



# Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2020 – 11:59 AM EDT

PDB ID : 2Q7N  
Title : Crystal structure of Leukemia inhibitory factor in complex with LIF receptor (domains 1-5)  
Authors : Huyton, T.; Zhang, J.G.; Nicola, N.A.; Garrett, T.P.J.  
Deposited on : 2007-06-07  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.10.1  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.10.1

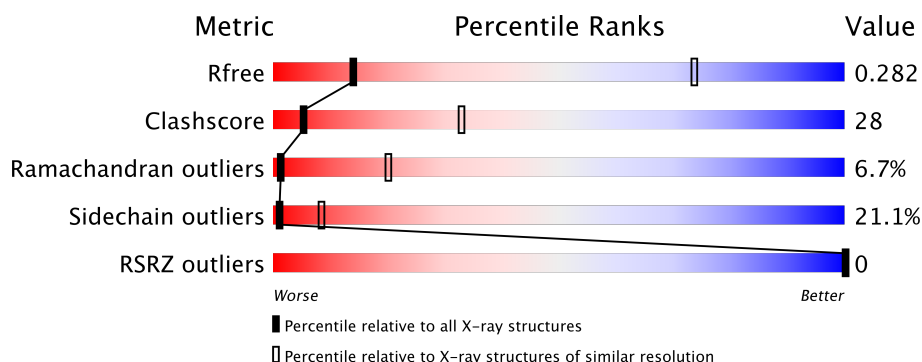
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1008 (4.38-3.62)
Clashscore	122126	1012 (4.34-3.66)
Ramachandran outliers	120053	1000 (4.36-3.64)
Sidechain outliers	120020	1023 (4.38-3.62)
RSRZ outliers	108989	1107 (4.40-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	488	
1	C	488	
2	B	180	
2	D	180	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	605	-	-	X	-
3	NAG	A	606	-	-	X	X
3	NAG	A	611	-	-	-	X
3	NAG	A	614	-	-	-	X
3	NAG	C	504	-	-	-	X
3	NAG	C	505	-	-	X	-
3	NAG	C	507	-	-	X	X
3	NAG	C	508	X	-	-	-
3	NAG	C	510	-	-	-	X
3	NAG	C	512	-	-	-	X
3	NAG	C	520	-	-	X	-
3	NAG	C	521	-	-	-	X
4	FUC	C	509	-	-	-	X
5	MAN	A	617	X	-	-	-
5	MAN	A	622	X	-	-	-
5	MAN	C	518	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10839 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leukemia inhibitory factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2369	642	711	17			
1	C	480	Total	C	N	O	S	0	0	0
			3739	2369	642	711	17			

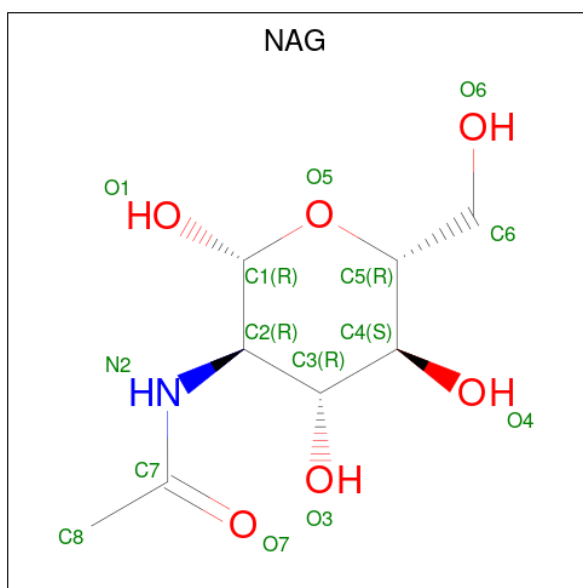
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	cloning artifact	UNP P42703
A	0	TYR	-	cloning artifact	UNP P42703
A	1	LYS	-	cloning artifact	UNP P42703
A	2	ASP	-	cloning artifact	UNP P42703
A	3	ASP	-	cloning artifact	UNP P42703
A	4	ASP	-	cloning artifact	UNP P42703
A	5	ASP	-	cloning artifact	UNP P42703
A	6	LYS	-	cloning artifact	UNP P42703
C	-1	ASP	-	cloning artifact	UNP P42703
C	0	TYR	-	cloning artifact	UNP P42703
C	1	LYS	-	cloning artifact	UNP P42703
C	2	ASP	-	cloning artifact	UNP P42703
C	3	ASP	-	cloning artifact	UNP P42703
C	4	ASP	-	cloning artifact	UNP P42703
C	5	ASP	-	cloning artifact	UNP P42703
C	6	LYS	-	cloning artifact	UNP P42703

- Molecule 2 is a protein called Leukemia inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1387	884	245	251	7			
2	D	180	Total	C	N	O	S	0	0	0
			1387	884	245	251	7			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



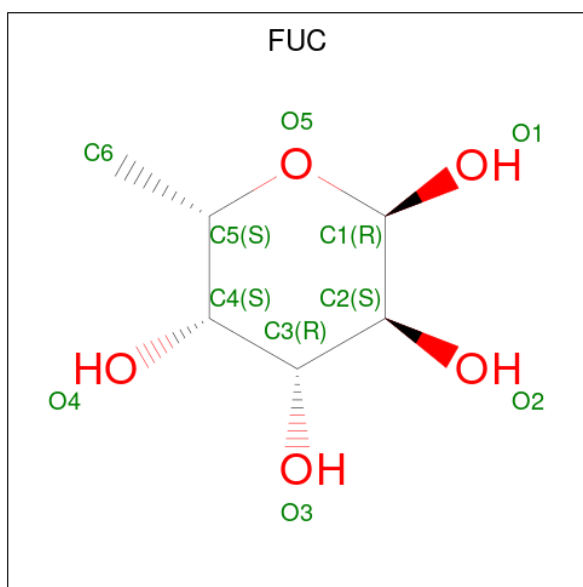
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1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

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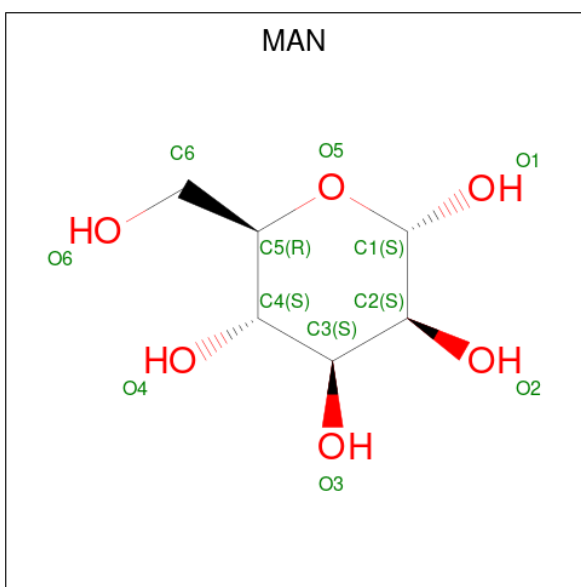
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

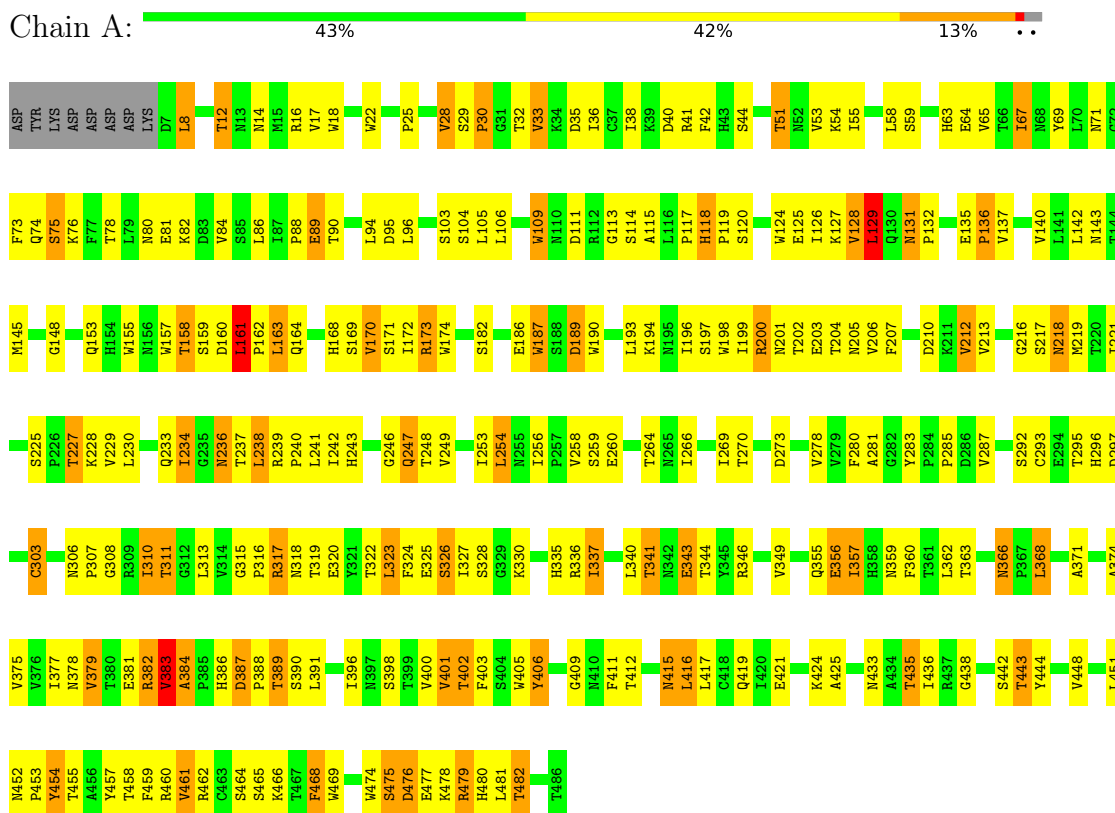


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

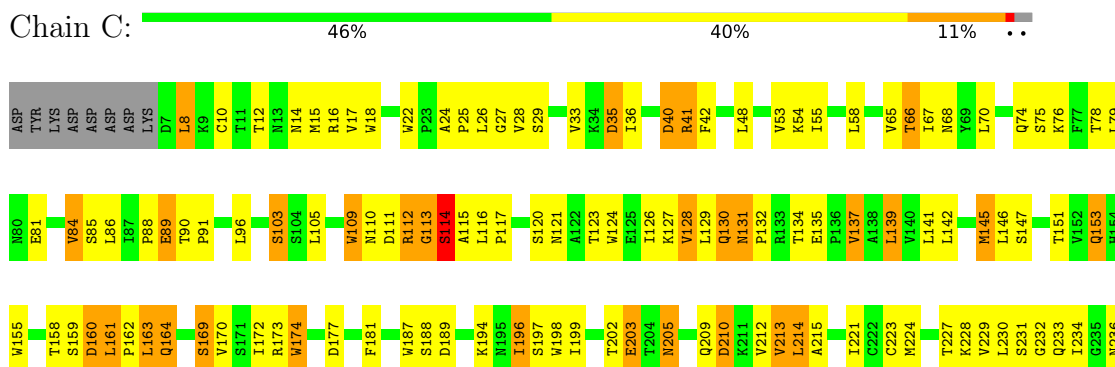
### 3 Residue-property plots

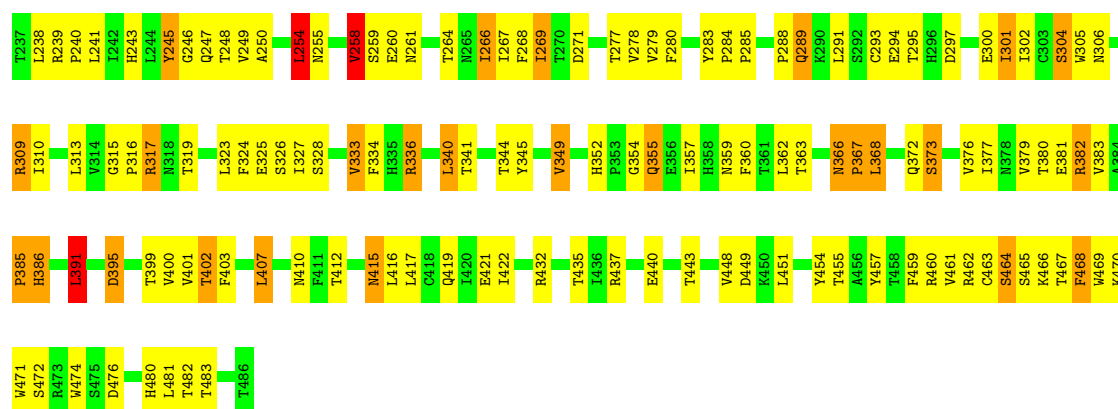
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Leukemia inhibitory factor receptor

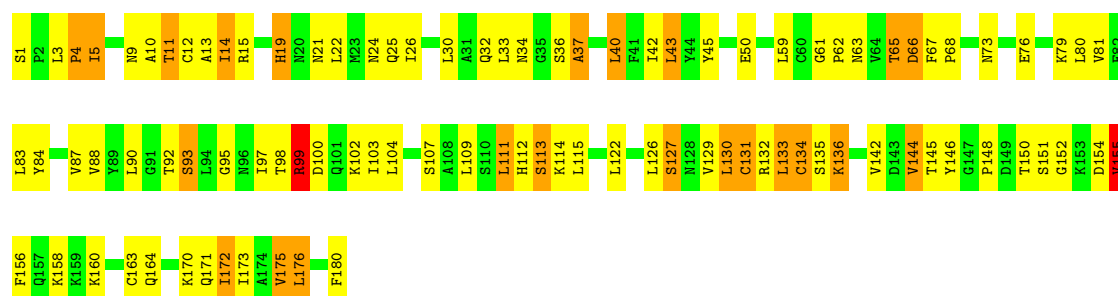


#### • Molecule 1: Leukemia inhibitory factor receptor

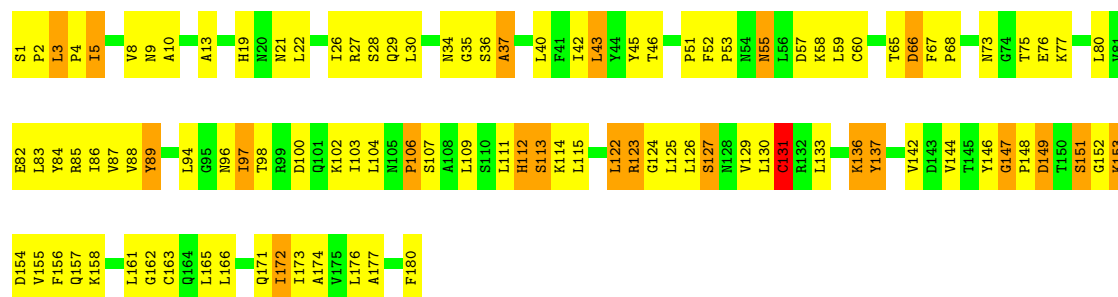




• Molecule 2: Leukemia inhibitory factor



• Molecule 2: Leukemia inhibitory factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.48Å 240.13Å 202.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 19.98 – 4.01	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-4.00) 93.6 (19.98-4.01)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.237 , 0.287 0.232 , 0.282	Depositor DCC
$R_{free}$ test set	1852 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 81.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10839	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, 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	0.76	2/3842 (0.1%)	0.82	2/5267 (0.0%)
1	C	0.73	0/3842	0.82	2/5267 (0.0%)
2	B	0.73	0/1416	0.77	0/1923
2	D	0.73	0/1416	0.81	0/1923
All	All	0.74	2/10516 (0.0%)	0.81	4/14380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	VAL	CA-CB	5.65	1.66	1.54
1	A	303	CYS	CB-SG	-5.65	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	LEU	CA-CB-CG	7.97	133.63	115.30
1	A	161	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	254	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	391	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ARG	Peptide
1	A	384	ALA	Peptide
1	C	28	VAL	Peptide
1	C	40	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3739	0	3568	210	0
1	C	3739	0	3568	205	0
2	B	1387	0	1417	78	0
2	D	1387	0	1417	83	0
3	A	238	0	207	20	0
3	C	224	0	197	16	0
4	A	40	0	40	7	0
4	C	30	0	30	0	0
5	A	33	0	29	0	0
5	C	22	0	19	0	0
All	All	10839	0	10492	596	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 28.

All (596) 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)
3:A:605:NAG:C6	3:A:606:NAG:H82	1.41	1.46
3:C:505:NAG:C6	3:C:507:NAG:H82	1.54	1.36
3:A:605:NAG:C6	3:A:606:NAG:C8	2.13	1.23
3:C:505:NAG:H61	3:C:507:NAG:C8	1.73	1.19
3:A:605:NAG:H62	3:A:606:NAG:C8	1.72	1.14
1:A:310:ILE:HD12	1:A:310:ILE:H	1.00	1.13
3:A:605:NAG:H62	3:A:606:NAG:H82	1.14	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:605:NAG:H61	3:A:606:NAG:H82	1.20	1.09
3:A:605:NAG:H61	3:A:606:NAG:C8	1.77	1.08
1:C:285:PRO:HD3	1:C:366:ASN:HB2	1.40	1.02
3:C:505:NAG:H61	3:C:507:NAG:H82	1.06	1.02
2:B:34:ASN:HD22	2:B:173:ILE:HG23	1.25	1.01
2:B:15:ARG:HD2	2:B:130:LEU:HD21	1.40	1.01
1:A:337:ILE:H	1:A:337:ILE:HD12	1.22	1.00
3:A:612:NAG:O5	4:A:613:FUC:H5	1.63	0.98
1:C:109:TRP:CH2	1:C:153:GLN:HB3	2.02	0.94
2:D:87:VAL:HG13	2:D:122:LEU:HD12	1.46	0.94
1:A:310:ILE:HD12	1:A:310:ILE:N	1.85	0.92
3:C:505:NAG:C6	3:C:507:NAG:C8	2.38	0.91
1:A:310:ILE:CD1	1:A:310:ILE:H	1.77	0.91
1:C:482:THR:HG22	1:C:483:THR:H	1.34	0.90
2:D:1:SER:N	2:D:2:PRO:HD3	1.88	0.89
1:A:225:SER:H	1:A:248:THR:HG22	1.38	0.89
3:C:505:NAG:H62	3:C:507:NAG:H82	1.50	0.88
2:B:88:VAL:O	2:B:92:THR:HG23	1.74	0.87
1:A:317:ARG:HH11	1:A:317:ARG:HG3	1.40	0.86
3:C:520:NAG:O4	3:C:521:NAG:C7	2.19	0.86
1:C:454:TYR:H	1:C:482:THR:HB	1.40	0.85
1:A:234:ILE:HG23	1:A:266:ILE:HG12	1.59	0.85
1:C:340:LEU:HG	1:C:345:TYR:HE1	1.42	0.84
1:C:285:PRO:HD3	1:C:366:ASN:CB	2.06	0.84
3:A:607:NAG:H61	3:A:608:NAG:C1	2.07	0.84
3:C:520:NAG:H62	3:C:521:NAG:O7	1.77	0.84
1:C:103:SER:HB2	1:C:163:LEU:HD13	1.57	0.84
1:C:145:MET:SD	1:C:145:MET:C	2.58	0.82
1:C:327:ILE:HD11	1:C:357:ILE:O	1.78	0.82
1:A:210:ASP:OD2	2:B:155:VAL:HG22	1.77	0.82
1:C:317:ARG:CG	1:C:317:ARG:HH11	1.93	0.81
1:A:12:THR:HG22	1:A:17:VAL:O	1.81	0.81
1:A:424:LYS:HG2	1:A:425:ALA:H	1.45	0.81
2:B:42:ILE:HA	2:B:45:TYR:CE2	2.14	0.80
1:C:109:TRP:CZ3	1:C:153:GLN:CB	2.64	0.80
1:A:131:ASN:H	1:A:132:PRO:CD	1.95	0.80
1:C:317:ARG:HG3	1:C:317:ARG:HH11	1.46	0.80
1:C:313:LEU:HB3	1:C:317:ARG:HB2	1.64	0.79
1:C:234:ILE:HG13	1:C:266:ILE:HG23	1.64	0.79
1:A:196:ILE:O	1:A:196:ILE:HD12	1.83	0.79
1:A:295:THR:OG1	1:A:297:ASP:O	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:THR:HG23	1:C:76:LYS:NZ	1.97	0.79
1:C:285:PRO:CD	1:C:366:ASN:HB2	2.11	0.79
1:A:128:VAL:O	1:A:129:LEU:HB2	1.83	0.78
1:C:109:TRP:CZ3	1:C:153:GLN:HB3	2.19	0.78
1:C:161:LEU:HB3	1:C:162:PRO:HD2	1.66	0.77
1:A:131:ASN:H	1:A:132:PRO:HD3	1.49	0.77
1:C:289:GLN:HB2	1:C:306:ASN:HB3	1.67	0.77
2:D:96:ASN:O	2:D:98:THR:N	2.18	0.77
1:A:161:LEU:HB2	1:A:162:PRO:HD3	1.67	0.76
1:A:337:ILE:H	1:A:337:ILE:CD1	1.98	0.76
1:A:163:LEU:O	1:A:198:TRP:HZ3	1.68	0.76
1:C:463:CYS:O	1:C:472:SER:HB3	1.86	0.76
2:D:84:TYR:CE2	2:D:142:VAL:HB	2.20	0.76
1:C:340:LEU:HG	1:C:345:TYR:CE1	2.20	0.75
1:A:258:VAL:HA	1:A:281:ALA:HB3	1.69	0.75
2:D:80:LEU:HB3	2:D:133:LEU:HD11	1.67	0.75
1:A:278:VAL:HB	2:B:155:VAL:HG21	1.68	0.75
2:B:26:ILE:O	2:B:30:LEU:HB2	1.86	0.75
1:C:223:CYS:HB2	1:C:268:PHE:CE1	2.21	0.75
1:C:366:ASN:O	1:C:368:LEU:N	2.20	0.74
1:C:22:TRP:CZ2	1:C:67:ILE:HD11	2.22	0.74
3:A:619:NAG:H61	4:A:620:FUC:O2	1.88	0.74
2:D:42:ILE:HA	2:D:45:TYR:CE2	2.22	0.74
1:A:317:ARG:HH11	1:A:317:ARG:CG	2.01	0.74
1:A:337:ILE:HD12	1:A:337:ILE:N	2.00	0.74
1:C:67:ILE:O	1:C:74:GLN:HA	1.87	0.73
2:D:1:SER:H3	2:D:2:PRO:HD3	1.51	0.73
1:C:123:THR:HG21	1:C:142:LEU:HD23	1.68	0.73
1:C:231:SER:O	1:C:269:ILE:HD12	1.88	0.73
1:C:239:ARG:HB3	1:C:240:PRO:HD2	1.71	0.72
1:C:288:PRO:HG2	1:C:373:SER:HB2	1.70	0.72
2:B:67:PHE:CD1	2:B:68:PRO:HD2	2.24	0.72
2:D:136:LYS:O	2:D:137:TYR:CD1	2.43	0.71
1:C:416:LEU:HB2	1:C:464:SER:O	1.90	0.71
1:A:462:ARG:HB2	1:A:474:TRP:CZ3	2.26	0.71
3:A:605:NAG:C6	3:A:606:NAG:H83	2.17	0.71
1:C:103:SER:CB	1:C:163:LEU:HD13	2.22	0.70
1:C:301:ILE:HD13	1:C:360:PHE:HZ	1.57	0.70
1:A:462:ARG:HB2	1:A:474:TRP:CE3	2.26	0.69
2:B:21:ASN:HD21	2:B:24:ASN:HB2	1.57	0.69
1:C:391:LEU:HD13	1:C:403:PHE:HZ	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:O	1:A:368:LEU:N	2.25	0.69
1:C:66:THR:HG23	1:C:76:LYS:HZ2	1.57	0.69
2:B:40:LEU:HB2	2:B:114:LYS:HD2	1.75	0.69
2:B:43:LEU:HD12	2:B:111:LEU:HG	1.76	0.68
1:A:233:GLN:HB3	1:A:238:LEU:HA	1.75	0.68
1:A:228:LYS:HA	1:A:247:GLN:HG2	1.75	0.68
1:A:459:PHE:HB2	1:A:478:LYS:CB	2.24	0.68
1:A:128:VAL:HG23	1:A:136:PRO:HD2	1.75	0.68
2:B:34:ASN:ND2	2:B:173:ILE:HG23	2.06	0.68
2:D:109:LEU:HD23	2:D:109:LEU:H	1.58	0.68
1:A:217:SER:H	1:A:256:ILE:HG22	1.59	0.68
1:C:131:ASN:N	1:C:132:PRO:CD	2.56	0.68
1:C:109:TRP:HZ3	1:C:153:GLN:HB2	1.60	0.67
1:C:120:SER:O	1:C:145:MET:HB3	1.92	0.67
1:C:228:LYS:HA	1:C:247:GLN:HG3	1.77	0.67
1:A:173:ARG:HG2	1:A:190:TRP:CZ3	2.30	0.67
1:C:395:ASP:N	1:C:395:ASP:OD1	2.26	0.67
1:C:231:SER:C	1:C:269:ILE:HD12	2.15	0.67
1:A:129:LEU:HA	1:A:136:PRO:HD3	1.76	0.66
1:A:424:LYS:HG2	1:A:425:ALA:N	2.10	0.66
1:C:10:CYS:HB2	1:C:84:VAL:HG13	1.76	0.66
1:A:198:TRP:CH2	1:A:207:PHE:CE2	2.83	0.66
1:A:259:SER:H	1:A:281:ALA:HB3	1.60	0.66
1:A:131:ASN:N	1:A:132:PRO:CD	2.58	0.66
1:A:313:LEU:HB3	1:A:317:ARG:HB2	1.76	0.66
1:C:212:VAL:HG12	1:C:280:PHE:HB2	1.77	0.66
3:A:619:NAG:C6	4:A:620:FUC:O2	2.44	0.65
1:C:454:TYR:N	1:C:482:THR:HB	2.10	0.65
1:A:25:PRO:HD3	1:A:69:TYR:OH	1.95	0.65
1:C:196:ILE:O	1:C:196:ILE:HG13	1.95	0.65
3:A:605:NAG:H61	3:A:606:NAG:H83	1.74	0.65
1:A:326:SER:HB3	1:A:359:ASN:HB3	1.77	0.65
1:C:88:PRO:HD2	1:C:188:SER:HA	1.78	0.65
1:A:285:PRO:HD3	1:A:366:ASN:HB3	1.78	0.65
1:A:435:THR:CG2	1:A:466:LYS:HD3	2.27	0.65
1:A:96:LEU:HD23	1:A:196:ILE:HG23	1.76	0.64
1:A:161:LEU:HB2	1:A:162:PRO:CD	2.27	0.64
1:C:145:MET:SD	1:C:147:SER:N	2.71	0.64
1:C:131:ASN:N	1:C:132:PRO:HD3	2.12	0.64
1:C:400:VAL:HG13	1:C:448:VAL:O	1.96	0.64
2:B:127:SER:O	2:B:131:CYS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:CB	1:A:162:PRO:HD3	2.27	0.64
1:A:323:LEU:HD12	1:A:362:LEU:HD13	1.78	0.63
1:C:129:LEU:HD13	1:C:169:SER:HB3	1.81	0.63
2:B:10:ALA:CB	2:B:84:TYR:OH	2.47	0.63
1:C:90:THR:HG23	1:C:189:ASP:HB3	1.80	0.63
1:A:246:GLY:C	1:A:248:THR:H	2.00	0.63
2:B:158:LYS:NZ	2:D:9:ASN:HB2	2.14	0.63
1:C:91:PRO:HG2	1:C:172:ILE:CD1	2.28	0.63
1:A:258:VAL:HG23	1:A:281:ALA:O	1.99	0.63
1:C:139:LEU:HD23	1:C:155:TRP:HZ2	1.63	0.63
2:D:96:ASN:HD22	2:D:149:ASP:HB2	1.63	0.63
1:A:128:VAL:HG21	1:A:137:VAL:HG22	1.80	0.62
2:D:65:THR:C	2:D:67:PHE:H	2.00	0.62
1:A:217:SER:O	1:A:219:MET:N	2.28	0.62
1:A:387:ASP:N	1:A:387:ASP:OD1	2.33	0.62
2:B:155:VAL:HG23	2:B:156:PHE:H	1.64	0.62
1:A:306:ASN:HB2	1:A:344:THR:HG22	1.81	0.62
2:B:88:VAL:HG21	2:B:144:VAL:HG11	1.82	0.62
1:C:130:GLN:HB2	1:C:132:PRO:HD3	1.81	0.62
1:C:24:ALA:HB1	1:C:25:PRO:HD2	1.80	0.62
2:D:1:SER:H2	2:D:2:PRO:HD3	1.64	0.62
2:B:40:LEU:HD12	2:B:114:LYS:HB3	1.82	0.62
1:C:245:TYR:HD1	1:C:246:GLY:H	1.47	0.62
2:B:154:ASP:O	2:B:155:VAL:C	2.37	0.62
2:B:83:LEU:CD2	2:B:129:VAL:HG21	2.29	0.62
1:C:128:VAL:HG23	1:C:137:VAL:H	1.65	0.62
1:C:317:ARG:NH1	1:C:317:ARG:CG	2.57	0.62
3:C:505:NAG:H61	3:C:507:NAG:C7	2.29	0.62
3:C:520:NAG:C6	3:C:521:NAG:O7	2.48	0.61
1:A:320:GLU:HG2	1:A:320:GLU:O	2.00	0.61
2:D:1:SER:N	2:D:2:PRO:CD	2.62	0.61
1:A:164:GLN:NE2	1:A:164:GLN:HA	2.14	0.61
1:C:391:LEU:HD13	1:C:403:PHE:CZ	2.36	0.61
1:C:480:HIS:CE1	1:C:481:LEU:O	2.53	0.61
3:C:520:NAG:O4	3:C:521:NAG:O7	2.18	0.61
1:C:313:LEU:HB3	1:C:317:ARG:CB	2.30	0.61
2:D:26:ILE:O	2:D:30:LEU:HB2	2.00	0.61
1:A:229:VAL:HA	1:A:270:THR:HG22	1.81	0.61
1:C:131:ASN:H	1:C:132:PRO:HD3	1.66	0.61
1:A:124:TRP:HB3	1:A:172:ILE:HD11	1.83	0.60
2:B:132:ARG:C	2:B:134:CYS:H	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:SER:OG	2:B:148:PRO:HG2	2.01	0.60
2:D:34:ASN:ND2	2:D:174:ALA:HA	2.16	0.60
2:D:96:ASN:ND2	2:D:149:ASP:HB2	2.17	0.60
1:A:366:ASN:C	1:A:366:ASN:HD22	2.04	0.59
2:D:34:ASN:HD22	2:D:173:ILE:HG23	1.67	0.59
2:B:158:LYS:HZ1	2:D:9:ASN:HB2	1.66	0.59
1:A:103:SER:OG	1:A:159:SER:HB3	2.03	0.59
1:A:421:GLU:HB3	1:A:460:ARG:HB2	1.82	0.59
1:C:35:ASP:HB2	1:C:68:ASN:HB2	1.84	0.59
1:C:126:ILE:HG12	1:C:172:ILE:HG22	1.84	0.59
1:A:315:GLY:HA2	1:A:337:ILE:HA	1.83	0.59
1:A:129:LEU:HA	1:A:136:PRO:CD	2.32	0.59
2:D:152:GLY:O	2:D:153:LYS:HB2	2.03	0.59
2:D:40:LEU:CD2	2:D:166:LEU:HD22	2.33	0.59
2:B:11:THR:HB	2:B:14:ILE:H	1.67	0.58
1:A:196:ILE:HD12	1:A:196:ILE:C	2.24	0.58
1:A:416:LEU:HA	1:A:465:SER:HA	1.86	0.58
1:A:189:ASP:OD2	1:A:189:ASP:N	2.34	0.58
1:A:8:LEU:HD21	1:A:22:TRP:HE3	1.68	0.58
1:C:173:ARG:HD2	1:C:187:TRP:CE3	2.38	0.58
1:A:458:THR:HA	1:A:479:ARG:HA	1.86	0.58
2:B:151:SER:OG	2:B:152:GLY:N	2.37	0.58
1:C:161:LEU:HB3	1:C:162:PRO:CD	2.34	0.58
1:C:422:ILE:HG23	1:C:459:PHE:HE2	1.68	0.58
2:D:10:ALA:HB3	2:D:84:TYR:OH	2.03	0.58
1:C:223:CYS:HB2	1:C:268:PHE:CD1	2.38	0.57
1:C:229:VAL:HG11	1:C:249:VAL:HG21	1.86	0.57
1:A:243:HIS:HA	1:A:249:VAL:HG12	1.86	0.57
1:C:464:SER:HB3	1:C:471:TRP:CE3	2.40	0.57
3:C:505:NAG:H62	3:C:507:NAG:C8	2.22	0.57
1:A:419:GLN:HG2	1:A:433:ASN:OD1	2.04	0.57
1:A:451:LEU:HD12	1:A:457:TYR:CE1	2.40	0.57
1:A:128:VAL:HG23	1:A:129:LEU:N	2.19	0.56
1:A:168:HIS:HB2	1:A:196:ILE:HD11	1.87	0.56
1:A:212:VAL:HG13	1:A:280:PHE:HB2	1.88	0.56
2:B:21:ASN:ND2	2:B:24:ASN:HB2	2.20	0.56
1:C:482:THR:HG22	1:C:483:THR:N	2.12	0.56
1:A:435:THR:HG21	1:A:466:LYS:HD3	1.85	0.56
1:A:258:VAL:HA	1:A:281:ALA:CB	2.35	0.56
1:A:18:TRP:CD1	1:A:84:VAL:HG11	2.40	0.56
1:A:30:PRO:HD2	1:A:32:THR:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:HB	2:B:155:VAL:CG2	2.35	0.56
1:C:103:SER:HB2	1:C:163:LEU:CD1	2.33	0.56
1:A:323:LEU:HD22	1:A:349:VAL:HG21	1.88	0.56
2:D:154:ASP:O	2:D:155:VAL:C	2.44	0.56
1:A:325:GLU:OE2	1:A:327:ILE:HG13	2.06	0.55
1:C:259:SER:CB	1:C:264:THR:OG1	2.53	0.55
1:A:403:PHE:HE2	1:A:461:VAL:CG2	2.20	0.55
1:C:66:THR:HG23	1:C:76:LYS:HZ3	1.70	0.55
1:C:174:TRP:O	1:C:188:SER:HB3	2.07	0.55
1:C:416:LEU:H	1:C:416:LEU:HD23	1.72	0.55
1:C:260:GLU:HG2	1:C:261:ASN:N	2.22	0.55
2:D:77:LYS:HB2	2:D:137:TYR:CE2	2.42	0.55
1:C:120:SER:HB2	1:C:145:MET:CE	2.37	0.55
1:A:328:SER:HB3	1:A:330:LYS:H	1.71	0.55
1:A:306:ASN:C	1:A:306:ASN:OD1	2.45	0.55
1:C:377:ILE:HG23	1:C:382:ARG:HD2	1.88	0.55
1:A:126:ILE:HG13	1:A:172:ILE:HD13	1.89	0.54
1:A:384:ALA:HB2	1:A:469:TRP:HD1	1.72	0.54
1:C:232:GLY:HA2	1:C:267:ILE:O	2.06	0.54
1:A:114:SER:HA	1:A:148:GLY:O	2.06	0.54
1:A:317:ARG:NH1	1:A:317:ARG:CG	2.63	0.54
1:C:174:TRP:CD1	1:C:174:TRP:N	2.76	0.54
2:D:42:ILE:HD13	2:D:45:TYR:HE2	1.72	0.54
3:A:619:NAG:H61	4:A:620:FUC:HO2	1.73	0.54
2:D:97:ILE:HD12	2:D:162:GLY:HA2	1.88	0.54
1:A:465:SER:OG	1:A:468:PHE:N	2.37	0.54
1:C:126:ILE:HG12	1:C:172:ILE:CG2	2.38	0.54
1:A:306:ASN:OD1	1:A:308:GLY:N	2.38	0.54
1:A:366:ASN:C	1:A:366:ASN:ND2	2.62	0.54
1:C:465:SER:C	1:C:467:THR:H	2.10	0.53
1:A:161:LEU:CB	1:A:162:PRO:CD	2.87	0.53
1:A:233:GLN:CB	1:A:238:LEU:HA	2.37	0.53
2:B:81:VAL:HA	2:B:133:LEU:HD21	1.91	0.53
1:A:379:VAL:O	1:A:382:ARG:N	2.36	0.53
1:A:403:PHE:CE1	1:A:459:PHE:HB3	2.44	0.53
3:C:520:NAG:C5	3:C:521:NAG:O7	2.56	0.53
1:A:406:TYR:CD2	1:A:406:TYR:C	2.82	0.53
1:C:223:CYS:SG	1:C:224:MET:N	2.82	0.53
2:D:96:ASN:C	2:D:98:THR:N	2.61	0.53
1:A:53:VAL:HG22	1:A:54:LYS:N	2.24	0.53
2:B:100:ASP:O	2:B:104:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:HE22	1:A:168:HIS:CE1	2.27	0.52
2:B:81:VAL:O	2:B:84:TYR:HB3	2.09	0.52
1:C:259:SER:HB2	1:C:264:THR:OG1	2.09	0.52
2:B:59:LEU:HD23	2:B:160:LYS:HG3	1.91	0.52
1:A:155:TRP:CH2	1:A:157:TRP:HB2	2.44	0.52
3:A:619:NAG:C6	3:A:621:NAG:C1	2.87	0.52
1:C:111:ASP:HB3	1:C:151:THR:O	2.10	0.52
2:D:153:LYS:O	2:D:154:ASP:C	2.48	0.52
1:C:205:ASN:HB3	1:C:224:MET:HB2	1.92	0.52
1:C:310:ILE:O	1:C:310:ILE:HD12	2.09	0.52
1:C:440:GLU:OE1	3:C:520:NAG:N2	2.42	0.52
1:C:66:THR:CG2	1:C:76:LYS:NZ	2.72	0.52
1:A:173:ARG:HG2	1:A:190:TRP:CH2	2.45	0.52
1:A:253:ILE:HD11	1:A:266:ILE:HD13	1.92	0.52
1:A:106:LEU:HB2	3:A:605:NAG:H82	1.92	0.52
1:C:403:PHE:CE2	1:C:461:VAL:CG2	2.92	0.52
1:A:18:TRP:HZ3	1:A:58:LEU:HD12	1.75	0.51
1:A:128:VAL:CG2	1:A:137:VAL:HG22	2.39	0.51
3:A:607:NAG:C6	3:A:608:NAG:C1	2.82	0.51
1:C:379:VAL:O	1:C:381:GLU:N	2.43	0.51
1:A:233:GLN:HB3	1:A:238:LEU:CA	2.39	0.51
3:A:612:NAG:C6	4:A:613:FUC:H5	2.41	0.51
1:C:128:VAL:CG2	1:C:137:VAL:H	2.23	0.51
1:C:305:TRP:CD2	1:C:362:LEU:HD21	2.46	0.51
1:A:126:ILE:HG22	1:A:127:LYS:N	2.25	0.51
1:A:405:TRP:O	1:A:443:THR:HA	2.10	0.51
1:C:451:LEU:HB3	1:C:457:TYR:CE1	2.46	0.51
2:D:65:THR:O	2:D:66:ASP:CG	2.49	0.51
1:A:59:SER:O	1:A:63:HIS:NE2	2.43	0.51
2:B:95:GLY:O	2:B:98:THR:HB	2.10	0.51
1:C:135:GLU:N	1:C:135:GLU:OE2	2.43	0.51
1:C:421:GLU:HB3	1:C:460:ARG:HB2	1.92	0.51
2:B:83:LEU:HD21	2:B:129:VAL:HG21	1.93	0.51
2:B:34:ASN:HD22	2:B:173:ILE:CG2	2.10	0.51
2:B:14:ILE:HG21	2:D:104:LEU:CD1	2.40	0.51
2:D:84:TYR:HE2	2:D:142:VAL:HB	1.71	0.51
1:A:406:TYR:HD2	1:A:406:TYR:C	2.14	0.51
2:B:61:GLY:O	2:B:63:ASN:N	2.44	0.51
1:C:352:HIS:HB3	1:C:355:GLN:HG3	1.94	0.51
1:A:163:LEU:O	1:A:198:TRP:CZ3	2.56	0.50
1:C:36:ILE:HB	1:C:48:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:HG21	1:C:18:TRP:CD1	2.47	0.50
1:C:198:TRP:CD1	1:C:199:ILE:O	2.64	0.50
2:D:27:ARG:C	2:D:29:GLN:H	2.14	0.50
1:A:468:PHE:C	1:A:468:PHE:CD2	2.84	0.50
1:C:422:ILE:HD12	1:C:432:ARG:HG3	1.93	0.50
2:B:21:ASN:HD21	2:B:24:ASN:CB	2.21	0.50
2:B:83:LEU:HD23	2:B:129:VAL:HG21	1.91	0.50
1:A:451:LEU:HD12	1:A:457:TYR:CZ	2.47	0.50
2:B:76:GLU:HA	2:B:79:LYS:HE3	1.94	0.50
1:C:86:LEU:HB2	1:C:181:PHE:CE2	2.47	0.50
1:A:16:ARG:HH21	1:A:115:ALA:C	2.15	0.50
1:A:296:HIS:CD2	1:A:296:HIS:N	2.79	0.50
1:A:293:CYS:HB2	1:A:377:ILE:HD13	1.94	0.50
1:A:236:ASN:HB2	2:B:50:GLU:OE1	2.12	0.50
2:D:40:LEU:HB2	2:D:114:LYS:HD2	1.92	0.50
1:A:118:HIS:HB3	1:A:119:PRO:HD2	1.93	0.50
1:A:403:PHE:HE2	1:A:461:VAL:HG23	1.76	0.50
1:C:315:GLY:O	1:C:317:ARG:N	2.44	0.50
2:D:154:ASP:C	2:D:156:PHE:N	2.63	0.50
1:C:278:VAL:HG12	1:C:279:VAL:N	2.27	0.50
1:C:461:VAL:HG13	1:C:462:ARG:N	2.27	0.50
2:D:30:LEU:HD21	2:D:176:LEU:HB3	1.95	0.49
1:A:155:TRP:CZ2	1:A:157:TRP:HB2	2.47	0.49
1:C:89:GLU:CD	1:C:112:ARG:HD3	2.32	0.49
1:A:287:VAL:HA	1:A:371:ALA:HB1	1.93	0.49
1:C:379:VAL:C	1:C:381:GLU:H	2.16	0.49
1:C:81:GLU:O	1:C:84:VAL:HG23	2.13	0.49
1:A:117:PRO:HB2	1:A:118:HIS:HD2	1.78	0.49
1:C:120:SER:HB2	1:C:145:MET:HE3	1.94	0.49
1:C:385:PRO:CG	1:C:464:SER:HA	2.42	0.49
1:C:395:ASP:HA	1:C:401:VAL:HG12	1.95	0.49
1:A:198:TRP:HH2	1:A:207:PHE:CE2	2.30	0.49
1:A:325:GLU:OE1	1:A:328:SER:N	2.39	0.49
1:A:86:LEU:O	1:A:88:PRO:HD3	2.13	0.49
1:C:402:THR:O	1:C:402:THR:HG22	2.12	0.49
1:C:159:SER:O	1:C:161:LEU:N	2.46	0.49
1:A:325:GLU:HB3	1:A:328:SER:HB2	1.94	0.49
1:C:325:GLU:HG2	1:C:360:PHE:CE2	2.48	0.49
2:D:77:LYS:HB2	2:D:137:TYR:HE2	1.76	0.49
2:D:151:SER:OG	2:D:152:GLY:N	2.46	0.49
1:A:128:VAL:HG22	1:A:137:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PHE:CE1	1:A:459:PHE:CB	2.96	0.48
1:C:22:TRP:CH2	1:C:67:ILE:HD11	2.48	0.48
1:A:111:ASP:C	1:A:113:GLY:H	2.17	0.48
1:A:315:GLY:O	1:A:316:PRO:C	2.51	0.48
1:C:462:ARG:HB2	1:C:474:TRP:CE3	2.48	0.48
1:C:210:ASP:CG	2:D:155:VAL:HG23	2.34	0.48
1:A:128:VAL:HG12	1:A:170:VAL:HG23	1.96	0.48
2:B:135:SER:O	2:B:136:LYS:C	2.51	0.48
1:A:405:TRP:O	1:A:443:THR:HG22	2.14	0.48
1:C:379:VAL:C	1:C:381:GLU:N	2.66	0.48
1:A:233:GLN:HB3	1:A:238:LEU:HB3	1.95	0.48
1:A:67:ILE:HD12	1:A:75:SER:HB3	1.94	0.48
2:B:79:LYS:HD2	2:B:180:PHE:HB3	1.95	0.48
2:B:155:VAL:HG23	2:B:156:PHE:N	2.28	0.48
1:A:233:GLN:HA	1:A:238:LEU:HA	1.96	0.48
1:C:113:GLY:O	1:C:114:SER:C	2.51	0.48
1:C:145:MET:O	1:C:145:MET:SD	2.72	0.48
2:D:84:TYR:CD2	2:D:142:VAL:HB	2.49	0.48
1:A:125:GLU:HA	1:A:140:VAL:HG12	1.96	0.47
1:A:82:LYS:HE2	1:A:182:SER:O	2.13	0.47
1:C:163:LEU:CD2	1:C:163:LEU:N	2.77	0.47
1:C:164:GLN:OE1	1:C:164:GLN:N	2.46	0.47
1:C:145:MET:SD	1:C:147:SER:HB3	2.55	0.47
1:A:378:ASN:O	1:A:379:VAL:C	2.52	0.47
1:C:285:PRO:CD	1:C:366:ASN:CB	2.81	0.47
1:C:366:ASN:O	1:C:367:PRO:C	2.53	0.47
2:D:96:ASN:C	2:D:98:THR:H	2.17	0.47
1:A:379:VAL:C	1:A:381:GLU:H	2.18	0.47
1:A:246:GLY:C	1:A:248:THR:N	2.67	0.47
1:A:464:SER:OG	1:A:465:SER:N	2.48	0.47
2:B:93:SER:O	2:B:97:ILE:HG12	2.15	0.47
1:A:438:GLY:HA2	1:A:444:TYR:HE2	1.80	0.47
1:A:438:GLY:HA2	1:A:444:TYR:CE2	2.49	0.47
1:A:80:ASN:CG	1:A:81:GLU:H	2.18	0.47
2:B:65:THR:O	2:B:67:PHE:N	2.47	0.47
1:C:12:THR:HG22	1:C:18:TRP:HA	1.97	0.47
1:A:117:PRO:O	1:A:118:HIS:O	2.33	0.47
1:A:129:LEU:N	1:A:136:PRO:HD2	2.29	0.47
1:A:253:ILE:HG21	1:A:256:ILE:HD12	1.96	0.47
2:B:84:TYR:CE2	2:B:142:VAL:HB	2.50	0.47
1:A:120:SER:HB2	1:A:145:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLY:N	1:A:256:ILE:O	2.48	0.47
1:A:283:TYR:O	1:A:311:THR:HB	2.15	0.47
1:A:303:CYS:O	1:A:346:ARG:HA	2.15	0.47
1:C:317:ARG:NH1	1:C:317:ARG:HG2	2.30	0.47
1:C:326:SER:HB3	1:C:359:ASN:HB3	1.97	0.47
1:A:401:VAL:HG23	1:A:448:VAL:HB	1.96	0.47
1:C:8:LEU:CD2	1:C:22:TRP:HB3	2.45	0.47
1:C:379:VAL:O	1:C:382:ARG:N	2.47	0.47
2:D:89:TYR:CE1	2:D:147:GLY:HA2	2.50	0.47
2:D:84:TYR:O	2:D:88:VAL:HG23	2.14	0.47
2:B:103:ILE:O	2:B:103:ILE:HG22	2.14	0.46
1:C:36:ILE:HD12	1:C:66:THR:O	2.15	0.46
1:C:482:THR:CG2	1:C:483:THR:H	2.10	0.46
2:D:124:GLY:O	2:D:125:LEU:C	2.53	0.46
1:A:391:LEU:HD13	1:A:403:PHE:CZ	2.50	0.46
3:A:612:NAG:C5	4:A:613:FUC:H5	2.43	0.46
2:B:93:SER:HB2	2:B:148:PRO:HD2	1.96	0.46
1:C:14:ASN:HD21	1:C:16:ARG:HB2	1.79	0.46
1:C:334:PHE:CZ	1:C:336:ARG:HB2	2.49	0.46
1:A:53:VAL:HG22	1:A:54:LYS:H	1.80	0.46
1:A:12:THR:HB	1:A:14:ASN:O	2.15	0.46
2:B:132:ARG:C	2:B:134:CYS:N	2.68	0.46
1:C:209:GLN:OE1	1:C:209:GLN:HA	2.15	0.46
1:C:81:GLU:HA	1:C:84:VAL:HG23	1.97	0.46
1:C:419:GLN:O	1:C:461:VAL:HA	2.15	0.46
2:D:129:VAL:O	2:D:133:LEU:HD12	2.16	0.46
1:C:229:VAL:HG11	1:C:249:VAL:CG2	2.45	0.46
1:C:363:THR:HG22	1:C:372:GLN:HB3	1.98	0.46
2:D:36:SER:O	2:D:37:ALA:C	2.54	0.46
1:A:415:ASN:N	1:A:415:ASN:OD1	2.49	0.45
3:C:511:NAG:H61	3:C:512:NAG:HN2	1.82	0.45
2:D:148:PRO:O	2:D:149:ASP:HB2	2.16	0.45
2:B:111:LEU:HD22	2:B:115:LEU:HD11	1.98	0.45
1:C:173:ARG:HB2	1:C:188:SER:OG	2.16	0.45
1:C:124:TRP:CD1	1:C:124:TRP:N	2.83	0.45
1:C:258:VAL:HG22	1:C:258:VAL:O	2.17	0.45
2:D:112:HIS:O	2:D:113:SER:C	2.55	0.45
1:C:116:LEU:HA	1:C:117:PRO:HD3	1.64	0.45
1:C:245:TYR:HD1	1:C:246:GLY:N	2.12	0.45
1:C:315:GLY:C	1:C:317:ARG:H	2.19	0.45
2:B:112:HIS:O	2:B:113:SER:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:SER:CB	2:B:148:PRO:HD2	2.47	0.45
2:B:175:VAL:O	2:B:176:LEU:C	2.54	0.45
1:A:40:ASP:HB3	1:A:58:LEU:HD22	1.99	0.45
1:C:383:VAL:HG21	1:C:465:SER:HB3	1.97	0.45
1:A:198:TRP:CZ2	1:A:207:PHE:CE2	3.03	0.45
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.76	0.45
1:A:128:VAL:CG2	1:A:137:VAL:H	2.30	0.45
1:C:12:THR:HG22	1:C:17:VAL:O	2.16	0.45
1:C:209:GLN:O	1:C:210:ASP:C	2.55	0.45
1:C:247:GLN:O	1:C:249:VAL:HG13	2.17	0.45
3:C:505:NAG:H61	3:C:507:NAG:N2	2.32	0.45
2:D:96:ASN:O	2:D:97:ILE:C	2.55	0.45
1:A:461:VAL:O	1:A:475:SER:HB3	2.16	0.45
3:A:612:NAG:C6	4:A:613:FUC:C5	2.94	0.45
2:B:155:VAL:HG13	2:D:13:ALA:HB1	1.99	0.45
1:C:315:GLY:C	1:C:317:ARG:N	2.68	0.45
2:B:83:LEU:HD22	2:B:180:PHE:HZ	1.82	0.44
2:D:123:ARG:O	2:D:126:LEU:HB3	2.17	0.44
1:A:198:TRP:CZ2	1:A:207:PHE:CZ	3.05	0.44
1:C:159:SER:C	1:C:161:LEU:N	2.70	0.44
1:A:137:VAL:HG21	1:A:157:TRP:CE2	2.52	0.44
1:C:385:PRO:HG3	1:C:464:SER:HA	1.98	0.44
3:A:619:NAG:H61	3:A:621:NAG:C1	2.48	0.44
1:C:130:GLN:HB2	1:C:131:ASN:H	1.55	0.44
1:C:469:TRP:CG	1:C:470:LYS:N	2.85	0.44
2:D:60:CYS:HB3	2:D:163:CYS:HB3	1.89	0.44
1:A:127:LYS:HE2	1:A:171:SER:HB3	2.00	0.44
1:A:126:ILE:CG2	1:A:127:LYS:N	2.80	0.44
2:B:172:ILE:HD13	2:B:172:ILE:HA	1.85	0.44
2:D:172:ILE:HD13	2:D:172:ILE:HA	1.84	0.44
2:D:94:LEU:HA	2:D:94:LEU:HD12	1.62	0.44
1:A:227:THR:O	1:A:228:LYS:C	2.55	0.44
1:A:118:HIS:HB3	1:A:119:PRO:CD	2.47	0.44
1:A:218:ASN:HA	1:A:254:LEU:O	2.18	0.44
1:A:480:HIS:ND1	1:A:481:LEU:O	2.51	0.44
1:C:10:CYS:CB	1:C:84:VAL:HG13	2.46	0.44
1:C:8:LEU:HD23	1:C:22:TRP:HB3	1.98	0.44
2:B:10:ALA:HB3	2:B:84:TYR:OH	2.17	0.44
1:C:407:LEU:HD21	1:C:463:CYS:HB2	1.99	0.44
2:D:127:SER:O	2:D:131:CYS:HB2	2.18	0.44
1:C:325:GLU:OE1	1:C:327:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:GLN:OE1	1:C:462:ARG:NH1	2.50	0.44
1:A:317:ARG:O	1:A:318:ASN:C	2.56	0.43
1:C:124:TRP:HA	1:C:174:TRP:HB3	1.99	0.43
1:C:53:VAL:HG22	1:C:54:LYS:N	2.33	0.43
2:B:14:ILE:HD11	2:D:158:LYS:CD	2.47	0.43
2:D:173:ILE:HD12	2:D:176:LEU:HD12	1.99	0.43
2:D:77:LYS:CD	2:D:137:TYR:HD2	2.31	0.43
1:C:233:GLN:O	1:C:266:ILE:CG2	2.66	0.43
1:C:403:PHE:HE2	1:C:461:VAL:CG2	2.31	0.43
1:A:409:GLY:HA3	1:A:411:PHE:CE1	2.52	0.43
1:A:403:PHE:CE2	1:A:461:VAL:HG23	2.53	0.43
2:D:103:ILE:HG22	2:D:103:ILE:O	2.18	0.43
2:D:147:GLY:HA3	2:D:148:PRO:HD3	1.61	0.43
1:A:377:ILE:HG23	1:A:382:ARG:HD2	2.01	0.43
1:C:145:MET:SD	1:C:146:LEU:N	2.91	0.43
1:C:109:TRP:HH2	1:C:153:GLN:HB3	1.72	0.43
2:B:13:ALA:HB1	2:D:155:VAL:HG22	2.00	0.43
1:A:198:TRP:CD1	1:A:200:ARG:HA	2.54	0.43
1:A:323:LEU:HD21	1:A:360:PHE:CD2	2.53	0.43
2:B:132:ARG:O	2:B:134:CYS:N	2.52	0.43
2:B:19:HIS:CD2	1:C:333:VAL:CG1	3.01	0.43
2:B:90:LEU:O	2:B:93:SER:N	2.51	0.43
1:C:132:PRO:HB2	1:C:134:THR:HG22	1.99	0.43
1:C:315:GLY:HA3	1:C:316:PRO:HD2	1.77	0.43
1:A:129:LEU:CA	1:A:136:PRO:CD	2.97	0.43
1:C:301:ILE:HD13	1:C:360:PHE:CZ	2.46	0.43
1:A:452:ASN:HA	1:A:453:PRO:HD3	1.84	0.43
1:C:15:MET:HE2	1:C:117:PRO:HD2	2.01	0.43
2:B:9:ASN:ND2	2:D:96:ASN:HB3	2.34	0.43
2:B:98:THR:C	2:B:100:ASP:H	2.21	0.43
1:C:25:PRO:O	1:C:27:GLY:O	2.37	0.43
1:C:277:THR:CG2	1:C:278:VAL:N	2.81	0.43
2:D:106:PRO:HG2	2:D:107:SER:H	1.83	0.43
1:A:109:TRP:CH2	1:A:153:GLN:HB3	2.53	0.43
2:B:87:VAL:O	2:B:88:VAL:C	2.56	0.43
2:D:52:PHE:N	2:D:53:PRO:HD2	2.34	0.43
2:B:65:THR:C	2:B:66:ASP:OD2	2.56	0.43
2:B:99:ARG:HG3	2:B:99:ARG:O	2.19	0.43
1:C:96:LEU:HD23	1:C:194:LYS:HB3	2.00	0.43
1:A:379:VAL:O	1:A:381:GLU:N	2.51	0.42
1:A:400:VAL:HG13	1:A:448:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:PHE:CE2	1:C:461:VAL:HG21	2.54	0.42
1:C:213:VAL:HG12	1:C:214:LEU:H	1.85	0.42
1:C:293:CYS:HA	1:C:302:ILE:O	2.19	0.42
1:A:33:VAL:HG13	1:A:69:TYR:CE2	2.55	0.42
1:A:36:ILE:HD11	1:A:65:VAL:CG1	2.49	0.42
2:B:98:THR:C	2:B:100:ASP:N	2.72	0.42
1:C:221:ILE:O	1:C:250:ALA:HB1	2.19	0.42
1:C:283:TYR:CD2	1:C:309:ARG:CZ	3.02	0.42
1:A:117:PRO:HB2	1:A:118:HIS:CD2	2.54	0.42
1:A:388:PRO:HB2	1:A:461:VAL:HG12	2.01	0.42
1:A:476:ASP:HB3	1:A:477:GLU:H	1.67	0.42
1:C:129:LEU:HD13	1:C:169:SER:CB	2.46	0.42
1:C:415:ASN:HB3	1:C:437:ARG:HA	2.01	0.42
1:A:341:THR:HB	1:A:343:GLU:H	1.85	0.42
1:A:389:THR:HG22	1:A:390:SER:N	2.33	0.42
1:A:38:ILE:HG22	1:A:65:VAL:HG22	2.00	0.42
1:C:278:VAL:CG1	1:C:279:VAL:N	2.83	0.42
1:C:432:ARG:HH12	1:C:449:ASP:H	1.67	0.42
2:D:68:PRO:HD3	2:D:89:TYR:CD1	2.54	0.42
1:A:462:ARG:HD2	1:A:474:TRP:CZ2	2.54	0.42
2:B:130:LEU:O	2:B:130:LEU:HG	2.09	0.42
1:C:40:ASP:O	1:C:41:ARG:HB2	2.19	0.42
1:A:199:ILE:O	1:A:200:ARG:C	2.58	0.42
1:C:113:GLY:O	1:C:116:LEU:N	2.40	0.42
1:C:120:SER:HB2	1:C:145:MET:HE2	2.02	0.42
1:C:128:VAL:HG22	1:C:137:VAL:O	2.19	0.42
2:D:42:ILE:HA	2:D:45:TYR:HE2	1.78	0.42
1:A:233:GLN:HB3	1:A:238:LEU:CB	2.49	0.42
1:C:291:LEU:HA	1:C:304:SER:O	2.19	0.42
2:D:55:ASN:HB3	2:D:58:LYS:HD2	2.02	0.42
1:A:89:GLU:HG3	1:A:89:GLU:H	1.44	0.42
1:A:402:THR:O	1:A:402:THR:HG22	2.20	0.42
1:C:109:TRP:CZ3	1:C:153:GLN:HB2	2.35	0.42
1:A:454:TYR:N	1:A:482:THR:OG1	2.53	0.41
2:D:165:LEU:O	2:D:166:LEU:C	2.57	0.41
2:B:65:THR:HB	2:B:66:ASP:H	1.80	0.41
1:C:126:ILE:HG22	1:C:127:LYS:N	2.35	0.41
2:B:3:LEU:HD13	2:D:3:LEU:HB2	2.02	0.41
2:D:29:GLN:OE1	2:D:125:LEU:HA	2.20	0.41
1:A:474:TRP:O	1:A:475:SER:O	2.38	0.41
1:A:36:ILE:HG21	1:A:53:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:SER:O	2:B:37:ALA:C	2.59	0.41
2:D:130:LEU:C	2:D:130:LEU:HD23	2.41	0.41
2:D:40:LEU:HD21	2:D:166:LEU:HD22	2.02	0.41
2:D:35:GLY:O	2:D:36:SER:C	2.58	0.41
2:D:149:ASP:OD1	2:D:151:SER:O	2.39	0.41
2:D:51:PRO:O	2:D:55:ASN:ND2	2.54	0.41
1:A:104:SER:HB3	1:A:158:THR:HG23	2.03	0.41
1:A:356:GLU:O	1:A:357:ILE:C	2.59	0.41
2:B:33:LEU:HD13	2:B:173:ILE:HD11	2.01	0.41
2:D:42:ILE:HA	2:D:45:TYR:CD2	2.55	0.41
2:D:43:LEU:HA	2:D:43:LEU:HD13	1.86	0.41
1:A:128:VAL:HG22	1:A:137:VAL:H	1.84	0.41
2:B:4:PRO:HB2	2:B:5:ILE:H	1.75	0.41
1:C:88:PRO:HD2	1:C:188:SER:CA	2.49	0.41
2:D:82:GLU:O	2:D:85:ARG:HB2	2.20	0.41
1:A:8:LEU:CD2	1:A:22:TRP:HB3	2.51	0.41
1:A:285:PRO:HD3	1:A:366:ASN:CB	2.48	0.41
1:C:14:ASN:ND2	1:C:16:ARG:HB2	2.36	0.41
1:C:323:LEU:HD23	1:C:349:VAL:HG22	2.02	0.41
2:D:166:LEU:HA	2:D:166:LEU:HD23	1.90	0.41
1:A:22:TRP:CE2	1:A:51:THR:O	2.74	0.41
1:A:225:SER:N	1:A:248:THR:HG22	2.20	0.41
1:A:306:ASN:HA	1:A:307:PRO:HD2	1.73	0.41
1:A:325:GLU:OE1	1:A:325:GLU:C	2.59	0.41
1:A:378:ASN:O	1:A:381:GLU:N	2.42	0.41
2:B:84:TYR:CD2	2:B:142:VAL:HG11	2.56	0.41
1:C:385:PRO:HG2	1:C:464:SER:HA	2.03	0.41
1:C:403:PHE:CE1	1:C:459:PHE:HB3	2.56	0.41
1:A:169:SER:HA	1:A:194:LYS:O	2.21	0.41
1:A:442:SER:O	1:A:444:TYR:CE1	2.74	0.41
1:A:448:VAL:HG12	1:A:451:LEU:HD21	2.02	0.41
1:C:40:ASP:O	1:C:41:ARG:CB	2.68	0.41
2:D:154:ASP:O	2:D:156:PHE:N	2.54	0.41
1:A:233:GLN:CA	1:A:238:LEU:HA	2.50	0.40
1:C:367:PRO:O	1:C:368:LEU:HB2	2.22	0.40
1:A:234:ILE:HG12	1:A:253:ILE:HG12	2.03	0.40
1:A:360:PHE:O	1:A:374:ALA:HA	2.20	0.40
2:B:11:THR:C	2:B:13:ALA:N	2.74	0.40
1:C:109:TRP:HB2	1:C:110:ASN:H	1.41	0.40
1:C:113:GLY:O	1:C:115:ALA:N	2.54	0.40
1:C:81:GLU:HA	1:C:84:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:ILE:HD13	2:D:45:TYR:CE2	2.55	0.40
2:B:93:SER:OG	2:B:148:PRO:HD2	2.20	0.40
2:B:98:THR:O	2:B:102:LYS:N	2.44	0.40
1:C:231:SER:OG	1:C:232:GLY:N	2.52	0.40
1:C:245:TYR:CE1	1:C:248:THR:OG1	2.69	0.40
2:D:84:TYR:HD2	2:D:142:VAL:HG11	1.86	0.40
2:D:82:GLU:O	2:D:86:ILE:HG13	2.22	0.40
1:A:173:ARG:HD3	1:A:187:TRP:CZ3	2.56	0.40
1:C:284:PRO:HD3	1:C:368:LEU:HD22	2.03	0.40
3:C:520:NAG:H5	3:C:521:NAG:O7	2.21	0.40
2:D:152:GLY:O	2:D:153:LYS:CB	2.68	0.40
1:A:379:VAL:C	1:A:381:GLU:N	2.74	0.40
1:A:382:ARG:O	1:A:383:VAL:C	2.59	0.40
1:C:159:SER:C	1:C:161:LEU:H	2.24	0.40
1:C:245:TYR:CD1	1:C:246:GLY:N	2.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/488 (98%)	374 (78%)	74 (16%)	30 (6%)	1	22
1	C	478/488 (98%)	383 (80%)	70 (15%)	25 (5%)	2	25
2	B	178/180 (99%)	125 (70%)	38 (21%)	15 (8%)	1	15
2	D	178/180 (99%)	115 (65%)	45 (25%)	18 (10%)	0	11
All	All	1312/1336 (98%)	997 (76%)	227 (17%)	88 (7%)	1	20

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	30	PRO
1	A	71	ASN
1	A	73	PHE
1	A	118	HIS
1	A	143	ASN
1	A	161	LEU
1	A	218	ASN
1	A	356	GLU
1	A	383	VAL
1	A	468	PHE
1	A	475	SER
1	A	479	ARG
2	B	4	PRO
2	B	37	ALA
2	B	136	LYS
1	C	26	LEU
1	C	114	SER
1	C	245	TYR
1	C	254	LEU
1	C	258	VAL
1	C	368	LEU
1	C	468	PHE
2	D	37	ALA
2	D	97	ILE
2	D	149	ASP
2	D	153	LYS
2	D	177	ALA
1	A	129	LEU
1	A	247	GLN
1	A	386	HIS
2	B	65	THR
2	B	66	ASP
2	B	155	VAL
1	C	41	ARG
1	C	113	GLY
1	C	161	LEU
1	C	203	GLU
1	C	215	ALA
1	C	367	PRO
2	D	19	HIS
2	D	21	ASN
2	D	89	TYR

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Mol	Chain	Res	Type
2	D	151	SER
1	A	51	THR
1	A	74	GLN
1	A	160	ASP
1	A	355	GLN
1	A	368	LEU
1	A	379	VAL
2	B	5	ILE
2	B	22	LEU
2	B	62	PRO
2	B	99	ARG
2	B	133	LEU
1	C	160	ASP
1	C	380	THR
1	C	385	PRO
1	C	466	LYS
2	D	59	LEU
2	D	147	GLY
1	A	136	PRO
1	A	204	THR
1	A	260	GLU
1	A	343	GLU
2	B	113	SER
2	B	176	LEU
1	C	89	GLU
1	C	121	ASN
1	C	386	HIS
2	D	22	LEU
1	A	128	VAL
1	A	200	ARG
2	B	19	HIS
1	C	410	ASN
2	D	4	PRO
2	D	100	ASP
2	D	131	CYS
2	D	137	TYR
1	A	131	ASN
1	A	240	PRO
1	C	289	GLN
1	C	131	ASN
2	B	175	VAL
1	C	29	SER

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Mol	Chain	Res	Type
1	C	354	GLY
2	D	5	ILE
2	D	106	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	419/443 (95%)	328 (78%)	91 (22%)	1	8
1	C	419/443 (95%)	329 (78%)	90 (22%)	1	8
2	B	154/154 (100%)	123 (80%)	31 (20%)	1	10
2	D	154/154 (100%)	124 (80%)	30 (20%)	1	11
All	All	1146/1194 (96%)	904 (79%)	242 (21%)	1	8

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	THR
1	A	29	SER
1	A	33	VAL
1	A	35	ASP
1	A	41	ARG
1	A	42	PHE
1	A	44	SER
1	A	55	ILE
1	A	64	GLU
1	A	67	ILE
1	A	75	SER
1	A	76	LYS
1	A	78	THR
1	A	89	GLU
1	A	90	THR
1	A	94	LEU
1	A	95	ASP

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	109	TRP
1	A	129	LEU
1	A	135	GLU
1	A	142	LEU
1	A	158	THR
1	A	163	LEU
1	A	170	VAL
1	A	173	ARG
1	A	174	TRP
1	A	186	GLU
1	A	187	TRP
1	A	189	ASP
1	A	193	LEU
1	A	197	SER
1	A	201	ASN
1	A	202	THR
1	A	203	GLU
1	A	205	ASN
1	A	206	VAL
1	A	212	VAL
1	A	213	VAL
1	A	221	ILE
1	A	227	THR
1	A	230	LEU
1	A	234	ILE
1	A	236	ASN
1	A	237	THR
1	A	238	LEU
1	A	241	LEU
1	A	242	ILE
1	A	264	THR
1	A	269	ILE
1	A	273	ASP
1	A	292	SER
1	A	310	ILE
1	A	311	THR
1	A	317	ARG
1	A	319	THR
1	A	322	THR
1	A	323	LEU
1	A	324	PHE

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Mol	Chain	Res	Type
1	A	326	SER
1	A	335	HIS
1	A	336	ARG
1	A	337	ILE
1	A	340	LEU
1	A	341	THR
1	A	357	ILE
1	A	363	THR
1	A	366	ASN
1	A	375	VAL
1	A	382	ARG
1	A	383	VAL
1	A	387	ASP
1	A	389	THR
1	A	396	ILE
1	A	398	SER
1	A	401	VAL
1	A	402	THR
1	A	406	TYR
1	A	412	THR
1	A	415	ASN
1	A	416	LEU
1	A	417	LEU
1	A	435	THR
1	A	436	ILE
1	A	443	THR
1	A	454	TYR
1	A	455	THR
1	A	461	VAL
1	A	476	ASP
1	A	482	THR
2	B	1	SER
2	B	11	THR
2	B	12	CYS
2	B	14	ILE
2	B	25	GLN
2	B	32	GLN
2	B	40	LEU
2	B	43	LEU
2	B	73	ASN
2	B	80	LEU
2	B	93	SER

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Mol	Chain	Res	Type
2	B	99	ARG
2	B	107	SER
2	B	109	LEU
2	B	111	LEU
2	B	122	LEU
2	B	126	LEU
2	B	127	SER
2	B	130	LEU
2	B	131	CYS
2	B	134	CYS
2	B	144	VAL
2	B	145	THR
2	B	146	TYR
2	B	150	THR
2	B	155	VAL
2	B	163	CYS
2	B	164	GLN
2	B	170	LYS
2	B	171	GLN
2	B	172	ILE
1	C	8	LEU
1	C	33	VAL
1	C	35	ASP
1	C	42	PHE
1	C	55	ILE
1	C	65	VAL
1	C	66	THR
1	C	70	LEU
1	C	75	SER
1	C	78	THR
1	C	79	LEU
1	C	84	VAL
1	C	85	SER
1	C	103	SER
1	C	105	LEU
1	C	109	TRP
1	C	112	ARG
1	C	114	SER
1	C	128	VAL
1	C	130	GLN
1	C	137	VAL
1	C	139	LEU

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Mol	Chain	Res	Type
1	C	141	LEU
1	C	145	MET
1	C	153	GLN
1	C	158	THR
1	C	160	ASP
1	C	163	LEU
1	C	164	GLN
1	C	169	SER
1	C	170	VAL
1	C	174	TRP
1	C	177	ASP
1	C	196	ILE
1	C	197	SER
1	C	202	THR
1	C	203	GLU
1	C	205	ASN
1	C	210	ASP
1	C	213	VAL
1	C	214	LEU
1	C	227	THR
1	C	230	LEU
1	C	236	ASN
1	C	238	LEU
1	C	241	LEU
1	C	243	HIS
1	C	254	LEU
1	C	255	ASN
1	C	258	VAL
1	C	266	ILE
1	C	269	ILE
1	C	271	ASP
1	C	294	GLU
1	C	295	THR
1	C	297	ASP
1	C	300	GLU
1	C	301	ILE
1	C	304	SER
1	C	309	ARG
1	C	317	ARG
1	C	319	THR
1	C	324	PHE
1	C	328	SER

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Mol	Chain	Res	Type
1	C	333	VAL
1	C	336	ARG
1	C	340	LEU
1	C	341	THR
1	C	344	THR
1	C	349	VAL
1	C	355	GLN
1	C	366	ASN
1	C	373	SER
1	C	376	VAL
1	C	382	ARG
1	C	386	HIS
1	C	391	LEU
1	C	395	ASP
1	C	399	THR
1	C	402	THR
1	C	407	LEU
1	C	412	THR
1	C	415	ASN
1	C	417	LEU
1	C	435	THR
1	C	443	THR
1	C	455	THR
1	C	464	SER
1	C	468	PHE
1	C	476	ASP
2	D	3	LEU
2	D	5	ILE
2	D	8	VAL
2	D	28	SER
2	D	43	LEU
2	D	46	THR
2	D	55	ASN
2	D	57	ASP
2	D	66	ASP
2	D	73	ASN
2	D	75	THR
2	D	76	GLU
2	D	83	LEU
2	D	102	LYS
2	D	111	LEU
2	D	112	HIS

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Mol	Chain	Res	Type
2	D	113	SER
2	D	115	LEU
2	D	122	LEU
2	D	123	ARG
2	D	127	SER
2	D	131	CYS
2	D	136	LYS
2	D	144	VAL
2	D	146	TYR
2	D	157	GLN
2	D	161	LEU
2	D	171	GLN
2	D	172	ILE
2	D	180	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	130	GLN
1	A	164	GLN
1	A	201	ASN
1	A	209	GLN
1	A	236	ASN
1	A	296	HIS
1	A	335	HIS
1	A	366	ASN
1	A	419	GLN
2	B	9	ASN
2	B	19	HIS
2	B	21	ASN
2	B	25	GLN
2	B	34	ASN
2	B	38	ASN
2	B	54	ASN
2	B	128	ASN
2	B	178	GLN
1	C	80	ASN
1	C	180	HIS
1	C	201	ASN
1	C	233	GLN
1	C	236	ASN

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Mol	Chain	Res	Type
1	C	255	ASN
1	C	261	ASN
1	C	370	GLN
1	C	480	HIS
2	D	34	ASN
2	D	55	ASN
2	D	71	HIS
2	D	96	ASN
2	D	171	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

45 ligands 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	$\# Z  > 2$
4	FUC	A	620	3	10,10,11	0.81	0	14,14,16	1.47	2 (14%)
3	NAG	C	505	1,3,4	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
5	MAN	A	622	3	11,11,12	0.72	0	15,15,17	1.37	3 (20%)
3	NAG	A	608	3	14,14,15	0.73	0	17,19,21	1.31	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	511	1,3	14,14,15	0.52	0	17,19,21	1.40	3 (17%)
4	FUC	C	506	3	10,10,11	0.73	0	14,14,16	1.55	3 (21%)
3	NAG	A	601	1	14,14,15	0.50	0	17,19,21	1.34	3 (17%)
3	NAG	C	507	3	14,14,15	0.58	0	17,19,21	0.80	0
4	FUC	A	613	3	10,10,11	0.83	0	14,14,16	1.01	1 (7%)
3	NAG	A	611	3	14,14,15	0.58	0	17,19,21	1.11	1 (5%)
4	FUC	A	610	3	10,10,11	0.71	0	14,14,16	1.08	2 (14%)
3	NAG	C	514	3	14,14,15	0.83	1 (7%)	17,19,21	1.86	3 (17%)
5	MAN	A	618	5	11,11,12	0.57	0	15,15,17	0.89	1 (6%)
3	NAG	A	604	3	14,14,15	0.58	0	17,19,21	1.09	1 (5%)
3	NAG	C	515	1,3,4	14,14,15	0.82	0	17,19,21	1.66	5 (29%)
3	NAG	A	621	3,5	14,14,15	0.54	0	17,19,21	0.82	0
5	MAN	A	617	3,5	11,11,12	0.62	0	15,15,17	1.83	4 (26%)
3	NAG	A	615	1,3	14,14,15	0.71	0	17,19,21	1.42	3 (17%)
3	NAG	A	606	3	14,14,15	0.62	0	17,19,21	1.44	3 (17%)
3	NAG	A	602	1,3,4	14,14,15	0.61	0	17,19,21	1.10	1 (5%)
3	NAG	A	609	1,3,4	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
3	NAG	A	623	1,3	14,14,15	0.58	0	17,19,21	1.40	3 (17%)
3	NAG	A	624	3	14,14,15	0.47	0	17,19,21	1.00	0
3	NAG	A	614	3	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
3	NAG	C	513	1,3	14,14,15	0.51	0	17,19,21	1.82	3 (17%)
3	NAG	C	517	3,5	14,14,15	0.68	0	17,19,21	1.10	2 (11%)
3	NAG	C	512	3	14,14,15	0.63	0	17,19,21	1.28	2 (11%)
3	NAG	A	605	1,3	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
3	NAG	C	501	1	14,14,15	0.49	0	17,19,21	0.87	1 (5%)
3	NAG	C	508	1,3,4	14,14,15	0.58	0	17,19,21	1.19	1 (5%)
3	NAG	A	612	1,3,4	14,14,15	0.60	0	17,19,21	1.20	2 (11%)
4	FUC	C	509	3	10,10,11	0.78	0	14,14,16	1.10	0
3	NAG	A	607	1,3	14,14,15	0.56	0	17,19,21	1.33	2 (11%)
3	NAG	C	510	3	14,14,15	0.61	0	17,19,21	0.92	1 (5%)
4	FUC	C	516	3	10,10,11	0.69	0	14,14,16	0.90	1 (7%)
3	NAG	C	503	1,3	14,14,15	0.53	0	17,19,21	1.86	3 (17%)
5	MAN	C	519	5	11,11,12	0.51	0	15,15,17	2.37	5 (33%)
3	NAG	C	502	1	14,14,15	0.46	0	17,19,21	1.36	1 (5%)
3	NAG	C	504	3	14,14,15	0.50	0	17,19,21	0.88	0
4	FUC	A	603	3	10,10,11	0.71	0	14,14,16	1.97	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	619	1,3,4	14,14,15	0.77	0	17,19,21	1.09	1 (5%)
3	NAG	C	521	3	14,14,15	0.52	0	17,19,21	1.31	3 (17%)
3	NAG	A	616	3,5	14,14,15	0.62	0	17,19,21	1.08	1 (5%)
5	MAN	C	518	3,5	11,11,12	0.91	0	15,15,17	2.15	6 (40%)
3	NAG	C	520	1,3	14,14,15	0.46	0	17,19,21	1.64	4 (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
4	FUC	A	620	3	-	-	0/1/1/1
3	NAG	C	505	1,3,4	-	4/6/23/26	0/1/1/1
5	MAN	A	622	3	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	A	608	3	-	4/6/23/26	0/1/1/1
3	NAG	C	511	1,3	-	4/6/23/26	0/1/1/1
4	FUC	A	610	3	-	-	0/1/1/1
3	NAG	A	601	1	-	5/6/23/26	0/1/1/1
3	NAG	C	513	1,3	-	4/6/23/26	0/1/1/1
4	FUC	A	613	3	-	-	0/1/1/1
3	NAG	A	611	3	-	3/6/23/26	0/1/1/1
4	FUC	C	506	3	-	-	0/1/1/1
3	NAG	C	514	3	-	4/6/23/26	0/1/1/1
5	MAN	A	618	5	-	1/2/19/22	0/1/1/1
3	NAG	A	604	3	-	0/6/23/26	0/1/1/1
3	NAG	C	515	1,3,4	-	4/6/23/26	0/1/1/1
3	NAG	A	621	3,5	-	0/6/23/26	0/1/1/1
5	MAN	A	617	3,5	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	A	615	1,3	-	3/6/23/26	0/1/1/1
3	NAG	A	606	3	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1,3,4	-	2/6/23/26	0/1/1/1
3	NAG	C	517	3,5	-	3/6/23/26	0/1/1/1
3	NAG	A	623	1,3	-	3/6/23/26	0/1/1/1
3	NAG	A	624	3	-	5/6/23/26	0/1/1/1
3	NAG	A	614	3	-	2/6/23/26	0/1/1/1
3	NAG	A	609	1,3,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	512	3	-	3/6/23/26	0/1/1/1
3	NAG	A	605	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	501	1	-	1/6/23/26	0/1/1/1
3	NAG	C	508	1,3,4	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	504	3	-	2/6/23/26	0/1/1/1
4	FUC	C	509	3	-	-	0/1/1/1
3	NAG	A	607	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	507	3	-	2/6/23/26	0/1/1/1
3	NAG	C	510	3	-	2/6/23/26	0/1/1/1
4	FUC	C	516	3	-	-	0/1/1/1
3	NAG	C	503	1,3	-	4/6/23/26	0/1/1/1
5	MAN	C	519	5	-	0/2/19/22	0/1/1/1
3	NAG	C	502	1	-	3/6/23/26	0/1/1/1
3	NAG	A	612	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	603	3	-	-	0/1/1/1
3	NAG	A	619	1,3,4	-	3/6/23/26	0/1/1/1
3	NAG	C	521	3	-	6/6/23/26	0/1/1/1
3	NAG	A	616	3,5	-	4/6/23/26	0/1/1/1
5	MAN	C	518	3,5	1/1/4/5	1/2/19/22	0/1/1/1
3	NAG	C	520	1,3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	514	NAG	C1-C2	2.44	1.56	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	519	MAN	C1-O5-C5	7.17	121.91	112.19
3	C	514	NAG	C1-O5-C5	5.45	119.58	112.19
4	A	603	FUC	C1-C2-C3	4.77	115.52	109.67
3	C	503	NAG	C4-C3-C2	-4.52	104.39	111.02
5	A	617	MAN	C3-C4-C5	4.37	118.04	110.24
3	C	502	NAG	C1-O5-C5	4.15	117.81	112.19
5	C	518	MAN	C3-C4-C5	4.10	117.55	110.24
3	C	513	NAG	C1-O5-C5	4.05	117.68	112.19
3	C	513	NAG	C4-C3-C2	3.77	116.54	111.02
4	A	603	FUC	O5-C1-C2	3.69	116.47	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	623	NAG	O5-C1-C2	-3.67	105.50	111.29
5	C	518	MAN	O5-C5-C6	3.63	112.90	107.20
3	C	508	NAG	O5-C5-C6	3.60	112.84	107.20
5	C	518	MAN	C1-O5-C5	-3.53	107.41	112.19
3	C	503	NAG	C1-O5-C5	3.52	116.96	112.19
3	C	515	NAG	O5-C1-C2	-3.50	105.76	111.29
3	A	606	NAG	O5-C5-C6	3.45	112.61	107.20
3	A	611	NAG	C1-O5-C5	3.42	116.83	112.19
4	A	620	FUC	C1-C2-C3	3.42	113.87	109.67
4	C	506	FUC	C1-C2-C3	-3.40	105.48	109.67
3	A	608	NAG	C4-C3-C2	3.30	115.85	111.02
5	A	622	MAN	C1-C2-C3	3.29	113.71	109.67
3	C	512	NAG	C2-N2-C7	3.27	127.56	122.90
3	C	513	NAG	C3-C4-C5	3.23	116.00	110.24
3	C	511	NAG	O5-C5-C6	3.23	112.26	107.20
3	A	615	NAG	C4-C3-C2	3.10	115.57	111.02
3	A	623	NAG	C2-N2-C7	-3.09	118.51	122.90
3	C	520	NAG	C4-C3-C2	-3.02	106.59	111.02
5	C	518	MAN	C1-C2-C3	3.02	113.38	109.67
3	A	615	NAG	O5-C5-C6	2.99	111.89	107.20
3	A	601	NAG	O5-C1-C2	-2.95	106.62	111.29
3	C	521	NAG	C2-N2-C7	-2.91	118.76	122.90
3	C	517	NAG	C4-C3-C2	2.89	115.25	111.02
3	C	520	NAG	C2-N2-C7	-2.89	118.79	122.90
5	A	617	MAN	C1-O5-C5	2.86	116.07	112.19
3	C	520	NAG	C1-O5-C5	2.82	116.02	112.19
3	A	604	NAG	O5-C5-C6	2.80	111.60	107.20
3	C	503	NAG	O4-C4-C5	2.80	116.26	109.30
3	C	514	NAG	O5-C1-C2	2.80	115.71	111.29
4	C	506	FUC	O5-C5-C4	2.76	114.47	109.52
3	A	612	NAG	C4-C3-C2	2.75	115.05	111.02
3	C	515	NAG	C2-N2-C7	-2.74	119.00	122.90
3	C	515	NAG	O3-C3-C2	-2.74	103.79	109.47
5	C	519	MAN	O5-C5-C4	2.70	117.39	110.83
5	A	617	MAN	C1-C2-C3	-2.68	106.37	109.67
3	A	607	NAG	O5-C5-C6	2.68	111.40	107.20
5	C	518	MAN	O4-C4-C3	-2.67	104.19	110.35
5	C	518	MAN	C2-C3-C4	2.65	115.48	110.89
3	A	619	NAG	O5-C5-C6	2.60	111.29	107.20
3	A	612	NAG	C1-O5-C5	2.59	115.70	112.19
3	A	608	NAG	O5-C1-C2	2.55	115.32	111.29
3	C	501	NAG	C1-O5-C5	2.46	115.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	511	NAG	O5-C1-C2	-2.44	107.43	111.29
4	C	506	FUC	C3-C4-C5	2.44	113.58	109.77
3	A	601	NAG	C4-C3-C2	2.44	114.59	111.02
4	A	610	FUC	C3-C4-C5	2.43	113.56	109.77
5	C	519	MAN	C3-C4-C5	2.41	114.55	110.24
3	C	512	NAG	C1-O5-C5	2.38	115.42	112.19
3	C	515	NAG	C4-C3-C2	2.35	114.46	111.02
3	A	605	NAG	O4-C4-C3	-2.33	104.97	110.35
5	A	622	MAN	C2-C3-C4	2.32	114.92	110.89
3	A	614	NAG	C1-O5-C5	2.32	115.33	112.19
3	A	602	NAG	C4-C3-C2	2.30	114.38	111.02
4	A	620	FUC	C2-C3-C4	2.28	114.84	110.89
4	A	613	FUC	C3-C4-C5	2.27	113.31	109.77
5	A	618	MAN	C1-O5-C5	2.26	115.25	112.19
3	C	517	NAG	C3-C4-C5	2.26	114.27	110.24
3	A	607	NAG	C4-C3-C2	2.24	114.31	111.02
3	A	616	NAG	C4-C3-C2	2.24	114.31	111.02
3	C	520	NAG	O5-C1-C2	-2.24	107.75	111.29
3	A	606	NAG	O7-C7-C8	-2.24	117.89	122.06
4	A	610	FUC	O5-C5-C4	2.22	113.50	109.52
3	C	521	NAG	C1-C2-N2	-2.21	106.71	110.49
3	A	623	NAG	C1-O5-C5	2.20	115.18	112.19
3	A	609	NAG	C1-O5-C5	2.18	115.15	112.19
3	A	606	NAG	C4-C3-C2	2.18	114.21	111.02
3	C	511	NAG	C4-C3-C2	2.18	114.21	111.02
5	C	519	MAN	O5-C1-C2	2.17	114.13	110.77
5	A	617	MAN	O5-C5-C4	2.17	116.10	110.83
3	C	514	NAG	O7-C7-C8	-2.15	118.06	122.06
3	C	521	NAG	O5-C5-C6	2.14	110.56	107.20
3	A	601	NAG	C1-O5-C5	2.14	115.09	112.19
4	C	516	FUC	C1-C2-C3	-2.12	107.05	109.67
5	C	519	MAN	O5-C5-C6	2.11	110.51	107.20
3	C	515	NAG	C1-O5-C5	2.08	115.01	112.19
3	A	615	NAG	O3-C3-C2	-2.05	105.22	109.47
3	C	505	NAG	C1-O5-C5	2.04	114.95	112.19
3	C	510	NAG	C4-C3-C2	2.03	113.99	111.02
4	A	603	FUC	C6-C5-C4	-2.02	109.34	113.07
5	A	622	MAN	C3-C4-C5	2.01	113.83	110.24

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
5	A	622	MAN	C1
5	A	617	MAN	C1
3	C	508	NAG	C1
5	C	518	MAN	C1

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	505	NAG	C8-C7-N2-C2
3	C	505	NAG	O7-C7-N2-C2
3	C	511	NAG	C8-C7-N2-C2
3	C	511	NAG	O7-C7-N2-C2
3	C	507	NAG	C8-C7-N2-C2
3	C	507	NAG	O7-C7-N2-C2
3	C	514	NAG	C8-C7-N2-C2
3	C	514	NAG	O7-C7-N2-C2
3	A	615	NAG	C3-C2-N2-C7
3	A	615	NAG	C8-C7-N2-C2
3	A	615	NAG	O7-C7-N2-C2
3	A	606	NAG	C8-C7-N2-C2
3	A	606	NAG	O7-C7-N2-C2
3	A	609	NAG	C8-C7-N2-C2
3	A	609	NAG	O7-C7-N2-C2
3	A	623	NAG	C8-C7-N2-C2
3	A	623	NAG	O7-C7-N2-C2
3	A	624	NAG	C8-C7-N2-C2
3	A	624	NAG	O7-C7-N2-C2
3	A	614	NAG	C8-C7-N2-C2
3	A	614	NAG	O7-C7-N2-C2
3	C	513	NAG	O7-C7-N2-C2
3	C	517	NAG	C8-C7-N2-C2
3	C	517	NAG	O7-C7-N2-C2
3	C	508	NAG	C8-C7-N2-C2
3	C	508	NAG	O7-C7-N2-C2
3	C	510	NAG	C8-C7-N2-C2
3	C	510	NAG	O7-C7-N2-C2
3	C	503	NAG	C8-C7-N2-C2
3	C	503	NAG	O7-C7-N2-C2
3	C	502	NAG	C8-C7-N2-C2
3	C	502	NAG	O7-C7-N2-C2
3	C	521	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	521	NAG	O7-C7-N2-C2
3	A	616	NAG	C8-C7-N2-C2
3	A	616	NAG	O7-C7-N2-C2
3	C	520	NAG	C8-C7-N2-C2
3	C	520	NAG	O7-C7-N2-C2
3	C	513	NAG	C8-C7-N2-C2
3	C	504	NAG	C8-C7-N2-C2
3	C	504	NAG	O7-C7-N2-C2
3	A	605	NAG	O5-C5-C6-O6
3	A	607	NAG	O5-C5-C6-O6
3	C	521	NAG	O5-C5-C6-O6
3	A	624	NAG	O5-C5-C6-O6
5	A	617	MAN	C4-C5-C6-O6
3	A	624	NAG	C1-C2-N2-C7
3	C	515	NAG	O5-C5-C6-O6
3	C	515	NAG	C4-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	A	624	NAG	C4-C5-C6-O6
3	C	521	NAG	C4-C5-C6-O6
3	A	608	NAG	C8-C7-N2-C2
3	A	601	NAG	C8-C7-N2-C2
3	A	619	NAG	C8-C7-N2-C2
3	C	511	NAG	C4-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6
3	C	503	NAG	O5-C5-C6-O6
3	C	511	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	C	514	NAG	C4-C5-C6-O6
3	A	607	NAG	C4-C5-C6-O6
3	C	521	NAG	C1-C2-N2-C7
3	A	611	NAG	C8-C7-N2-C2
3	A	608	NAG	O7-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
3	A	611	NAG	O7-C7-N2-C2
3	C	515	NAG	C8-C7-N2-C2
3	C	512	NAG	C8-C7-N2-C2
3	A	616	NAG	O5-C5-C6-O6
5	A	617	MAN	O5-C5-C6-O6
5	A	618	MAN	O5-C5-C6-O6
3	A	619	NAG	O7-C7-N2-C2
3	C	514	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	512	NAG	O7-C7-N2-C2
5	C	518	MAN	C4-C5-C6-O6
3	C	501	NAG	O5-C5-C6-O6
3	C	502	NAG	O5-C5-C6-O6
3	C	503	NAG	C4-C5-C6-O6
3	C	512	NAG	O5-C5-C6-O6
3	C	513	NAG	C1-C2-N2-C7
3	C	505	NAG	O5-C5-C6-O6
3	A	601	NAG	C3-C2-N2-C7
3	C	515	NAG	O7-C7-N2-C2
3	A	623	NAG	O5-C5-C6-O6
3	A	608	NAG	O5-C5-C6-O6
3	A	619	NAG	O5-C5-C6-O6
3	A	608	NAG	C4-C5-C6-O6
3	C	505	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	A	616	NAG	C4-C5-C6-O6
3	C	517	NAG	O5-C5-C6-O6
3	A	611	NAG	C4-C5-C6-O6
3	C	513	NAG	C3-C2-N2-C7
3	C	521	NAG	C3-C2-N2-C7

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	620	FUC	3	0
3	C	505	NAG	8	0
3	A	608	NAG	2	0
3	C	511	NAG	1	0
4	A	613	FUC	4	0
3	A	621	NAG	2	0
3	A	606	NAG	8	0
3	C	512	NAG	1	0
3	A	605	NAG	9	0
3	A	607	NAG	2	0
3	C	507	NAG	8	0
3	A	612	NAG	4	0
3	A	619	NAG	5	0
3	C	521	NAG	6	0
3	C	520	NAG	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	480/488 (98%)	-0.60	0 100 100	78, 100, 119, 144	0
1	C	480/488 (98%)	-0.64	0 100 100	80, 100, 119, 141	0
2	B	180/180 (100%)	-0.74	0 100 100	83, 100, 122, 138	0
2	D	180/180 (100%)	-0.75	0 100 100	85, 101, 122, 137	0
All	All	1320/1336 (98%)	-0.66	0 100 100	78, 100, 120, 144	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FUC	C	509	10/11	0.54	0.52	135,136,137,137	10
3	NAG	C	512	14/15	0.57	0.68	110,112,113,113	14
3	NAG	A	611	14/15	0.65	0.58	105,107,108,109	14
3	NAG	C	514	14/15	0.67	0.40	105,107,108,109	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	504	14/15	0.73	0.56	109,109,109,109	14
3	NAG	A	614	14/15	0.74	0.47	114,114,115,115	14
3	NAG	C	510	14/15	0.74	0.60	128,129,129,130	14
3	NAG	A	606	14/15	0.76	0.54	87,89,90,90	14
3	NAG	C	507	14/15	0.76	0.47	103,105,105,105	14
3	NAG	C	521	14/15	0.78	0.43	96,96,97,97	14
3	NAG	C	501	14/15	0.79	0.38	89,92,93,94	14
3	NAG	C	511	14/15	0.82	0.23	101,102,105,108	14
3	NAG	C	513	14/15	0.82	0.28	102,102,104,105	14
4	FUC	A	620	10/11	0.83	0.32	57,59,59,59	10
3	NAG	C	508	14/15	0.83	0.28	123,126,130,133	14
5	MAN	A	618	11/12	0.84	0.42	105,105,106,106	11
3	NAG	A	604	14/15	0.84	0.38	75,76,76,76	14
4	FUC	A	610	10/11	0.84	0.41	100,101,101,101	10
5	MAN	A	622	11/12	0.84	0.35	63,64,64,64	11
3	NAG	A	616	14/15	0.84	0.35	92,93,95,98	14
4	FUC	C	506	10/11	0.85	0.35	102,103,103,103	10
3	NAG	C	502	14/15	0.85	0.27	94,97,99,99	14
3	NAG	A	601	14/15	0.85	0.28	77,86,87,88	14
3	NAG	A	607	14/15	0.85	0.22	92,94,96,98	14
5	MAN	A	617	11/12	0.86	0.39	100,101,102,104	11
3	NAG	A	608	14/15	0.86	0.38	100,101,103,103	14
3	NAG	A	609	14/15	0.86	0.25	96,98,100,102	14
3	NAG	A	605	14/15	0.87	0.42	90,91,93,95	14
3	NAG	A	624	14/15	0.87	0.35	87,87,87,87	14
5	MAN	C	519	11/12	0.87	0.29	67,68,69,69	11
3	NAG	A	621	14/15	0.87	0.24	59,60,62,63	14
3	NAG	A	602	14/15	0.87	0.24	71,74,76,77	14
4	FUC	A	613	10/11	0.87	0.45	104,105,106,106	10
3	NAG	C	517	14/15	0.88	0.29	73,78,80,81	14
4	FUC	C	516	10/11	0.89	0.35	83,84,84,84	10
4	FUC	A	603	10/11	0.89	0.37	68,69,69,70	10
3	NAG	C	503	14/15	0.89	0.33	103,107,108,108	14
3	NAG	C	505	14/15	0.89	0.20	96,98,102,102	14
3	NAG	A	623	14/15	0.90	0.25	85,88,88,89	14
3	NAG	C	520	14/15	0.90	0.18	92,93,94,95	14
3	NAG	C	515	14/15	0.92	0.20	80,81,83,83	14
3	NAG	A	612	14/15	0.92	0.25	107,112,112,113	14
5	MAN	C	518	11/12	0.94	0.25	68,69,70,71	11
3	NAG	A	619	14/15	0.94	0.22	56,60,62,64	14
3	NAG	A	615	14/15	0.95	0.14	81,88,90,90	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.