



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:41 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

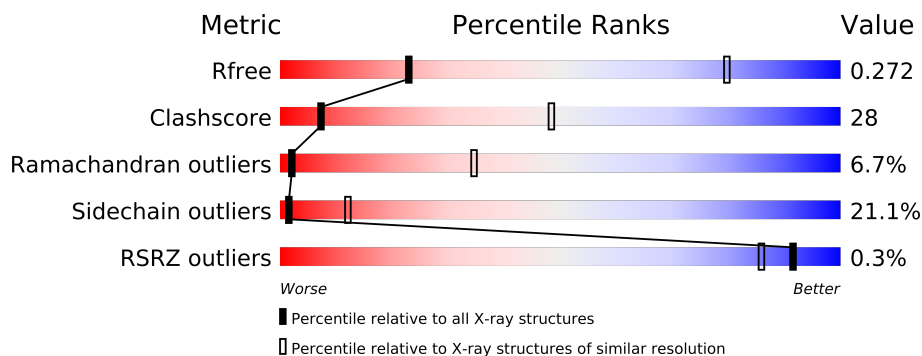
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	601	-	X
5	NAG	C	501	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10839 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

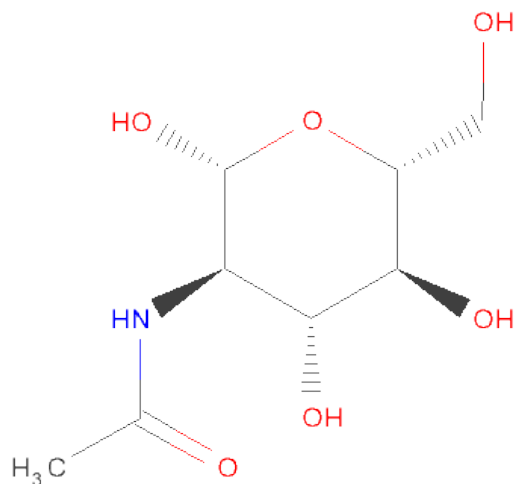
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	3	Total	C	N	O	0	0
			38	22	2	14		
3	H	3	Total	C	N	O	0	0
			38	22	2	14		
3	I	3	Total	C	N	O	0	0
			38	22	2	14		
3	N	3	Total	C	N	O	0	0
			38	22	2	14		
3	O	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

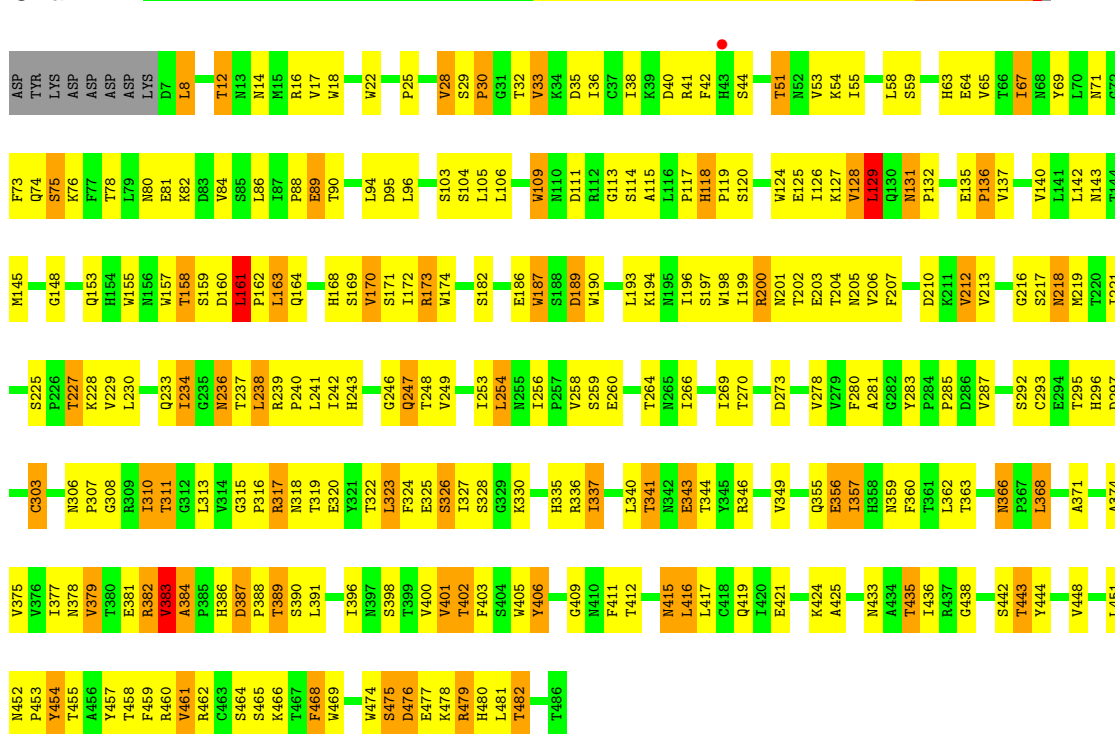
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	R	5	Total	C	N	O	0	0
			60	34	2	24		

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 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.

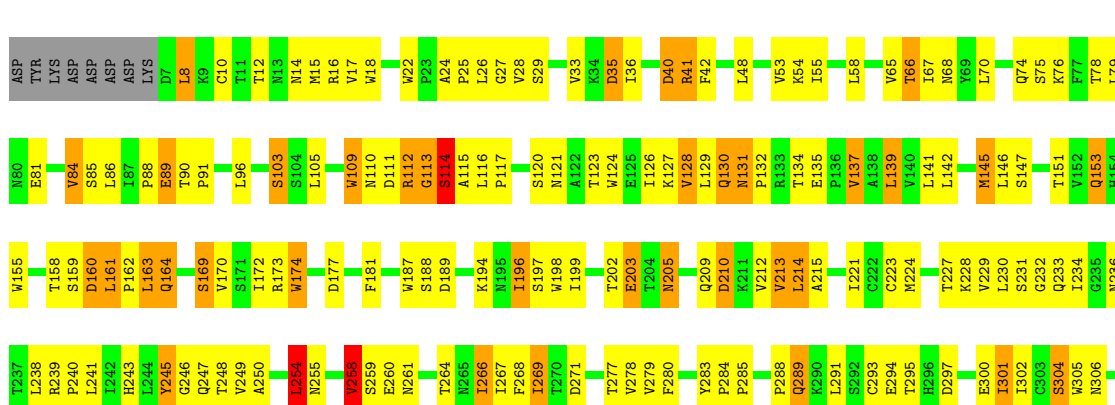
- Molecule 1: Leukemia inhibitory factor receptor

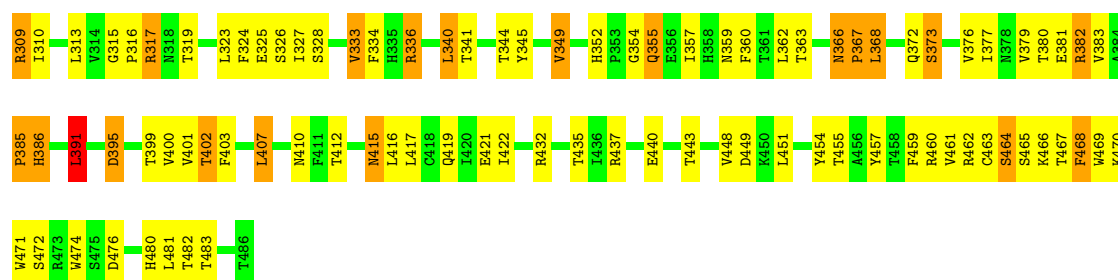
Chain A:



- Molecule 1: Leukemia inhibitory factor receptor

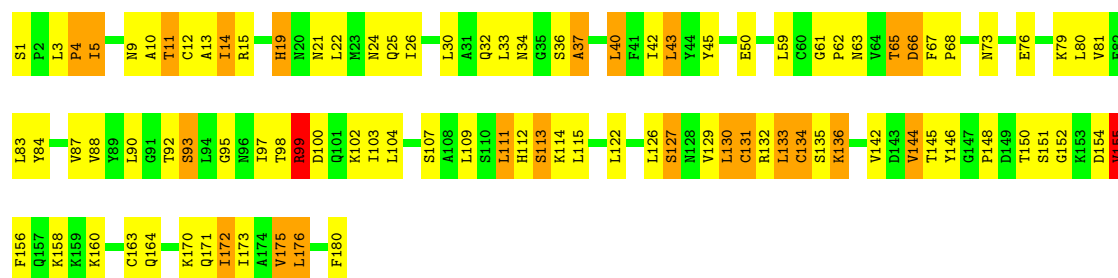
Chain C:





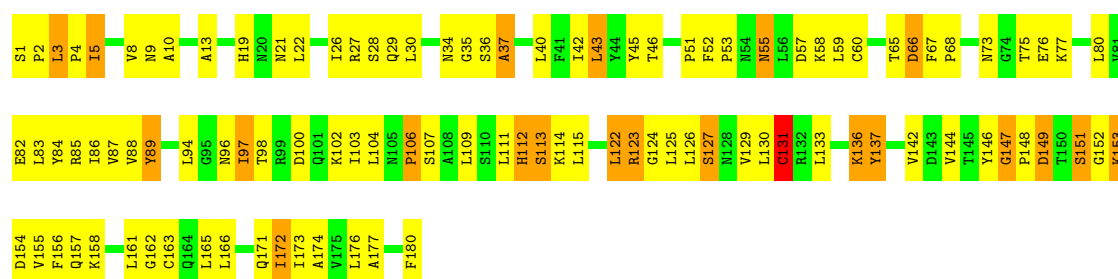
- Molecule 2: Leukemia inhibitory factor

Chain B:



- Molecule 2: Leukemia inhibitory factor

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.287 0.231 , 0.272	Depositor DCC
R_{free} test set	1852 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	119.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 95.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 37091 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10839	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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
3	O	1	0
6	J	1	0
7	K	1	0
8	R	1	0
All	All	4	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	J	703	MAN	C1
7	K	804	MAN	C1
3	O	501	NAG	C1
8	R	804	MAN	C1

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	E	38	0	34	0	0
3	H	38	0	34	0	0
3	I	38	0	34	4	0
3	N	38	0	34	8	0
3	O	38	0	34	0	0
4	F	28	0	25	9	0
4	G	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	S	28	0	25	7	0
5	A	14	0	13	0	0
5	C	28	0	26	0	0
6	J	50	0	43	0	0
7	K	49	0	43	5	0
8	R	60	0	52	0	0
All	All	10839	0	10492	596	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (596) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:201:NAG:C6	4:F:203:NAG:H82	1.41	1.46
3:N:401:NAG:C6	3:N:403:NAG:H82	1.54	1.36
4:F:201:NAG:C6	4:F:203:NAG:C8	2.13	1.23
3:N:401:NAG:H61	3:N:403:NAG:C8	1.73	1.19
4:F:201:NAG:H62	4:F:203:NAG:C8	1.72	1.14
1:A:310:ILE:HD12	1:A:310:ILE:H	1.00	1.13
4:F:201:NAG:H62	4:F:203:NAG:H82	1.14	1.13
4:F:201:NAG:H61	4:F:203:NAG:H82	1.20	1.09
4:F:201:NAG:H61	4:F:203:NAG:C8	1.77	1.08
1:C:285:PRO:HD3	1:C:366:ASN:HB2	1.40	1.02
3:N:401:NAG:H61	3:N:403: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:I:501:NAG:O5	3:I:502:FUC:H5	1.63	0.98
2:D:87:VAL:HG13	2:D:122:LEU:HD12	1.46	0.94
1:C:109:TRP:CH2	1:C:153:GLN:HB3	2.02	0.94
1:A:310:ILE:HD12	1:A:310:ILE:N	1.85	0.92
3:N:401:NAG:C6	3:N:403: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:N:401:NAG:H62	3:N:403:NAG:H82	1.50	0.88
2:B:88:VAL:O	2:B:92:THR:HG23	1.74	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:ARG:HH11	1:A:317:ARG:HG3	1.40	0.86
4:S:901:NAG:O4	4:S:902: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:285:PRO:HD3	1:C:366:ASN:CB	2.06	0.84
1:C:340:LEU:HG	1:C:345:TYR:HE1	1.42	0.84
4:S:901:NAG:H62	4:S:902:NAG:O7	1.77	0.84
4:G:301:NAG:H61	4:G:302:NAG:C1	2.07	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:424:LYS:HG2	1:A:425:ALA:H	1.45	0.81
1:A:12:THR:HG22	1:A:17:VAL:O	1.81	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
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
2:D:96:ASN:O	2:D:98:THR:N	2.18	0.77
1:C:289:GLN:HB2	1:C:306:ASN:HB3	1.67	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
2:D:80:LEU:HB3	2:D:133:LEU:HD11	1.67	0.75
1:A:258:VAL:HA	1:A:281:ALA:HB3	1.69	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
7:K:801:NAG:H61	7:K:802: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
4:F:201:NAG:C6	4:F:203: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
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:424:LYS:HG2	1:A:425:ALA:N	2.10	0.66
1:A:129:LEU:HA	1:A:136:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
7:K:801:NAG:C6	7:K:802: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
4:F:201:NAG:H61	4:F:203: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
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
1:C:90:THR:HG23	1:C:189:ASP:HB3	1.80	0.63
2:B:10:ALA:CB	2:B:84:TYR:OH	2.47	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
2:D:96:ASN:HD22	2:D:149:ASP:HB2	1.63	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
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
2:B:155:VAL:HG23	2:B:156:PHE:H	1.64	0.62
1:A:387:ASP:N	1:A:387:ASP:OD1	2.33	0.62
1:A:306:ASN:HB2	1:A:344:THR:HG22	1.81	0.62
2:D:1:SER:H2	2:D:2:PRO:HD3	1.64	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:N:401:NAG:H61	3:N:403:NAG:C7	2.29	0.62
1:C:317:ARG:NH1	1:C:317:ARG:CG	2.57	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
4:S:901:NAG:C6	4:S:902: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
4:S:901:NAG:O4	4:S:902: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:C:131:ASN:H	1:C:132:PRO:HD3	1.66	0.61
1:A:229:VAL:HA	1:A:270:THR:HG22	1.81	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
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:C	1:A:196:ILE:HD12	2.24	0.58
1:A:416:LEU:HA	1:A:465:SER:HA	1.86	0.58
1:C:173:ARG:HD2	1:C:187:TRP:CE3	2.38	0.58
1:A:8:LEU:HD21	1:A:22:TRP:HE3	1.68	0.58
1:A:189:ASP:OD2	1:A:189:ASP:N	2.34	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
3:N:401:NAG:H62	3:N:403:NAG:C8	2.22	0.57
1:C:464:SER:HB3	1:C:471:TRP:CE3	2.40	0.57
1:A:243:HIS:HA	1:A:249:VAL:HG12	1.86	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:168:HIS:HB2	1:A:196:ILE:HD11	1.87	0.56
1:A:128:VAL:HG23	1:A:129:LEU:N	2.19	0.56
1:C:482:THR:HG22	1:C:483:THR:N	2.12	0.56
2:B:21:ASN:ND2	2:B:24:ASN:HB2	2.20	0.56
1:A:212:VAL:HG13	1:A:280:PHE:HB2	1.88	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:C:103:SER:HB2	1:C:163:LEU:CD1	2.33	0.56
1:A:278:VAL:HB	2:B:155:VAL:CG2	2.35	0.56
1:A:30:PRO:HD2	1:A:32:THR:HG23	1.86	0.56
2:D:154:ASP:O	2:D:155:VAL:C	2.44	0.56
1:A:323:LEU:HD22	1:A:349:VAL:HG21	1.88	0.56
1:C:259:SER:CB	1:C:264:THR:OG1	2.53	0.55
1:A:325:GLU:OE2	1:A:327:ILE:HG13	2.06	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
2:D:77:LYS:HB2	2:D:137:TYR:CE2	2.42	0.55
1:C:260:GLU:HG2	1:C:261:ASN:N	2.22	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:C:232:GLY:HA2	1:C:267:ILE:O	2.06	0.54
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: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
2:D:42:ILE:HD13	2:D:45:TYR:HE2	1.72	0.54
1:C:174:TRP:N	1:C:174:TRP:CD1	2.76	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:97:ILE:HD12	2:D:162:GLY:HA2	1.88	0.54
7:K:801:NAG:H61	7:K:802:FUC:HO2	1.73	0.54
1:C:126:ILE:HG12	1:C:172:ILE:CG2	2.38	0.54
1:A:465:SER:OG	1:A:468:PHE:N	2.37	0.54
1:A:366:ASN:C	1:A:366:ASN:ND2	2.62	0.54
1:A:306:ASN:OD1	1:A:308:GLY:N	2.38	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
4:S:901:NAG:C5	4:S:902:NAG:O7	2.56	0.53
1:A:403:PHE:CE1	1:A:459:PHE:HB3	2.44	0.53
1:A:379:VAL:O	1:A:382:ARG:N	2.36	0.53
1:C:223:CYS:SG	1:C:224:MET:N	2.82	0.53
1:A:406:TYR:CD2	1:A:406:TYR:C	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
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
7:K:801:NAG:C6	7:K:803: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	4:S:901:NAG:N2	2.42	0.52
1:C:66:THR:CG2	1:C:76:LYS:NZ	2.72	0.52
1:A:253:ILE:HD11	1:A:266:ILE:HD13	1.92	0.52
1:A:173:ARG:HG2	1:A:190:TRP:CH2	2.45	0.52
1:A:106:LEU:HB2	4:F:201: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
4:G:301:NAG:C6	4:G:302:NAG:C1	2.82	0.51
1:A:128:VAL:CG2	1:A:137:VAL:HG22	2.39	0.51
1:C:379:VAL:O	1:C:381:GLU:N	2.43	0.51
3:I:501:NAG:C6	3:I:502:FUC:H5	2.41	0.51
1:A:233:GLN:HB3	1:A:238:LEU:CA	2.39	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:ILE:HG22	1:A:127:LYS:N	2.25	0.51
1:C:451:LEU:HB3	1:C:457:TYR:CE1	2.46	0.51
1:A:405:TRP:O	1:A:443:THR:HA	2.10	0.51
2:D:65:THR:O	2:D:66:ASP:CG	2.49	0.51
2:B:95:GLY:O	2:B:98:THR:HB	2.10	0.51
1:C:421:GLU:HB3	1:C:460:ARG:HB2	1.92	0.51
1:A:59:SER:O	1:A:63:HIS:NE2	2.43	0.51
1:C:135:GLU:OE2	1:C:135:GLU:N	2.43	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
2:B:83:LEU:HD21	2:B:129:VAL:HG21	1.93	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:C:36:ILE:HB	1:C:48:LEU:HD11	1.93	0.50
1:A:163:LEU:O	1:A:198:TRP:CZ3	2.56	0.50
2:D:27:ARG:C	2:D:29:GLN:H	2.14	0.50
1:C:198:TRP:CD1	1:C:199:ILE:O	2.64	0.50
1:C:12:THR:HG21	1:C:18:TRP:CD1	2.47	0.50
1:C:422:ILE:HD12	1:C:432:ARG:HG3	1.93	0.50
1:A:468:PHE:C	1:A:468:PHE:CD2	2.84	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
2:B:76:GLU:HA	2:B:79:LYS:HE3	1.94	0.50
1:A:451:LEU:HD12	1:A:457:TYR:CZ	2.47	0.50
1:C:86:LEU:HB2	1:C:181:PHE:CE2	2.47	0.50
2:D:40:LEU:HB2	2:D:114:LYS:HD2	1.92	0.50
1:A:293:CYS:HB2	1:A:377:ILE:HD13	1.94	0.50
1:A:296:HIS:CD2	1:A:296:HIS:N	2.79	0.50
1:A:236:ASN:HB2	2:B:50:GLU:OE1	2.12	0.50
1:A:16:ARG:HH21	1:A:115:ALA:C	2.15	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:A:403:PHE:HE2	1:A:461:VAL:HG23	1.76	0.50
1:A:118:HIS:HB3	1:A:119:PRO:HD2	1.93	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:C:81:GLU:O	1:C:84:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:379:VAL:C	1:C:381:GLU:H	2.16	0.49
1:A:287:VAL:HA	1:A:371:ALA:HB1	1.93	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:117:PRO:HB2	1:A:118:HIS:HD2	1.78	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:C:325:GLU:HG2	1:C:360:PHE:CE2	2.48	0.49
2:D:151:SER:OG	2:D:152:GLY:N	2.46	0.49
2:D:77:LYS:HB2	2:D:137:TYR:HE2	1.76	0.49
1:A:325:GLU:HB3	1:A:328:SER:HB2	1.94	0.49
1:A:128:VAL:HG22	1:A:137:VAL:O	2.13	0.48
1:C:22:TRP:CH2	1:C:67:ILE:HD11	2.48	0.48
1:A:403:PHE:CE1	1:A:459:PHE:CB	2.96	0.48
1:A:315:GLY:O	1:A:316:PRO:C	2.51	0.48
1:A:111:ASP:C	1:A:113:GLY:H	2.17	0.48
1:C:210:ASP:CG	2:D:155:VAL:HG23	2.34	0.48
1:C:462:ARG:HB2	1:C:474:TRP:CE3	2.48	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:C:379:VAL:C	1:C:381:GLU:N	2.66	0.48
1:A:405:TRP:O	1:A:443:THR:HG22	2.14	0.48
1:A:233:GLN:HB3	1:A:238:LEU:HB3	1.95	0.48
2:B:79:LYS:HD2	2:B:180:PHE:HB3	1.95	0.48
1:A:67:ILE:HD12	1:A:75:SER:HB3	1.94	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:C:163:LEU:CD2	1:C:163:LEU:N	2.77	0.47
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: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: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
1:A:378:ASN:O	1:A:379:VAL:C	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:93:SER:O	2:B:97:ILE:HG12	2.15	0.47
1:A:464:SER:OG	1:A:465:SER:N	2.48	0.47
1:A:129:LEU:N	1:A:136:PRO:HD2	2.29	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:438:GLY:HA2	1:A:444:TYR:CE2	2.49	0.47
1:A:438:GLY:HA2	1:A:444:TYR:HE2	1.80	0.47
1:A:80:ASN:CG	1:A:81:GLU:H	2.18	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:216:GLY:N	1:A:256:ILE:O	2.48	0.47
1:C:317:ARG:HG2	1:C:317:ARG:NH1	2.30	0.47
1:C:326:SER:HB3	1:C:359:ASN:HB3	1.97	0.47
1:A:283:TYR:O	1:A:311:THR:HB	2.15	0.47
1:A:120:SER:HB2	1:A:145:MET:HE3	1.96	0.47
1:A:303:CYS:O	1:A:346:ARG:HA	2.15	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
1:C:8:LEU:CD2	1:C:22:TRP:HB3	2.45	0.47
1:A:401:VAL:HG23	1:A:448:VAL:HB	1.96	0.47
1:C:379:VAL:O	1:C:382:ARG:N	2.47	0.47
1:C:482:THR:CG2	1:C:483:THR:H	2.10	0.46
1:C:36:ILE:HD12	1:C:66:THR:O	2.15	0.46
2:D:124:GLY:O	2:D:125:LEU:C	2.53	0.46
2:B:103:ILE:HG22	2:B:103:ILE:O	2.14	0.46
3:I:501:NAG:C5	3:I:502:FUC:H5	2.43	0.46
1:A:391:LEU:HD13	1:A:403:PHE:CZ	2.50	0.46
2:B:93:SER:HB2	2:B:148:PRO:HD2	1.96	0.46
1:C:334:PHE:CZ	1:C:336:ARG:HB2	2.49	0.46
1:C:14:ASN:HD21	1:C:16:ARG:HB2	1.79	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
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
2:B:132:ARG:C	2:B:134:CYS:N	2.68	0.46
2:D:129:VAL:O	2:D:133:LEU:HD12	2.16	0.46
1:C:419:GLN:O	1:C:461:VAL:HA	2.15	0.46
1:C:229:VAL:HG11	1:C:249:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:D:148:PRO:O	2:D:149:ASP:HB2	2.16	0.45
4:P:601:NAG:H61	4:P:603:NAG:HN2	1.82	0.45
1:A:415:ASN:N	1:A:415:ASN:OD1	2.49	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:315:GLY:C	1:C:317:ARG:H	2.19	0.45
1:C:245:TYR:HD1	1:C:246:GLY:N	2.12	0.45
1:C:116:LEU:HA	1:C:117:PRO:HD3	1.64	0.45
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
2:B:112:HIS:O	2:B:113:SER:C	2.53	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: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
1:C:12:THR:HG22	1:C:17:VAL:O	2.16	0.45
3:N:401:NAG:H61	3:N:403:NAG:N2	2.32	0.45
2:D:96:ASN:O	2:D:97:ILE:C	2.55	0.45
3:I:501:NAG:C6	3:I:502: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
1:A:461:VAL:O	1:A:475:SER:HB3	2.16	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:C:159:SER:C	1:C:161:LEU:N	2.70	0.44
1:A:198:TRP:CZ2	1:A:207:PHE:CZ	3.05	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
7:K:801:NAG:H61	7:K:803: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:126:ILE:CG2	1:A:127:LYS:N	2.80	0.44
1:A:127:LYS:HE2	1:A:171:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:172:ILE:HA	2:D:172:ILE:HD13	1.84	0.44
2:B:172:ILE:HD13	2:B:172:ILE:HA	1.85	0.44
2:D:94:LEU:HD12	2:D:94:LEU:HA	1.62	0.44
1:A:227:THR:O	1:A:228:LYS:C	2.55	0.44
1:C:8:LEU:HD23	1:C:22:TRP:HB3	1.98	0.44
1:C:10:CYS:CB	1:C:84:VAL:HG13	2.46	0.44
1:A:118:HIS:HB3	1:A:119:PRO:CD	2.47	0.44
1:A:480:HIS:ND1	1:A:481:LEU:O	2.51	0.44
1:A:218:ASN:HA	1:A:254:LEU:O	2.18	0.44
1:C:407:LEU:HD21	1:C:463:CYS:HB2	1.99	0.44
2:B:10:ALA:HB3	2:B:84:TYR:OH	2.17	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
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
2:B:14:ILE:HD11	2:D:158:LYS:CD	2.47	0.43
2:D:77:LYS:CD	2:D:137:TYR:HD2	2.31	0.43
1:C:124:TRP:HA	1:C:174:TRP:HB3	1.99	0.43
2:D:173:ILE:HD12	2:D:176:LEU:HD12	1.99	0.43
1:C:53:VAL:HG22	1:C:54:LYS:N	2.33	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
2:D:147:GLY:HA3	2:D:148:PRO:HD3	1.61	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
1:A:409:GLY:HA3	1:A:411:PHE:CE1	2.52	0.43
1:C:109:TRP:HH2	1:C:153:GLN:HB3	1.72	0.43
1:C:145:MET:SD	1:C:146:LEU:N	2.91	0.43
2:B:13:ALA:HB1	2:D:155:VAL:HG22	2.00	0.43
1:A:377:ILE:HG23	1:A:382:ARG:HD2	2.01	0.43
1:C:315:GLY:HA3	1:C:316:PRO:HD2	1.77	0.43
1:A:198:TRP:CD1	1:A:200:ARG:HA	2.54	0.43
1:C:132:PRO:HB2	1:C:134:THR:HG22	1.99	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:90:LEU:O	2:B:93:SER:N	2.51	0.43
2:B:19:HIS:CD2	1:C:333:VAL:CG1	3.01	0.43
1:C:301:ILE:HD13	1:C:360:PHE:CZ	2.46	0.43
1:A:129:LEU:CA	1:A:136:PRO:CD	2.97	0.43
2:B:9:ASN:ND2	2:D:96:ASN:HB3	2.34	0.43
1:C:15:MET:HE2	1:C:117:PRO:HD2	2.01	0.43
1:A:452:ASN:HA	1:A:453:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:25:PRO:O	1:C:27:GLY:O	2.37	0.43
2:B:98:THR:C	2:B:100:ASP:H	2.21	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
2:B:87:VAL:O	2:B:88:VAL:C	2.56	0.43
1:A:109:TRP:CH2	1:A:153:GLN:HB3	2.53	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:C:403:PHE:CE2	1:C:461:VAL:HG21	2.54	0.42
1:A:400:VAL:HG13	1:A:448:VAL:O	2.19	0.42
1:A:379:VAL:O	1:A:381:GLU:N	2.51	0.42
1:C:293:CYS:HA	1:C:302:ILE:O	2.19	0.42
1:C:213:VAL:HG12	1:C:214:LEU:H	1.85	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:283:TYR:CD2	1:C:309:ARG:CZ	3.02	0.42
1:C:221:ILE:O	1:C:250:ALA:HB1	2.19	0.42
1:A:388:PRO:HB2	1:A:461:VAL:HG12	2.01	0.42
1:C:129:LEU:HD13	1:C:169:SER:CB	2.46	0.42
1:A:117:PRO:HB2	1:A:118:HIS:CD2	2.54	0.42
1:C:415:ASN:HB3	1:C:437:ARG:HA	2.01	0.42
1:A:476:ASP:HB3	1:A:477:GLU:H	1.67	0.42
2:D:68:PRO:HD3	2:D:89:TYR:CD1	2.54	0.42
1:C:432:ARG:HH12	1:C:449:ASP:H	1.67	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:A:389:THR:HG22	1:A:390:SER:N	2.33	0.42
1:A:341:THR:HB	1:A:343:GLU:H	1.85	0.42
2:B:130:LEU:O	2:B:130:LEU:HG	2.09	0.42
1:A:462:ARG:HD2	1:A:474:TRP:CZ2	2.54	0.42
1:C:40:ASP:O	1:C:41:ARG:HB2	2.19	0.42
1:C:120:SER:HB2	1:C:145:MET:HE2	2.02	0.42
1:A:199:ILE:O	1:A:200:ARG:C	2.58	0.42
2:D:42:ILE:HA	2:D:45:TYR:HE2	1.78	0.42
1:C:128:VAL:HG22	1:C:137:VAL:O	2.19	0.42
1:C:113:GLY:O	1:C:116:LEU:N	2.40	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:89:GLU:HG3	1:A:89:GLU:H	1.44	0.42
1:C:109:TRP:CZ3	1:C:153:GLN:HB2	2.35	0.42
1:A:402:THR:HG22	1:A:402:THR:O	2.20	0.42
2:D:165:LEU:O	2:D:166:LEU:C	2.57	0.41
1:A:454:TYR:N	1:A:482:THR:OG1	2.53	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:D:29:GLN:OE1	2:D:125:LEU:HA	2.20	0.41
2:B:3:LEU:HD13	2:D:3:LEU:HB2	2.02	0.41
1:A:474:TRP:O	1:A:475:SER:O	2.38	0.41
2:D:40:LEU:HD21	2:D:166:LEU:HD22	2.02	0.41
1:A:36:ILE:HG21	1:A:53:VAL:HG11	2.02	0.41
2:D:35:GLY:O	2:D:36:SER:C	2.58	0.41
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: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
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
1:A:356:GLU:O	1:A:357:ILE:C	2.59	0.41
1:A:104:SER:HB3	1:A:158:THR:HG23	2.03	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
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
2:B:4:PRO:HB2	2:B:5:ILE:H	1.75	0.41
1:A:225:SER:N	1:A:248:THR:HG22	2.20	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:285:PRO:HD3	1:A:366:ASN:CB	2.48	0.41
2:B:84:TYR:CD2	2:B:142:VAL:HG11	2.56	0.41
1:A:306:ASN:HA	1:A:307:PRO:HD2	1.73	0.41
2:D:166:LEU:HA	2:D:166:LEU:HD23	1.90	0.41
1:A:8:LEU:CD2	1:A:22:TRP:HB3	2.51	0.41
1:A:22:TRP:CE2	1:A:51:THR:O	2.74	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
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:154:ASP:O	2:D:156:PHE:N	2.54	0.41
1:A:448:VAL:HG12	1:A:451:LEU:HD21	2.02	0.41
1:A:442:SER:O	1:A:444:TYR:CE1	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:40:ASP:O	1:C:41:ARG:CB	2.68	0.41
1:A:169:SER:HA	1:A:194:LYS:O	2.21	0.41
1:C:367:PRO:O	1:C:368:LEU:HB2	2.22	0.40
1:A:233:GLN:CA	1:A:238:LEU:HA	2.50	0.40
1:C:109:TRP:HB2	1:C:110:ASN:H	1.41	0.40
1:A:234:ILE:HG12	1:A:253:ILE:HG12	2.03	0.40
2:B:11:THR:C	2:B:13:ALA:N	2.74	0.40
2:D:42:ILE:HD13	2:D:45:TYR:CE2	2.55	0.40
1:C:81:GLU:HA	1:C:84:VAL:CG2	2.51	0.40
1:A:360:PHE:O	1:A:374:ALA:HA	2.20	0.40
1:C:113:GLY:O	1:C:115:ALA:N	2.54	0.40
2:D:84:TYR:HD2	2:D:142:VAL:HG11	1.86	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: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
2:D:82:GLU:O	2:D:86:ILE:HG13	2.22	0.40
1:C:284:PRO:HD3	1:C:368:LEU:HD22	2.03	0.40
4:S:901:NAG:H5	4:S:902:NAG:O7	2.21	0.40
2:D:152:GLY:O	2:D:153:LYS:CB	2.68	0.40
1:A:173:ARG:HD3	1:A:187:TRP:CZ3	2.56	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
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

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%)	2	37
1	C	478/488 (98%)	383 (80%)	70 (15%)	25 (5%)	3	42
2	B	178/180 (99%)	125 (70%)	38 (21%)	15 (8%)	1	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	178/180 (99%)	115 (65%)	45 (25%)	18 (10%)	1	20
All	All	1312/1336 (98%)	997 (76%)	227 (17%)	88 (7%)	2	34

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	11
1	C	419/443 (95%)	329 (78%)	90 (22%)	1	11
2	B	154/154 (100%)	123 (80%)	31 (20%)	2	14
2	D	154/154 (100%)	124 (80%)	30 (20%)	2	15
All	All	1146/1194 (96%)	904 (79%)	242 (21%)	1	12

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

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Mol	Chain	Res	Type
1	A	76	LYS
1	A	78	THR
1	A	89	GLU
1	A	90	THR
1	A	94	LEU
1	A	95	ASP
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

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Mol	Chain	Res	Type
1	A	311	THR
1	A	317	ARG
1	A	319	THR
1	A	322	THR
1	A	323	LEU
1	A	324	PHE
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

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Mol	Chain	Res	Type
2	B	32	GLN
2	B	40	LEU
2	B	43	LEU
2	B	73	ASN
2	B	80	LEU
2	B	93	SER
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

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Mol	Chain	Res	Type
1	C	112	ARG
1	C	114	SER
1	C	128	VAL
1	C	130	GLN
1	C	137	VAL
1	C	139	LEU
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

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Mol	Chain	Res	Type
1	C	304	SER
1	C	309	ARG
1	C	317	ARG
1	C	319	THR
1	C	324	PHE
1	C	328	SER
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

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Mol	Chain	Res	Type
2	D	75	THR
2	D	76	GLU
2	D	83	LEU
2	D	102	LYS
2	D	111	LEU
2	D	112	HIS
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

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Mol	Chain	Res	Type
2	B	178	GLN
1	C	80	ASN
1	C	180	HIS
1	C	201	ASN
1	C	233	GLN
1	C	236	ASN
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 chains 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 ⓘ

42 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	$\# Z > 2$
3	NAG	E	101	1,3	12,14,15	0.65	0	15,19,21	1.11	1 (6%)
3	FUC	E	102	3	9,10,11	0.96	1 (11%)	10,14,16	1.36	1 (10%)
3	NAG	E	103	3	12,14,15	0.53	0	15,19,21	1.41	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	201	1,4	12,14,15	0.73	1 (8%)	15,19,21	1.27	3 (20%)
4	NAG	F	203	4	12,14,15	0.66	0	15,19,21	1.69	2 (13%)
4	NAG	G	301	1,4	12,14,15	0.67	0	15,19,21	1.51	2 (13%)
4	NAG	G	302	4	12,14,15	0.76	1 (8%)	15,19,21	1.16	2 (13%)
3	NAG	H	401	1,3	12,14,15	0.66	0	15,19,21	0.82	1 (6%)
3	FUC	H	402	3	9,10,11	0.81	0	10,14,16	1.03	2 (20%)
3	NAG	H	403	3	12,14,15	0.61	0	15,19,21	0.93	0
3	NAG	I	501	1,3	12,14,15	0.62	0	15,19,21	1.15	2 (13%)
3	FUC	I	502	3	9,10,11	0.94	0	10,14,16	1.04	2 (20%)
3	NAG	I	503	3	12,14,15	0.64	0	15,19,21	0.87	1 (6%)
6	NAG	J	701	1,6	12,14,15	0.88	1 (8%)	15,19,21	1.64	3 (20%)
6	NAG	J	702	6	12,14,15	0.71	1 (8%)	15,19,21	0.98	0
6	MAN	J	703	6	10,11,12	0.69	0	11,15,17	2.10	3 (27%)
6	MAN	J	704	6	10,11,12	0.69	0	11,15,17	0.96	0
7	NAG	K	801	1,7	12,14,15	0.94	1 (8%)	15,19,21	1.57	2 (13%)
7	FUC	K	802	7	9,10,11	0.93	0	10,14,16	1.35	1 (10%)
7	NAG	K	803	7	12,14,15	0.66	0	15,19,21	0.77	0
7	MAN	K	804	7	10,11,12	0.79	0	11,15,17	1.36	2 (18%)
4	NAG	L	901	1,4	12,14,15	0.68	0	15,19,21	1.07	2 (13%)
4	NAG	L	902	4	12,14,15	0.60	0	15,19,21	0.95	1 (6%)
4	NAG	M	101	1,4	12,14,15	0.46	0	15,19,21	1.50	3 (20%)
4	NAG	M	102	4	12,14,15	0.64	0	15,19,21	1.04	1 (6%)
3	NAG	N	401	1,3	12,14,15	0.69	0	15,19,21	1.28	2 (13%)
3	FUC	N	402	3	9,10,11	0.82	0	10,14,16	1.30	2 (20%)
3	NAG	N	403	3	12,14,15	0.66	0	15,19,21	0.90	1 (6%)
3	NAG	O	501	1,3	12,14,15	0.58	0	15,19,21	1.69	1 (6%)
3	FUC	O	502	3	9,10,11	0.79	0	10,14,16	1.16	0
3	NAG	O	503	3	12,14,15	0.63	0	15,19,21	0.93	1 (6%)
4	NAG	P	601	1,4	12,14,15	0.62	0	15,19,21	1.60	1 (6%)
4	NAG	P	603	4	12,14,15	0.62	0	15,19,21	1.21	2 (13%)
4	NAG	Q	701	1,4	12,14,15	0.62	0	15,19,21	1.60	3 (20%)
4	NAG	Q	703	4	12,14,15	0.70	0	15,19,21	1.23	2 (13%)
8	NAG	R	801	1,8	12,14,15	1.01	1 (8%)	15,19,21	1.76	4 (26%)
8	FUC	R	802	8	9,10,11	0.78	0	10,14,16	0.59	0
8	NAG	R	803	8	12,14,15	0.82	1 (8%)	15,19,21	1.19	1 (6%)
8	MAN	R	804	8	10,11,12	0.99	1 (10%)	11,15,17	2.58	4 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	R	805	8	10,11,12	0.53	0	11,15,17	2.19	3 (27%)
4	NAG	S	901	1,4	12,14,15	0.59	0	15,19,21	1.33	2 (13%)
4	NAG	S	902	4	12,14,15	0.54	0	15,19,21	1.34	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	101	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	102	3	-	0/0/17/20	0/1/1/1
3	NAG	E	103	3	-	0/6/23/26	0/1/1/1
4	NAG	F	201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	203	4	-	0/6/23/26	0/1/1/1
4	NAG	G	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	302	4	-	0/6/23/26	0/1/1/1
3	NAG	H	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	H	402	3	-	0/0/17/20	0/1/1/1
3	NAG	H	403	3	-	0/6/23/26	0/1/1/1
3	NAG	I	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	I	502	3	-	0/0/17/20	0/1/1/1
3	NAG	I	503	3	-	0/6/23/26	0/1/1/1
6	NAG	J	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	702	6	-	0/6/23/26	0/1/1/1
6	MAN	J	703	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	J	704	6	-	0/2/19/22	0/1/1/1
7	NAG	K	801	1,7	-	0/6/23/26	0/1/1/1
7	FUC	K	802	7	-	0/0/17/20	0/1/1/1
7	NAG	K	803	7	-	0/6/23/26	0/1/1/1
7	MAN	K	804	7	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	L	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	902	4	-	0/6/23/26	0/1/1/1
4	NAG	M	101	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	102	4	-	0/6/23/26	0/1/1/1
3	NAG	N	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	N	402	3	-	0/0/17/20	0/1/1/1
3	NAG	N	403	3	-	0/6/23/26	0/1/1/1
3	NAG	O	501	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	FUC	O	502	3	-	0/0/17/20	0/1/1/1
3	NAG	O	503	3	-	0/6/23/26	0/1/1/1
4	NAG	P	601	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	P	603	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	703	4	-	1/6/23/26	0/1/1/1
8	NAG	R	801	1,8	-	0/6/23/26	0/1/1/1
8	FUC	R	802	8	-	0/0/17/20	0/1/1/1
8	NAG	R	803	8	-	0/6/23/26	0/1/1/1
8	MAN	R	804	8	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	R	805	8	-	0/2/19/22	0/1/1/1
4	NAG	S	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	902	4	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	801	NAG	C2-N2	-2.63	1.43	1.46
8	R	803	NAG	O5-C5	-2.42	1.40	1.45
7	K	801	NAG	O5-C5	-2.29	1.41	1.45
6	J	701	NAG	O5-C5	-2.20	1.41	1.45
3	E	102	FUC	O5-C5	-2.18	1.41	1.45
4	F	201	NAG	O5-C5	-2.15	1.41	1.45
8	R	804	MAN	O5-C5	-2.13	1.41	1.45
6	J	702	NAG	O5-C5	-2.05	1.41	1.45
4	G	302	NAG	O5-C5	-2.02	1.41	1.45

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	804	MAN	O5-C5-C6	5.64	112.90	106.98
3	O	501	NAG	O5-C5-C6	5.58	112.84	106.98
4	F	203	NAG	O5-C5-C6	5.36	112.61	106.98
8	R	805	MAN	O5-C5-C4	5.31	117.39	110.65
4	P	601	NAG	O5-C5-C6	5.03	112.26	106.98
6	J	701	NAG	O5-C5-C6	4.68	111.89	106.98
8	R	801	NAG	C3-C2-N2	-4.43	105.02	111.76
3	E	103	NAG	O5-C5-C6	4.40	111.60	106.98
6	J	703	MAN	C3-C4-C5	4.39	118.04	110.20
6	J	703	MAN	O5-C5-C4	4.29	116.10	110.65
4	G	301	NAG	O5-C5-C6	4.21	111.40	106.98
8	R	804	MAN	C3-C4-C5	4.11	117.55	110.20
7	K	801	NAG	O5-C5-C6	4.10	111.29	106.98
8	R	804	MAN	C4-C3-C2	3.70	115.48	110.50
3	N	401	NAG	O5-C5-C4	-3.68	105.99	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	701	NAG	O5-C5-C4	3.57	115.19	110.65
4	S	902	NAG	O5-C5-C6	3.41	110.56	106.98
8	R	805	MAN	O5-C5-C6	3.36	110.51	106.98
7	K	804	MAN	C4-C3-C2	3.29	114.92	110.50
7	K	801	NAG	C3-C2-N2	-3.26	106.80	111.76
4	Q	701	NAG	C3-C4-C5	3.25	116.00	110.20
7	K	802	FUC	C4-C3-C2	3.23	114.84	110.50
4	M	102	NAG	O5-C5-C6	3.17	110.31	106.98
3	I	501	NAG	O5-C5-C6	2.94	110.07	106.98
4	Q	703	NAG	O5-C5-C6	2.85	109.97	106.98
4	M	101	NAG	C4-C3-C2	-2.83	104.39	111.32
3	N	402	FUC	O5-C5-C4	2.81	114.47	110.22
8	R	804	MAN	O4-C4-C3	-2.75	104.19	110.35
4	L	901	NAG	C2-N2-C7	-2.73	118.51	123.09
4	P	603	NAG	C2-N2-C7	2.66	127.56	123.09
4	M	101	NAG	O4-C4-C5	2.65	116.26	109.28
4	S	902	NAG	C2-N2-C7	-2.58	118.76	123.09
8	R	801	NAG	O5-C5-C6	2.57	109.68	106.98
4	S	901	NAG	C2-N2-C7	-2.56	118.79	123.09
8	R	801	NAG	O3-C3-C2	-2.52	103.79	109.09
3	E	101	NAG	O5-C5-C6	2.48	109.58	106.98
8	R	801	NAG	C2-N2-C7	-2.44	119.00	123.09
8	R	805	MAN	C3-C4-C5	2.43	114.55	110.20
4	F	201	NAG	O4-C4-C3	-2.40	104.97	110.35
6	J	703	MAN	C4-C3-C2	2.40	113.73	110.50
4	M	101	NAG	O5-C5-C6	2.36	109.46	106.98
3	O	503	NAG	O5-C5-C6	2.36	109.46	106.98
4	P	603	NAG	O5-C5-C6	2.32	109.42	106.98
4	L	901	NAG	O5-C5-C6	2.32	109.41	106.98
3	I	501	NAG	C3-C2-N2	-2.31	108.24	111.76
3	I	503	NAG	O5-C5-C6	2.30	109.39	106.98
3	E	102	FUC	C6-C5-C4	-2.29	109.34	113.06
8	R	803	NAG	C3-C4-C5	2.28	114.27	110.20
4	G	302	NAG	O5-C5-C6	2.27	109.37	106.98
4	L	902	NAG	O5-C5-C6	2.25	109.34	106.98
3	N	402	FUC	C3-C4-C5	2.24	113.58	109.84
3	H	402	FUC	C3-C4-C5	2.23	113.56	109.84
3	H	401	NAG	O5-C5-C6	2.23	109.32	106.98
4	F	201	NAG	C3-C2-N2	-2.22	108.38	111.76
4	S	901	NAG	O5-C5-C6	2.22	109.31	106.98
4	G	302	NAG	O5-C5-C4	-2.22	107.84	110.65
3	N	403	NAG	O5-C5-C6	2.21	109.30	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	502	FUC	C4-C3-C2	2.21	113.47	110.50
3	H	402	FUC	O5-C5-C4	2.17	113.50	110.22
4	Q	701	NAG	C4-C3-C2	2.13	116.54	111.32
4	F	203	NAG	O7-C7-C8	-2.13	117.89	122.04
4	F	201	NAG	O5-C5-C6	2.11	109.19	106.98
3	I	502	FUC	C3-C4-C5	2.09	113.31	109.84
6	J	701	NAG	O5-C5-C4	-2.06	108.03	110.65
3	N	401	NAG	O5-C5-C6	2.05	109.13	106.98
4	Q	703	NAG	O7-C7-C8	-2.04	118.06	122.04
7	K	804	MAN	C3-C4-C5	2.03	113.83	110.20
6	J	701	NAG	C3-C2-N2	-2.03	108.67	111.76
4	G	301	NAG	C3-C4-C5	2.01	113.79	110.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	R	804	MAN	C1
6	J	703	MAN	C1
3	O	501	NAG	C1
7	K	804	MAN	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	703	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry

3 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
5	NAG	A	601	1	12,14,15	0.58	0	15,19,21	1.15	2 (13%)
5	NAG	C	501	1	12,14,15	0.59	0	15,19,21	0.90	1 (6%)
5	NAG	C	601	1	12,14,15	0.55	0	15,19,21	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	NAG	O5-C5-C6	2.44	109.54	106.98
5	A	601	NAG	O5-C5-C6	2.37	109.47	106.98
5	A	601	NAG	C3-C2-N2	-2.14	108.50	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/488 (98%)	-0.30	1 (0%) 93 88	78, 100, 119, 144	0
1	C	480/488 (98%)	-0.31	0 100 100	80, 100, 119, 141	0
2	B	180/180 (100%)	-0.43	0 100 100	83, 100, 122, 138	0
2	D	180/180 (100%)	-0.41	0 100 100	85, 101, 122, 137	0
All	All	1320/1336 (98%)	-0.33	1 (0%) 91 90	78, 100, 120, 144	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	F	203	14/15	0.56	15.93	87,89,90,90	14
4	NAG	P	601	14/15	0.23	7.60	101,102,105,108	14
4	NAG	L	902	14/15	0.29	3.28	87,87,87,87	14
4	NAG	G	302	14/15	0.31	3.00	100,101,103,103	14

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	K	801	14/15	0.23	2.84	56,60,62,64	14
4	NAG	S	902	14/15	0.33	2.49	96,96,97,97	14
4	NAG	M	101	14/15	0.28	2.40	103,107,108,108	14
3	FUC	E	102	10/11	0.27	2.35	68,69,69,70	10
7	NAG	K	803	14/15	0.20	1.99	59,60,62,63	14
3	FUC	I	502	10/11	0.41	1.94	104,105,106,106	10
3	NAG	N	401	14/15	0.18	1.84	96,98,102,102	14
4	NAG	Q	701	14/15	0.24	1.79	102,102,104,105	14
8	NAG	R	803	14/15	0.22	1.52	73,78,80,81	14
3	NAG	H	401	14/15	0.19	1.18	96,98,100,102	14
3	NAG	I	501	14/15	0.18	1.01	107,112,112,113	14
4	NAG	L	901	14/15	0.22	0.75	85,88,88,89	14
3	NAG	O	501	14/15	0.21	0.63	123,126,130,133	14
6	NAG	J	701	14/15	0.17	0.49	81,88,90,90	14
4	NAG	F	201	14/15	0.30	0.47	90,91,93,95	14
4	NAG	S	901	14/15	0.19	0.43	92,93,94,95	14
8	NAG	R	801	14/15	0.16	0.14	80,81,83,83	14
4	NAG	G	301	14/15	0.17	-0.60	92,94,96,98	14
3	NAG	E	101	14/15	0.17	-0.86	71,74,76,77	14
7	FUC	K	802	10/11	0.28	-	57,59,59,59	10
6	MAN	J	703	11/12	0.29	-	100,101,102,104	11
3	NAG	H	403	14/15	0.54	-	105,107,108,109	14
8	MAN	R	805	11/12	0.24	-	67,68,69,69	11
7	MAN	K	804	11/12	0.22	-	63,64,64,64	11
3	NAG	O	503	14/15	0.62	-	128,129,129,130	14
8	FUC	R	802	10/11	0.24	-	83,84,84,84	10
6	MAN	J	704	11/12	0.33	-	105,105,106,106	11
3	NAG	I	503	14/15	0.48	-	114,114,115,115	14
8	MAN	R	804	11/12	0.21	-	68,69,70,71	11
3	NAG	N	403	14/15	0.39	-	103,105,105,105	14
6	NAG	J	702	14/15	0.30	-	92,93,95,98	14
4	NAG	P	603	14/15	0.62	-	110,112,113,113	14
3	FUC	N	402	10/11	0.23	-	102,103,103,103	10
3	FUC	O	502	10/11	0.47	-	135,136,137,137	10
4	NAG	M	102	14/15	0.42	-	109,109,109,109	14
3	NAG	E	103	14/15	0.33	-	75,76,76,76	14
3	FUC	H	402	10/11	0.33	-	100,101,101,101	10
4	NAG	Q	703	14/15	0.42	-	105,107,108,109	14

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	C	501	14/15	0.34	3.56	89,92,93,94	14
5	NAG	A	601	14/15	0.23	3.03	77,86,87,88	14
5	NAG	C	601	14/15	0.16	-	94,97,99,99	14

6.5 Other polymers

There are no such residues in this entry.