A:489:TRP:H	1:A:509:LEU:HD22	1.63	0.63
1:A:531:LEU:HD12	1:A:533:LEU:HG	1.80	0.62
1:A:597:THR:HA	2:A:2598:NAG:H83	1.80	0.62
1:B:237:GLY:HA3	1:B:242:ILE:HD11	1.82	0.61
1:B:428:ILE:HG22	1:B:450:LEU:HD21	1.82	0.61
1:A:523:SER:HA	1:A:546:LEU:HD23	1.83	0.61
1:A:741:ILE:HG12	1:A:769:LEU:HD12	1.82	0.61
1:A:475:LEU:HD12	1:A:497:VAL:HG11	1.83	0.61
1:A:211:ARG:HH21	1:A:214:VAL:HG13	1.66	0.61
1:B:169:LEU:HB3	1:B:172:LEU:HB2	1.83	0.61
1:A:312:LYS:HD3	1:A:312:LYS:H	1.65	0.61
1:A:163:HIS:ND1	1:A:165:SER:HB3	2.16	0.60
1:B:163:HIS:ND1	1:B:165:SER:HB3	2.16	0.60
1:A:428:ILE:HG22	1:A:450:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HD12	1:A:479:PHE:HB2	1.84	0.60
1:A:479:PHE:HA	1:A:503:HIS:HB3	1.83	0.60
1:A:386:LEU:HD23	1:A:405:ILE:HD11	1.83	0.60
1:A:372:ILE:HB	1:A:395:ALA:HB2	1.84	0.60
1:B:479:PHE:HA	1:B:503:HIS:HB3	1.82	0.60
1:B:435:LEU:HD13	1:B:440:ILE:HD11	1.84	0.59
1:A:135:VAL:HG22	1:A:137:LYS:H	1.68	0.59
1:B:522:PHE:HE2	1:B:531:LEU:HG	1.67	0.58
1:A:267:ALA:HB3	1:A:303:LEU:HA	1.86	0.58
1:A:475:LEU:HD11	1:A:478:LEU:HB2	1.85	0.58
1:B:454:ILE:HD12	1:B:479:PHE:HB2	1.85	0.58
1:A:435:LEU:HD13	1:A:440:ILE:HD11	1.85	0.58
1:A:190:LEU:HB3	1:A:193:LEU:HD12	1.85	0.58
1:B:372:ILE:HB	1:B:395:ALA:HB2	1.87	0.57
1:A:362:VAL:HG13	1:A:386:LEU:HD13	1.87	0.57
1:A:76:GLU:HG3	1:A:101:ASP:HB2	1.86	0.57
1:B:78:GLY:HA3	1:B:102:LEU:HA	1.87	0.57
1:A:752:ARG:HG3	1:A:753:LYS:HD2	1.86	0.57
1:A:505:GLN:HG2	1:A:506:VAL:HG12	1.87	0.57
1:A:697:LEU:HD22	1:A:711:LEU:HD21	1.87	0.57
1:B:75:LEU:HG	1:B:77:LEU:HG	1.87	0.57
1:B:176:ASP:HA	1:B:204:ALA:HB3	1.86	0.57
1:A:478:LEU:HG	1:A:480:LEU:HD21	1.87	0.56
1:A:735:VAL:HB	1:A:738:GLU:HB2	1.87	0.56
1:A:493:LEU:HD23	1:A:493:LEU:H	1.71	0.56
1:A:356:PHE:HB3	1:A:359:LEU:HD12	1.88	0.56
1:A:522:PHE:HE2	1:A:531:LEU:HG	1.71	0.56
1:B:161:TYR:HD1	1:B:189:GLU:HA	1.71	0.56
1:B:645:VAL:HA	1:B:648:VAL:HG22	1.88	0.56
1:A:428:ILE:HG23	1:A:453:LEU:HD13	1.86	0.56
1:A:541:LEU:HB2	1:A:560:LEU:HD13	1.87	0.55
1:A:361:LYS:HA	1:A:385:LYS:HD2	1.89	0.55
1:B:312:LYS:HD3	1:B:312:LYS:H	1.72	0.55
1:B:428:ILE:HG23	1:B:453:LEU:HD13	1.89	0.55
1:B:580:LYS:HD3	1:B:611:VAL:HG21	1.88	0.55
1:B:404:SER:HA	1:B:424:THR:HG21	1.89	0.55
1:B:507:LEU:HB2	1:B:509:LEU:HG	1.87	0.54
1:B:478:LEU:HG	1:B:480:LEU:HD21	1.87	0.54
1:A:511:HIS:HA	1:A:514:LEU:HD12	1.90	0.54
1:B:135:VAL:HG22	1:B:137:LYS:H	1.71	0.54
1:B:489:TRP:H	1:B:509:LEU:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PHE:HB2	1:A:571:LEU:HB2	1.90	0.54
1:A:121:LEU:HD23	1:A:144:LEU:HD22	1.88	0.54
1:A:834:GLN:O	1:A:838:LYS:HG2	2.08	0.54
1:A:755:VAL:HG21	1:A:836:ILE:HD11	1.91	0.53
1:B:505:GLN:HG2	1:B:506:VAL:HG12	1.90	0.53
1:B:365:ILE:HD13	1:B:365:ILE:H	1.73	0.53
1:A:404:SER:HA	1:A:424:THR:HG21	1.90	0.53
1:A:460:PHE:HB3	1:A:484:MET:O	2.08	0.53
1:B:361:LYS:HA	1:B:385:LYS:HD2	1.90	0.53
1:A:78:GLY:HA3	1:A:102:LEU:HA	1.90	0.52
1:B:387:GLN:HG3	1:B:388:THR:HG22	1.90	0.52
1:A:537:ARG:HH21	1:B:34:ARG:HH12	1.56	0.52
1:A:303:LEU:H	1:A:326:LYS:HB3	1.73	0.52
1:A:88:LYS:H	1:A:88:LYS:HD3	1.74	0.52
1:A:169:LEU:HB3	1:A:172:LEU:HB2	1.91	0.52
1:A:363:ALA:HA	1:A:386:LEU:HA	1.90	0.52
1:B:184:LEU:HD13	1:B:185:VAL:N	2.25	0.52
1:B:453:LEU:HG	1:B:455:LEU:HD11	1.92	0.52
1:A:368:GLN:HG3	1:A:392:ARG:HB3	1.92	0.52
1:A:563:PRO:HD3	1:A:590:PHE:HB2	1.91	0.51
1:A:362:VAL:HG11	1:A:383:LEU:HD22	1.92	0.51
1:B:175:ILE:HD12	1:B:201:PHE:HE1	1.76	0.51
1:B:110:LEU:HB3	1:B:140:TYR:HE1	1.75	0.51
1:A:338:LEU:HD23	1:A:359:LEU:HD13	1.93	0.51
1:A:364:TYR:HA	1:A:388:THR:HG23	1.92	0.51
1:A:357:TYR:HA	1:A:382:PHE:HB2	1.92	0.51
1:A:176:ASP:HA	1:A:204:ALA:HB3	1.92	0.51
1:A:744:ILE:O	1:A:748:ILE:HG13	2.11	0.51
1:B:469:PRO:HG3	1:B:493:LEU:HB2	1.93	0.51
1:B:460:PHE:H	1:B:483:ASN:HB2	1.76	0.51
1:A:426:ASN:H	1:A:426:ASN:ND2	2.08	0.50
1:A:72:LEU:HD13	1:A:75:LEU:HD13	1.93	0.50
1:B:406:PRO:HA	1:B:425:ALA:HA	1.91	0.50
1:B:29:ARG:HG2	1:B:50:ARG:HD2	1.92	0.50
1:B:426:ASN:H	1:B:426:ASN:ND2	2.08	0.50
1:A:460:PHE:H	1:A:483:ASN:HB2	1.76	0.50
1:B:563:PRO:HB3	1:B:590:PHE:HA	1.93	0.50
1:B:163:HIS:CE1	1:B:165:SER:HB3	2.47	0.50
1:B:554:ASP:HA	1:B:575:ASP:HB3	1.93	0.50
1:B:317:LEU:HB2	1:B:338:LEU:HD11	1.94	0.50
1:B:268:GLY:HA2	1:B:304:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:O	1:B:160:LEU:HD13	2.12	0.50
1:B:269:PHE:HE2	1:B:306:ARG:HH21	1.59	0.50
1:A:69:LEU:H	1:A:69:LEU:HD12	1.77	0.50
1:B:511:HIS:HB2	1:B:539:THR:HG22	1.94	0.50
1:A:694:ASP:O	1:A:752:ARG:HB3	2.12	0.50
1:A:268:GLY:HA2	1:A:304:ASN:HB2	1.93	0.50
1:A:439:ASP:O	1:A:443:PHE:HB3	2.12	0.49
1:B:25:SER:HB2	1:B:29:ARG:HB2	1.93	0.49
1:A:310:THR:HG23	1:A:311:LEU:HG	1.95	0.49
1:A:441:LEU:HD13	1:A:467:GLN:C	2.32	0.49
1:B:172:LEU:HD11	1:B:175:ILE:HD11	1.94	0.49
1:B:69:LEU:HD12	1:B:69:LEU:H	1.78	0.49
1:A:258:LEU:O	1:A:293:LEU:HD12	2.12	0.49
1:A:365:ILE:H	1:A:365:ILE:HD13	1.78	0.49
1:A:229:GLU:HG3	1:A:230:ILE:HG13	1.93	0.49
1:A:441:LEU:O	1:A:445:LEU:HG	2.13	0.48
1:B:190:LEU:HB3	1:B:193:LEU:HD12	1.94	0.48
1:A:460:PHE:HB2	1:A:483:ASN:HB2	1.94	0.48
1:B:509:LEU:HB3	1:B:514:LEU:HD21	1.95	0.48
1:A:571:LEU:HD11	1:A:574:LEU:HB2	1.95	0.48
1:A:75:LEU:O	1:A:100:LEU:HD12	2.13	0.48
1:A:511:HIS:HB2	1:A:539:THR:HG22	1.95	0.48
1:A:508:TYR:HA	1:A:537:ARG:HD3	1.96	0.48
1:B:460:PHE:HB3	1:B:484:MET:O	2.13	0.48
1:A:160:LEU:O	1:A:160:LEU:HD13	2.13	0.48
1:A:593:TRP:O	1:A:597:THR:HG23	2.14	0.48
1:A:347:LEU:HB3	1:A:348:LEU:H	1.56	0.47
1:B:75:LEU:O	1:B:100:LEU:HD12	2.14	0.47
1:A:552:ILE:HG22	1:A:573:VAL:HB	1.96	0.47
1:A:475:LEU:HB3	1:A:497:VAL:HG13	1.97	0.47
1:A:324:ILE:HG12	1:A:346:ASN:HB2	1.96	0.47
1:A:292:HIS:HA	1:A:316:VAL:O	2.14	0.47
1:A:237:GLY:HA3	1:A:242:ILE:HD11	1.97	0.47
1:A:546:LEU:HB3	1:A:547:PRO:HD3	1.95	0.47
1:B:399:ILE:HG23	1:B:402:ILE:HD13	1.96	0.47
1:A:399:ILE:HG23	1:A:402:ILE:HD13	1.96	0.47
1:B:428:ILE:HG21	1:B:443:PHE:CE1	2.49	0.47
1:A:440:ILE:HA	1:A:443:PHE:HD2	1.79	0.47
1:A:428:ILE:HG21	1:A:443:PHE:CE1	2.49	0.47
1:B:644:ILE:O	1:B:648:VAL:HG13	2.13	0.47
1:B:357:TYR:HA	1:B:382:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:O	1:A:406:PRO:HD2	2.15	0.47
1:A:740:ARG:O	1:A:743:ASN:HB2	2.14	0.47
1:A:543:HIS:HD2	1:A:564:ASN:HB2	1.78	0.47
1:A:91:PHE:HB2	1:A:118:LEU:HD21	1.95	0.47
1:A:274:ILE:HB	1:A:277:PRO:HD2	1.97	0.47
1:B:493:LEU:H	1:B:493:LEU:HD23	1.80	0.47
1:A:75:LEU:HG	1:A:77:LEU:HG	1.97	0.47
1:B:48:THR:HB	1:B:69:LEU:HD23	1.97	0.47
1:B:206:ASN:HB3	1:B:236:ASN:ND2	2.29	0.47
1:B:240:VAL:HB	1:B:273:ASN:HD22	1.79	0.47
1:B:275:LYS:HA	1:B:278:ASP:OD2	2.15	0.47
1:A:577:THR:HB	1:A:607:ASP:HB2	1.96	0.47
1:A:504:LEU:HD22	1:A:533:LEU:HD21	1.96	0.47
1:A:531:LEU:O	1:A:553:LEU:HD12	2.15	0.47
1:B:237:GLY:CA	1:B:242:ILE:HD11	2.44	0.46
1:A:383:LEU:HB2	1:A:403:PRO:HG2	1.98	0.46
1:A:504:LEU:HD13	1:A:531:LEU:HD11	1.98	0.46
1:B:439:ASP:O	1:B:443:PHE:HB3	2.16	0.46
1:A:163:HIS:CE1	1:A:165:SER:HB3	2.50	0.46
1:B:404:SER:CA	1:B:424:THR:HG21	2.44	0.46
1:A:415:LEU:HD13	1:A:434:ARG:O	2.16	0.46
1:A:408:ILE:N	1:A:408:ILE:HD13	2.30	0.46
1:A:559:GLN:HG2	1:A:580:LYS:HG3	1.97	0.46
1:A:58:ILE:HD13	1:A:58:ILE:O	2.15	0.46
1:B:559:GLN:HG2	1:B:580:LYS:HG3	1.98	0.46
1:A:712:LEU:HD13	1:A:729:PHE:HZ	1.81	0.46
1:A:271:PHE:HA	1:A:278:ASP:OD2	2.16	0.46
1:B:317:LEU:HD23	1:B:338:LEU:HD13	1.98	0.46
1:B:447:VAL:N	1:B:448:PRO:HD3	2.31	0.46
1:A:472:ASN:HD22	1:A:475:LEU:HG	1.81	0.46
1:A:683:PRO:HG2	1:A:686:THR:OG1	2.16	0.46
1:B:314:LEU:HD13	1:B:317:LEU:HD21	1.98	0.46
1:B:428:ILE:HD13	1:B:429:HIS:N	2.30	0.46
1:A:406:PRO:HA	1:A:425:ALA:HA	1.96	0.46
1:A:759:SER:H	1:A:762:PHE:HB3	1.81	0.46
1:A:175:ILE:HD12	1:A:201:PHE:HE1	1.81	0.46
1:A:763:LEU:HD21	1:A:800:LEU:HA	1.97	0.46
1:B:310:THR:HG23	1:B:311:LEU:HG	1.98	0.45
1:B:121:LEU:HD23	1:B:144:LEU:HD22	1.97	0.45
1:B:546:LEU:HB3	1:B:547:PRO:HD3	1.98	0.45
1:A:224:ARG:HD3	1:A:225:ASN:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HD13	1:B:467:GLN:C	2.37	0.45
1:B:391:LEU:HB2	1:B:410:LEU:HD13	1.98	0.45
1:B:510:ASN:O	1:B:514:LEU:HG	2.17	0.45
1:A:99:ILE:HG22	1:A:123:GLU:HB2	1.98	0.45
1:A:563:PRO:HB3	1:A:590:PHE:HD1	1.82	0.45
1:B:274:ILE:HB	1:B:277:PRO:HD2	1.98	0.45
1:A:754:ILE:HD12	1:A:780:LEU:HD21	1.98	0.45
1:B:224:ARG:HD3	1:B:225:ASN:HB2	1.99	0.45
1:B:191:GLU:O	1:B:194:GLN:HG2	2.16	0.45
1:B:184:LEU:HD12	1:B:186:CYS:SG	2.57	0.45
1:A:191:GLU:HB2	1:A:192:PRO:HD3	1.99	0.45
1:A:455:LEU:HB2	1:A:479:PHE:O	2.16	0.45
1:B:184:LEU:HD22	1:B:213:SER:O	2.17	0.45
1:A:184:LEU:HD13	1:A:185:VAL:N	2.31	0.45
1:A:579:ASN:HB2	1:A:581:PHE:CE2	2.52	0.45
1:A:114:ALA:HB3	1:A:140:TYR:CE2	2.52	0.45
1:B:362:VAL:HG13	1:B:386:LEU:HD13	1.99	0.45
1:A:580:LYS:HA	1:A:611:VAL:HG21	1.98	0.45
1:B:58:ILE:O	1:B:58:ILE:HD13	2.17	0.45
1:A:126:LEU:HB2	1:A:152:LEU:HD23	1.99	0.45
1:A:453:LEU:HG	1:A:455:LEU:HD11	1.98	0.44
1:A:752:ARG:HG3	1:A:753:LYS:CD	2.47	0.44
1:A:404:SER:CA	1:A:424:THR:HG21	2.47	0.44
1:A:711:LEU:O	1:A:715:LEU:HD13	2.18	0.44
1:A:428:ILE:HD13	1:A:429:HIS:N	2.32	0.44
1:A:684:GLN:HA	1:A:687:GLU:OE2	2.18	0.44
1:A:293:LEU:HB3	1:A:317:LEU:CD1	2.48	0.44
1:A:206:ASN:HB3	1:A:236:ASN:ND2	2.32	0.44
1:A:356:PHE:HB2	1:A:383:LEU:HD21	2.00	0.44
1:B:98:ARG:O	1:B:121:LEU:HD12	2.18	0.44
1:A:426:ASN:HD22	1:A:426:ASN:N	2.09	0.44
1:A:184:LEU:HD12	1:A:186:CYS:SG	2.57	0.44
1:A:757:LEU:HD22	1:A:757:LEU:N	2.33	0.44
1:A:391:LEU:HB2	1:A:410:LEU:HD13	2.00	0.44
1:B:91:PHE:HB2	1:B:118:LEU:HD21	2.00	0.44
1:A:269:PHE:HE2	1:A:306:ARG:HH21	1.65	0.44
1:B:408:ILE:N	1:B:408:ILE:HD13	2.32	0.44
1:B:571:LEU:HD11	1:B:574:LEU:HB2	1.99	0.44
1:B:518:PRO:O	1:B:521:VAL:HG23	2.18	0.44
1:A:98:ARG:O	1:A:121:LEU:HD12	2.17	0.44
1:B:230:ILE:HA	1:B:257:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG13	1:A:138:ASP:OD2	2.18	0.44
1:A:316:VAL:HG12	1:A:340:VAL:H	1.83	0.44
1:A:514:LEU:CD1	1:A:538:LEU:HG	2.46	0.44
1:A:341:LEU:O	1:A:365:ILE:HA	2.18	0.43
1:B:202:SER:HB3	1:B:230:ILE:HB	1.99	0.43
1:B:426:ASN:N	1:B:426:ASN:HD22	2.09	0.43
1:B:563:PRO:HB3	1:B:590:PHE:HD1	1.82	0.43
1:A:655:MET:O	1:A:659:THR:HG23	2.18	0.43
1:B:541:LEU:HB2	1:B:560:LEU:HD22	1.99	0.43
1:A:216:TRP:O	1:A:218:LYS:HG2	2.19	0.43
1:A:94:LEU:HB3	1:A:97:LEU:HB2	1.98	0.43
1:B:383:LEU:HB2	1:B:403:PRO:HG2	2.00	0.43
1:B:146:ALA:O	1:B:148:THR:HG23	2.18	0.43
1:B:398:THR:HG22	1:B:400:HIS:CD2	2.53	0.43
1:B:450:LEU:HD13	1:B:451:GLN:N	2.34	0.43
1:A:175:ILE:HD12	1:A:201:PHE:CE1	2.54	0.43
1:A:399:ILE:HD12	1:A:402:ILE:HG12	2.01	0.43
1:B:318:ASN:OD1	1:B:342:ASN:HB2	2.18	0.43
1:A:72:LEU:HD12	1:A:94:LEU:CD2	2.48	0.43
1:B:114:ALA:HB3	1:B:140:TYR:CE2	2.53	0.43
1:A:397:THR:HG21	1:A:410:LEU:HD12	2.00	0.43
1:B:126:LEU:HB2	1:B:152:LEU:HD23	2.01	0.43
1:B:415:LEU:HD13	1:B:434:ARG:O	2.18	0.43
1:A:231:LEU:HD23	1:A:258:LEU:HD13	2.00	0.43
1:B:72:LEU:HD13	1:B:75:LEU:HD13	2.01	0.43
1:B:77:LEU:O	1:B:102:LEU:HD23	2.19	0.43
1:A:463:CYS:HB2	1:A:485:LEU:HD22	2.00	0.43
1:A:190:LEU:HD22	1:A:193:LEU:HD11	2.01	0.43
1:B:72:LEU:HD13	1:B:75:LEU:HD22	1.99	0.43
1:B:380:PHE:HB3	1:B:383:LEU:HD12	1.99	0.43
1:B:605:PRO:HA	1:B:608:ILE:HD12	1.99	0.43
1:B:387:GLN:O	1:B:406:PRO:HD2	2.19	0.42
1:A:563:PRO:HB3	1:A:590:PHE:HA	2.01	0.42
1:A:240:VAL:HB	1:A:273:ASN:HD22	1.84	0.42
1:A:172:LEU:HD21	1:A:175:ILE:HD11	2.02	0.42
1:A:110:LEU:HB3	1:A:140:TYR:HE1	1.84	0.42
1:A:177:PHE:O	1:A:205:ALA:HA	2.19	0.42
1:A:327:ILE:N	1:A:327:ILE:HD12	2.35	0.42
1:A:416:VAL:HB	1:A:439:ASP:OD1	2.19	0.42
1:A:264:ILE:HD12	1:A:295:LEU:HD22	2.02	0.42
1:A:767:TRP:NE1	1:A:771:ALA:HB2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HD13	1:A:365:ILE:N	2.34	0.42
1:A:398:THR:HG22	1:A:400:HIS:CD2	2.54	0.42
1:B:100:LEU:HB3	1:B:124:LEU:HD12	2.02	0.42
1:B:268:GLY:O	1:B:307:VAL:HA	2.20	0.42
1:B:53:LEU:HB3	1:B:81:TYR:HE2	1.84	0.42
1:B:568:PHE:HB2	1:B:571:LEU:HB2	2.02	0.42
1:A:518:PRO:O	1:A:521:VAL:HG23	2.20	0.42
1:A:447:VAL:N	1:A:448:PRO:HD3	2.34	0.42
1:B:229:GLU:O	1:B:256:PHE:HB3	2.19	0.42
1:A:293:LEU:HB3	1:A:317:LEU:HD13	2.01	0.42
1:B:264:ILE:HD12	1:B:295:LEU:HD22	2.02	0.42
1:A:171:SER:O	1:A:173:LYS:HG3	2.19	0.42
1:B:365:ILE:N	1:B:365:ILE:HD13	2.33	0.42
1:A:504:LEU:HB2	1:A:533:LEU:HD23	2.01	0.42
1:A:545:ASP:HA	1:A:568:PHE:CE2	2.54	0.42
1:A:191:GLU:O	1:A:194:GLN:HG2	2.19	0.42
1:A:184:LEU:HD13	1:A:185:VAL:H	1.85	0.42
1:A:389:LEU:HB2	1:A:405:ILE:HD13	2.02	0.42
1:A:442:TYR:HA	1:A:445:LEU:HD12	2.02	0.42
1:B:58:ILE:HB	1:B:81:TYR:CE1	2.54	0.42
1:B:555:ILE:O	1:B:576:ILE:HA	2.20	0.42
1:B:347:LEU:HB2	1:B:370:ASN:HB3	2.02	0.41
1:B:171:SER:O	1:B:173:LYS:HG3	2.19	0.41
1:A:833:SER:O	1:A:837:LEU:HD13	2.20	0.41
1:B:88:LYS:HB3	1:B:111:HIS:CD2	2.55	0.41
1:B:94:LEU:HB3	1:B:97:LEU:HB2	2.02	0.41
1:A:203:LEU:O	1:A:231:LEU:HA	2.20	0.41
1:A:362:VAL:CG1	1:A:383:LEU:HD22	2.50	0.41
1:A:51:LEU:HD22	1:A:69:LEU:HD22	2.01	0.41
1:A:537:ARG:HH21	1:B:34:ARG:NH1	2.17	0.41
1:A:160:LEU:HB2	1:A:182:ILE:HG21	2.03	0.41
1:B:303:LEU:HD22	1:B:331:ALA:HB1	2.01	0.41
1:A:311:LEU:HB3	1:A:314:LEU:HG	2.02	0.41
1:B:571:LEU:HD11	1:B:574:LEU:HD23	2.02	0.41
1:A:598:ASN:HB2	1:A:600:THR:HG22	2.03	0.41
1:B:44:VAL:HG21	1:B:69:LEU:HD11	2.03	0.41
1:B:190:LEU:HD22	1:B:193:LEU:HD11	2.02	0.41
1:B:455:LEU:HB2	1:B:479:PHE:O	2.20	0.41
1:A:184:LEU:HD22	1:A:213:SER:O	2.21	0.41
1:B:76:GLU:HG3	1:B:101:ASP:HB2	2.03	0.41
1:B:375:ILE:HG23	1:B:398:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:O	1:A:553:LEU:HA	2.21	0.41
1:A:644:ILE:O	1:A:648:VAL:HG13	2.21	0.41
1:B:180:ASN:HB2	1:B:209:TYR:CE2	2.56	0.41
1:B:223:PHE:HD2	1:B:250:ILE:HA	1.85	0.41
1:A:180:ASN:HB2	1:A:209:TYR:CE2	2.56	0.41
1:A:450:LEU:HD13	1:A:451:GLN:N	2.35	0.40
1:A:152:LEU:HD12	1:A:177:PHE:HE1	1.86	0.40
1:B:444:LEU:HA	1:B:447:VAL:HG22	2.01	0.40
1:A:579:ASN:HB2	1:A:581:PHE:CZ	2.56	0.40
1:A:444:LEU:HA	1:A:447:VAL:HG22	2.03	0.40
1:B:538:LEU:HB2	1:B:560:LEU:HD21	2.03	0.40
1:A:338:LEU:HB3	1:A:359:LEU:HD22	2.04	0.40
1:B:389:LEU:HB2	1:B:405:ILE:HD13	2.04	0.40
1:A:77:LEU:O	1:A:102:LEU:HD23	2.20	0.40
1:A:229:GLU:O	1:A:256:PHE:HB3	2.20	0.40
1:B:656:THR:HG23	1:B:657:ILE:N	2.35	0.40
1:A:340:VAL:HG13	1:A:364:TYR:HD2	1.86	0.40
1:A:489:TRP:N	1:A:509:LEU:HD22	2.32	0.40
1:A:571:LEU:HD13	1:A:572:SER:N	2.36	0.40
1:A:53:LEU:HB3	1:A:81:TYR:HE2	1.86	0.40
1:B:211:ARG:NH2	1:B:246:PHE:HB2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	791/844 (94%)	621 (78%)	151 (19%)	19 (2%)	7	47
1	B	628/844 (74%)	471 (75%)	135 (22%)	22 (4%)	4	39
All	All	1419/1688 (84%)	1092 (77%)	286 (20%)	41 (3%)	9	43

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	397	THR
1	B	182	ILE
1	B	506	VAL
1	A	181	GLN
1	A	469	PRO
1	A	506	VAL
1	A	561	LEU
1	B	397	THR
1	B	663	PHE
1	A	34	ARG
1	A	59	ARG
1	A	263	HIS
1	A	403	PRO
1	A	468	THR
1	B	59	ARG
1	B	181	GLN
1	B	263	HIS
1	B	270	GLY
1	B	403	PRO
1	B	468	THR
1	B	469	PRO
1	B	561	LEU
1	A	270	GLY
1	A	306	ARG
1	A	348	LEU
1	A	394	ASN
1	A	801	MET
1	B	306	ARG
1	B	348	LEU
1	B	482	GLU
1	A	235	GLY
1	A	598	ASN
1	B	27	ASP
1	B	346	ASN
1	B	369	LYS
1	B	576	ILE
1	B	598	ASN
1	B	350	GLU
1	B	235	GLY
1	A	576	ILE

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 PDB entries followed by that with respect to all EM entries.

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	727/770 (94%)	697 (96%)	30 (4%)	37	71
1	B	576/770 (75%)	551 (96%)	25 (4%)	35	70
All	All	1303/1540 (85%)	1248 (96%)	55 (4%)	41	70

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	58	ILE
1	A	81	TYR
1	A	88	LYS
1	A	137	LYS
1	A	145	LYS
1	A	154	LYS
1	A	184	LEU
1	A	216	TRP
1	A	224	ARG
1	A	287	ARG
1	A	312	LYS
1	A	325	ASN
1	A	346	ASN
1	A	348	LEU
1	A	352	TYR
1	A	365	ILE
1	A	388	THR
1	A	408	ILE
1	A	426	ASN
1	A	428	ILE
1	A	443	PHE
1	A	460	PHE
1	A	531	LEU
1	A	571	LEU
1	A	650	LEU
1	A	655	MET

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Mol	Chain	Res	Type
1	A	738	GLU
1	A	739	ASN
1	A	802	LYS
1	B	40	GLN
1	B	58	ILE
1	B	81	TYR
1	B	88	LYS
1	B	137	LYS
1	B	145	LYS
1	B	184	LEU
1	B	216	TRP
1	B	224	ARG
1	B	287	ARG
1	B	312	LYS
1	B	325	ASN
1	B	346	ASN
1	B	348	LEU
1	B	365	ILE
1	B	388	THR
1	B	408	ILE
1	B	426	ASN
1	B	428	ILE
1	B	443	PHE
1	B	460	PHE
1	B	469	PRO
1	B	531	LEU
1	B	653	PHE
1	B	655	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	43	GLN
1	A	96	ASN
1	A	111	HIS
1	A	155	ASN
1	A	156	GLN
1	A	180	ASN
1	A	206	ASN
1	A	221	ASN
1	A	248	ASN

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Mol	Chain	Res	Type
1	A	273	ASN
1	A	279	GLN
1	A	325	ASN
1	A	337	ASN
1	A	339	GLN
1	A	346	ASN
1	A	378	GLN
1	A	387	GLN
1	A	426	ASN
1	A	456	ASN
1	A	486	GLN
1	A	510	ASN
1	A	543	HIS
1	A	549	ASN
1	A	743	ASN
1	A	745	GLN
1	A	804	GLN
1	A	823	GLN
1	B	40	GLN
1	B	80	GLN
1	B	96	ASN
1	B	111	HIS
1	B	155	ASN
1	B	156	GLN
1	B	206	ASN
1	B	221	ASN
1	B	248	ASN
1	B	262	HIS
1	B	273	ASN
1	B	279	GLN
1	B	325	ASN
1	B	337	ASN
1	B	346	ASN
1	B	378	GLN
1	B	387	GLN
1	B	426	ASN
1	B	456	ASN
1	B	486	GLN
1	B	505	GLN
1	B	510	ASN
1	B	549	ASN
1	B	592	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

28 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1037	1,2	14,14,15	1.51	2 (14%)	15,19,21	1.29	2 (13%)
2	FUC	A	1038	2	10,10,11	1.69	3 (30%)	13,14,16	2.05	4 (30%)
2	NAG	A	1245	1,2	14,14,15	1.66	3 (21%)	15,19,21	1.72	4 (26%)
2	FUC	A	1246	2	10,10,11	1.39	1 (10%)	13,14,16	1.25	1 (7%)
2	NAG	A	1342	1,2	14,14,15	1.39	4 (28%)	15,19,21	1.09	0
2	FUC	A	1343	2	10,10,11	1.60	3 (30%)	13,14,16	1.87	4 (30%)
2	NAG	A	1422	1,2	14,14,15	1.93	2 (14%)	15,19,21	1.39	2 (13%)
2	FUC	A	1423	2	10,10,11	1.69	2 (20%)	13,14,16	1.50	2 (15%)
2	NAG	A	1595	1,2	14,14,15	1.37	2 (14%)	15,19,21	1.42	2 (13%)
2	FUC	A	1596	2	10,10,11	1.90	3 (30%)	13,14,16	2.04	2 (15%)
2	NAG	A	2046	1,2	14,14,15	1.76	4 (28%)	15,19,21	1.26	1 (6%)
2	FUC	A	2047	2	10,10,11	1.61	3 (30%)	13,14,16	1.50	3 (23%)
2	NAG	A	2598	1,2	14,14,15	1.43	2 (14%)	15,19,21	1.08	1 (6%)
2	FUC	A	2599	2	10,10,11	1.83	3 (30%)	13,14,16	2.26	6 (46%)
2	NAG	B	1037	1,2	14,14,15	1.60	2 (14%)	15,19,21	1.39	3 (20%)
2	FUC	B	1038	2	10,10,11	1.61	2 (20%)	13,14,16	1.36	3 (23%)
2	NAG	B	1245	1,2	14,14,15	1.91	3 (21%)	15,19,21	1.11	1 (6%)
2	FUC	B	1246	2	10,10,11	1.70	3 (30%)	13,14,16	1.74	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1342	1,2	14,14,15	1.56	3 (21%)	15,19,21	1.36	2 (13%)
2	FUC	B	1343	2	10,10,11	1.60	2 (20%)	13,14,16	1.68	2 (15%)
2	NAG	B	1422	1,2	14,14,15	1.96	2 (14%)	15,19,21	1.38	2 (13%)
2	FUC	B	1423	2	10,10,11	1.69	2 (20%)	13,14,16	1.49	2 (15%)
2	NAG	B	1595	1,2	14,14,15	1.76	4 (28%)	15,19,21	1.13	1 (6%)
2	FUC	B	1596	2	10,10,11	1.95	3 (30%)	13,14,16	2.74	5 (38%)
2	NAG	B	2046	1,2	14,14,15	1.25	1 (7%)	15,19,21	1.21	3 (20%)
2	FUC	B	2047	2	10,10,11	1.47	3 (30%)	13,14,16	1.20	2 (15%)
2	NAG	B	2598	1,2	14,14,15	1.69	3 (21%)	15,19,21	1.49	3 (20%)
2	FUC	B	2599	2	10,10,11	1.79	3 (30%)	13,14,16	2.06	3 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1037	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1038	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1245	1,2	-	1/6/23/26	0/1/1/1
2	FUC	A	1246	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1342	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1343	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1422	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1423	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1595	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1596	2	-	0/0/17/20	0/1/1/1
2	NAG	A	2046	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	2047	2	-	0/0/17/20	0/1/1/1
2	NAG	A	2598	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	2599	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1037	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1038	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1245	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1246	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1342	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1343	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1422	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1423	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1595	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	B	1596	2	-	0/0/17/20	0/1/1/1
2	NAG	B	2046	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	2047	2	-	0/0/17/20	0/1/1/1
2	NAG	B	2598	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	2599	2	-	0/0/17/20	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2047	FUC	C2-C3	2.02	1.55	1.52
2	A	2598	NAG	C3-C2	2.03	1.57	1.52
2	A	1342	NAG	C1-C2	2.03	1.55	1.52
2	A	1422	NAG	O5-C5	2.04	1.47	1.43
2	A	1245	NAG	C8-C7	2.05	1.54	1.50
2	B	1422	NAG	O5-C5	2.06	1.48	1.43
2	A	2047	FUC	C1-C2	2.07	1.57	1.52
2	B	1595	NAG	O5-C1	2.07	1.47	1.43
2	B	2047	FUC	C4-C5	2.10	1.57	1.53
2	B	1245	NAG	O5-C5	2.11	1.48	1.43
2	A	1342	NAG	O5-C5	2.11	1.48	1.43
2	B	1595	NAG	C4-C3	2.11	1.58	1.52
2	B	1596	FUC	O5-C1	2.12	1.47	1.43
2	B	1037	NAG	O5-C1	2.14	1.47	1.43
2	A	2046	NAG	C4-C5	2.18	1.57	1.53
2	A	1596	FUC	C6-C5	2.19	1.56	1.51
2	A	1037	NAG	C3-C2	2.20	1.57	1.52
2	A	1342	NAG	C4-C3	2.20	1.58	1.52
2	B	2599	FUC	O5-C1	2.23	1.47	1.43
2	B	2598	NAG	C4-C3	2.26	1.58	1.52
2	B	1038	FUC	C1-C2	2.27	1.57	1.52
2	A	1342	NAG	C4-C5	2.28	1.58	1.53
2	A	1343	FUC	C2-C3	2.29	1.55	1.52
2	B	1246	FUC	C2-C3	2.31	1.55	1.52
2	B	2598	NAG	O5-C5	2.32	1.48	1.43
2	A	1595	NAG	C4-C3	2.32	1.58	1.52
2	A	1595	NAG	C1-C2	2.34	1.55	1.52
2	A	1343	FUC	C4-C5	2.39	1.57	1.53
2	B	1343	FUC	C4-C5	2.48	1.57	1.53
2	B	1342	NAG	O5-C5	2.51	1.49	1.43
2	A	1245	NAG	O5-C1	2.53	1.47	1.43
2	A	1596	FUC	C1-C2	2.54	1.58	1.52
2	A	1038	FUC	C1-C2	2.56	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2047	FUC	C1-C2	2.56	1.58	1.52
2	B	1246	FUC	C1-C2	2.57	1.58	1.52
2	A	2047	FUC	C4-C5	2.62	1.58	1.53
2	B	1596	FUC	C4-C3	2.66	1.59	1.52
2	B	1246	FUC	O5-C1	2.67	1.48	1.43
2	B	2599	FUC	C2-C3	2.67	1.56	1.52
2	A	1038	FUC	C4-C5	2.70	1.58	1.53
2	A	1038	FUC	O5-C1	2.75	1.48	1.43
2	A	1343	FUC	C1-C2	2.78	1.59	1.52
2	A	2598	NAG	O5-C5	2.79	1.49	1.43
2	A	2046	NAG	C3-C2	2.80	1.58	1.52
2	A	2599	FUC	C4-C5	2.82	1.58	1.53
2	A	1246	FUC	C2-C3	2.84	1.56	1.52
2	A	1423	FUC	C4-C5	2.86	1.58	1.53
2	B	1423	FUC	C4-C5	2.87	1.58	1.53
2	A	2599	FUC	C1-C2	2.87	1.59	1.52
2	B	1342	NAG	C3-C2	2.93	1.59	1.52
2	B	1342	NAG	C4-C5	2.93	1.59	1.53
2	A	2046	NAG	O5-C5	2.94	1.49	1.43
2	B	2046	NAG	C1-C2	2.97	1.56	1.52
2	A	1037	NAG	C1-C2	3.01	1.56	1.52
2	B	1595	NAG	C4-C5	3.04	1.59	1.53
2	B	1245	NAG	O5-C1	3.08	1.48	1.43
2	B	1423	FUC	C2-C3	3.11	1.56	1.52
2	A	2599	FUC	C2-C3	3.16	1.56	1.52
2	A	1423	FUC	C2-C3	3.17	1.56	1.52
2	A	2047	FUC	C2-C3	3.22	1.56	1.52
2	B	1343	FUC	C2-C3	3.38	1.57	1.52
2	B	1037	NAG	C1-C2	3.50	1.57	1.52
2	B	1038	FUC	C2-C3	3.58	1.57	1.52
2	A	2046	NAG	C1-C2	3.60	1.57	1.52
2	B	2599	FUC	C4-C5	3.81	1.60	1.53
2	B	1595	NAG	C1-C2	4.03	1.58	1.52
2	B	2598	NAG	C1-C2	4.09	1.58	1.52
2	A	1245	NAG	C4-C5	4.25	1.62	1.53
2	B	1596	FUC	C2-C3	4.35	1.58	1.52
2	A	1596	FUC	C4-C5	4.60	1.61	1.53
2	B	1245	NAG	C1-C2	4.84	1.59	1.52
2	A	1422	NAG	O5-C1	5.47	1.52	1.43
2	B	1422	NAG	O5-C1	5.53	1.52	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1245	NAG	C2-N2-C7	-3.80	118.16	123.11
2	B	2598	NAG	C2-N2-C7	-3.59	118.44	123.11
2	B	1342	NAG	C2-N2-C7	-3.34	118.76	123.11
2	B	1595	NAG	C2-N2-C7	-3.06	119.13	123.11
2	A	1422	NAG	O7-C7-C8	-2.99	116.56	122.07
2	B	1422	NAG	O7-C7-C8	-2.99	116.57	122.07
2	A	1422	NAG	C2-N2-C7	-2.83	119.43	123.11
2	B	1422	NAG	C2-N2-C7	-2.78	119.49	123.11
2	A	1037	NAG	C2-N2-C7	-2.75	119.53	123.11
2	A	1595	NAG	C2-N2-C7	-2.67	119.63	123.11
2	A	1245	NAG	O7-C7-C8	-2.62	117.24	122.07
2	A	2598	NAG	C2-N2-C7	-2.52	119.82	123.11
2	B	1037	NAG	C2-N2-C7	-2.51	119.83	123.11
2	B	2046	NAG	C2-N2-C7	-2.46	119.90	123.11
2	B	2047	FUC	O5-C5-C4	2.02	113.08	109.58
2	B	1342	NAG	C3-C4-C5	2.02	113.84	110.23
2	B	1037	NAG	O5-C5-C6	2.05	111.74	107.34
2	B	1038	FUC	C3-C4-C5	2.08	112.77	109.66
2	A	2599	FUC	O2-C2-C1	2.09	113.43	109.23
2	B	1245	NAG	O5-C5-C6	2.14	111.92	107.34
2	A	2046	NAG	C4-C3-C2	2.21	114.77	111.34
2	B	2599	FUC	O5-C5-C4	2.22	113.43	109.58
2	B	2598	NAG	O5-C5-C6	2.23	112.11	107.34
2	B	2046	NAG	C4-C3-C2	2.23	114.80	111.34
2	A	2599	FUC	C2-C3-C4	2.24	114.96	111.05
2	A	2599	FUC	O3-C3-C2	2.25	114.12	110.01
2	B	2598	NAG	C4-C3-C2	2.25	114.83	111.34
2	B	1038	FUC	O5-C5-C4	2.25	113.48	109.58
2	A	1343	FUC	O3-C3-C2	2.33	114.28	110.01
2	A	1245	NAG	C3-C4-C5	2.35	114.41	110.23
2	B	2047	FUC	C1-C2-C3	2.36	112.41	109.55
2	B	1343	FUC	C3-C4-C5	2.38	113.21	109.66
2	A	1038	FUC	O5-C5-C4	2.39	113.72	109.58
2	A	2047	FUC	O5-C5-C4	2.39	113.72	109.58
2	A	2599	FUC	C6-C5-C4	2.41	117.68	113.02
2	B	2046	NAG	C1-O5-C5	2.43	115.72	112.14
2	B	1037	NAG	C1-O5-C5	2.48	115.79	112.14
2	A	1245	NAG	C1-O5-C5	2.52	115.85	112.14
2	A	1038	FUC	O2-C2-C1	2.55	114.34	109.23
2	B	1246	FUC	O2-C2-C1	2.56	114.37	109.23
2	A	1343	FUC	C6-C5-C4	2.70	118.25	113.02
2	B	1246	FUC	C6-C5-C4	2.71	118.26	113.02
2	A	1423	FUC	C1-C2-C3	2.72	112.85	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1423	FUC	C1-C2-C3	2.74	112.87	109.55
2	A	2047	FUC	C1-C2-C3	2.78	112.92	109.55
2	A	1037	NAG	C1-O5-C5	2.85	116.33	112.14
2	B	1596	FUC	O5-C5-C4	2.85	114.51	109.58
2	A	1038	FUC	C3-C4-C5	2.89	113.98	109.66
2	B	1038	FUC	C1-C2-C3	2.91	113.08	109.55
2	A	2047	FUC	C2-C3-C4	2.97	116.22	111.05
2	A	1343	FUC	C1-C2-C3	2.98	113.16	109.55
2	B	1423	FUC	C3-C4-C5	2.98	114.11	109.66
2	A	1246	FUC	C6-C5-C4	2.99	118.81	113.02
2	A	1596	FUC	C3-C4-C5	3.02	114.17	109.66
2	A	1423	FUC	C3-C4-C5	3.03	114.19	109.66
2	A	1595	NAG	C6-C5-C4	3.24	121.10	112.99
2	A	1343	FUC	C3-C4-C5	3.41	114.75	109.66
2	B	1246	FUC	C1-C2-C3	3.70	114.04	109.55
2	B	1596	FUC	C2-C3-C4	3.84	117.74	111.05
2	A	2599	FUC	C3-C4-C5	4.09	115.78	109.66
2	A	2599	FUC	C1-C2-C3	4.22	114.66	109.55
2	B	1343	FUC	C1-C2-C3	4.29	114.75	109.55
2	B	2599	FUC	C6-C5-C4	4.33	121.41	113.02
2	B	1596	FUC	C1-C2-C3	4.42	114.91	109.55
2	B	1596	FUC	C6-C5-C4	4.51	121.74	113.02
2	B	2599	FUC	C1-C2-C3	4.91	115.50	109.55
2	B	1596	FUC	C3-C4-C5	5.49	117.86	109.66
2	A	1596	FUC	C6-C5-C4	5.57	123.80	113.02
2	A	1038	FUC	C1-C2-C3	5.66	116.41	109.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1245	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1342	NAG	1	0
2	A	2598	NAG	1	0
2	B	1342	NAG	1	0
2	B	2598	NAG	1	0

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.