Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:53 AM GMT

PDB ID	:	3CIY
Title	:	Mouse Toll-like receptor 3 ectodomain complexed with double-stranded RNA
Authors	:	Liu, L.; Botos, I.; Wang, Y.; Leonard, J.N.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on	:	2008-03-12
Resolution	:	3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

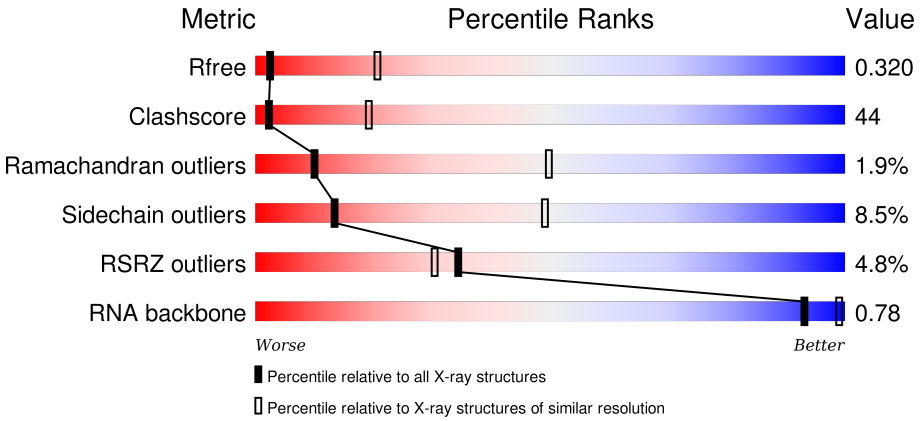
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)
RNA backbone	2183	1042 (4.02-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	46	48% 52%
2	D	46	37% 63%
3	A	697	4% 35% 54% 5% 5%
3	B	697	6% 34% 56% 6% .

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13194 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 RNA chain called 46-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	46	Total	C	N	O	P	0	0	0
			978	439	176	318	45			

- Molecule 2 is a RNA chain called 46-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	46	Total	C	N	O	P	0	0	0
			968	435	166	322	45			

- Molecule 3 is a protein called Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	661	Total	C	N	O	S	0	0	0
			5310	3392	905	999	14			
3	B	668	Total	C	N	O	S	0	0	0
			5360	3422	914	1010	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	ASN	-	EXPRESSION TAG	UNP Q99MB1
A	705	LEU	-	EXPRESSION TAG	UNP Q99MB1
A	706	TYR	-	EXPRESSION TAG	UNP Q99MB1
A	707	PHE	-	EXPRESSION TAG	UNP Q99MB1
A	708	GLN	-	EXPRESSION TAG	UNP Q99MB1
A	709	GLY	-	EXPRESSION TAG	UNP Q99MB1
A	710	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	711	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	712	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	713	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	714	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	715	HIS	-	EXPRESSION TAG	UNP Q99MB1

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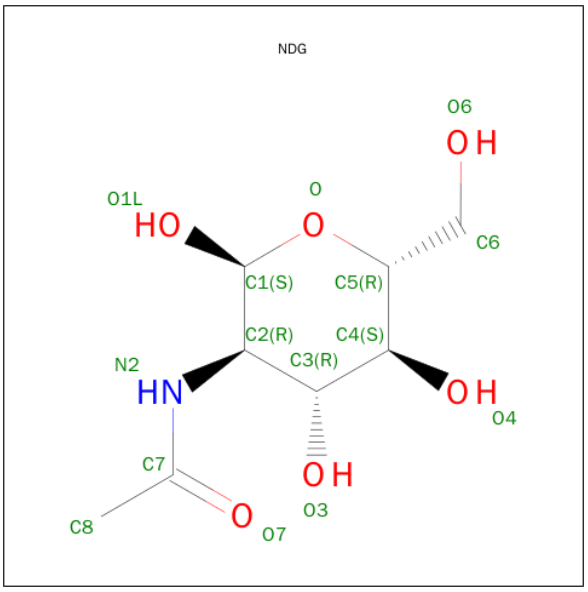
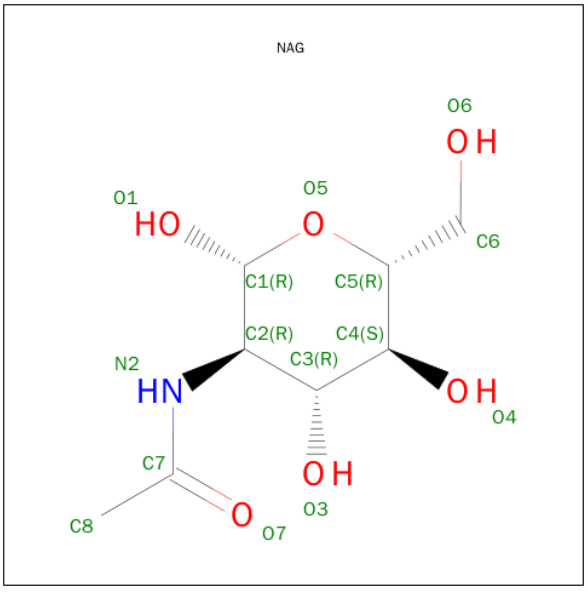
Chain	Residue	Modelled	Actual	Comment	Reference
A	716	TRP	-	EXPRESSION TAG	UNP Q99MB1
A	717	SER	-	EXPRESSION TAG	UNP Q99MB1
A	718	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	719	PRO	-	EXPRESSION TAG	UNP Q99MB1
A	720	GLN	-	EXPRESSION TAG	UNP Q99MB1
A	721	PHE	-	EXPRESSION TAG	UNP Q99MB1
A	722	GLU	-	EXPRESSION TAG	UNP Q99MB1
A	723	LYS	-	EXPRESSION TAG	UNP Q99MB1
B	704	ASN	-	EXPRESSION TAG	UNP Q99MB1
B	705	LEU	-	EXPRESSION TAG	UNP Q99MB1
B	706	TYR	-	EXPRESSION TAG	UNP Q99MB1
B	707	PHE	-	EXPRESSION TAG	UNP Q99MB1
B	708	GLN	-	EXPRESSION TAG	UNP Q99MB1
B	709	GLY	-	EXPRESSION TAG	UNP Q99MB1
B	710	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	711	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	712	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	713	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	714	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	715	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	716	TRP	-	EXPRESSION TAG	UNP Q99MB1
B	717	SER	-	EXPRESSION TAG	UNP Q99MB1
B	718	HIS	-	EXPRESSION TAG	UNP Q99MB1
B	719	PRO	-	EXPRESSION TAG	UNP Q99MB1
B	720	GLN	-	EXPRESSION TAG	UNP Q99MB1
B	721	PHE	-	EXPRESSION TAG	UNP Q99MB1
B	722	GLU	-	EXPRESSION TAG	UNP Q99MB1
B	723	LYS	-	EXPRESSION TAG	UNP Q99MB1

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SUGAR (2-MER) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (ALPHA-L-FUCOSE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	3	Total	C	N	O	0	0
			39	22	2	15		
10	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 14 is a polymer of unknown type called SUGAR (5-MER).

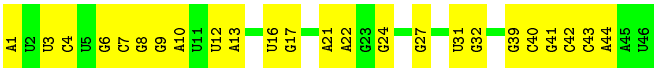
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	5	Total	C	N	O	0	0
			61	34	2	25		

3 Residue-property plots (i)

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.

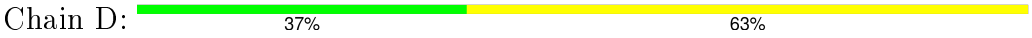
- Molecule 1: 46-MER

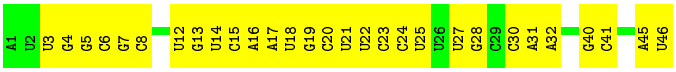
Chain C:



- Molecule 2: 46-MER

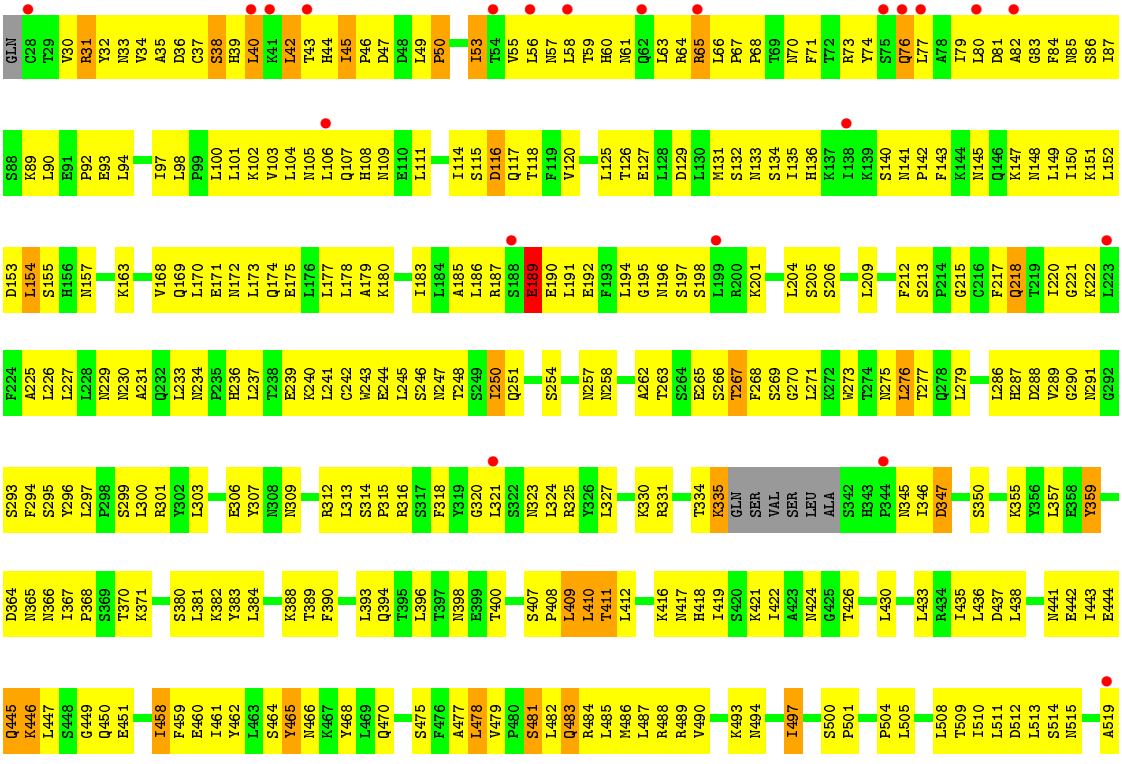
Chain D:

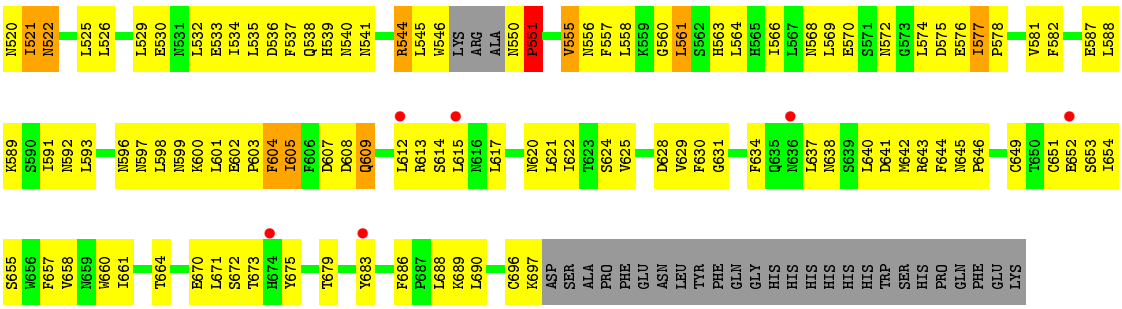




- Molecule 3: Toll-like receptor 3

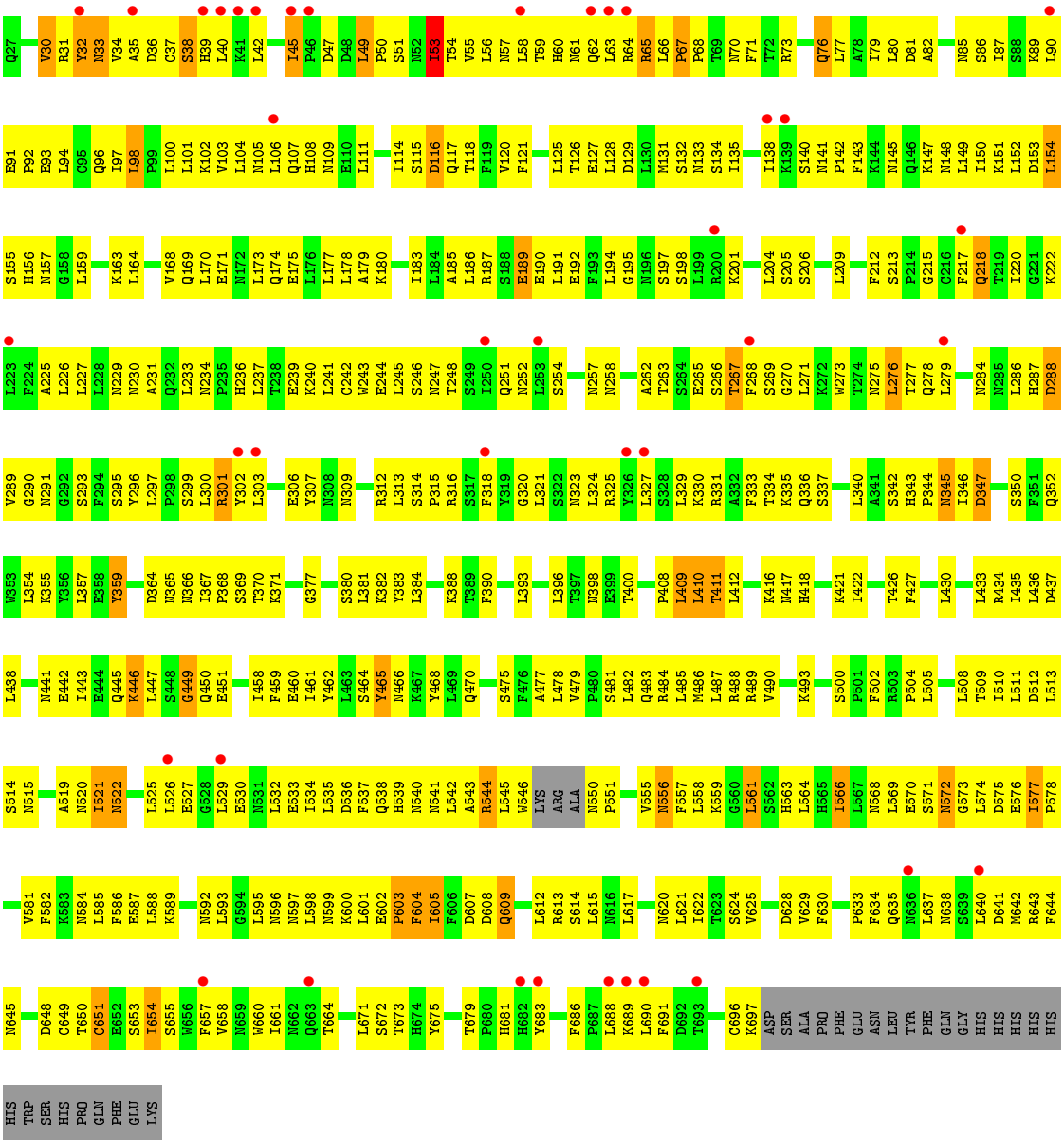
Chain A:





• Molecule 3: Toll-like receptor 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	117.85Å 225.88Å 259.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 3.41 47.29 – 3.41	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.29-3.41) 97.6 (47.29-3.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.288 , 0.333 0.307 , 0.320	Depositor DCC
R_{free} test set	2355 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	119.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 65.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 46429 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13194	wwPDB-VP
Average B, all atoms (Å^2)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, NDG, FUC, FUL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.40	0/1094	0.70	0/1703
2	D	0.43	0/1080	0.70	0/1679
3	A	0.46	1/5421 (0.0%)	0.69	1/7360 (0.0%)
3	B	0.48	1/5472 (0.0%)	0.70	0/7431
All	All	0.46	2/13067 (0.0%)	0.70	1/18173 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	53	ILE	CA-CB	5.48	1.67	1.54
3	A	189	GLU	N-CA	5.34	1.57	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	560	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	978	0	496	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	968	0	494	33	0
3	A	5310	0	5311	512	0
3	B	5360	0	5363	522	0
4	A	14	0	13	1	0
5	A	14	0	13	1	0
5	B	28	0	26	1	0
6	A	56	0	50	9	0
6	B	56	0	50	9	0
7	A	39	0	34	6	0
8	A	38	0	34	4	0
9	A	61	0	52	6	0
10	A	39	0	34	6	0
10	B	39	0	34	6	0
11	A	28	0	25	3	0
11	B	28	0	25	2	0
12	B	39	0	34	3	0
13	B	38	0	34	1	0
14	B	61	0	52	1	0
All	All	13194	0	12174	1111	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 44.

All (1111) 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:B:650:THR:O	3:B:654:ILE:HD12	1.41	1.21
3:A:605:ILE:HD11	3:A:629:VAL:HG13	1.19	1.13
3:B:450:GLN:HG3	10:B:4241:NDG:H6C2	1.29	1.12
3:A:536:ASP:HB3	3:A:538:GLN:HE22	1.20	1.06
3:B:108:HIS:HA	3:B:132:SER:HB2	1.32	1.06
3:A:108:HIS:HA	3:A:132:SER:HB2	1.32	1.06
3:A:277:THR:HG21	6:A:2521:NAG:H82	1.37	1.05
3:A:56:LEU:HD11	3:A:58:LEU:HG	1.38	1.05
3:B:605:ILE:HD11	3:B:629:VAL:HG13	1.07	1.05
3:B:536:ASP:HB3	3:B:538:GLN:HE22	1.23	1.00
3:B:468:TYR:HE1	3:B:470:GLN:HB2	1.29	0.97
3:B:650:THR:O	3:B:654:ILE:CD1	2.13	0.97
3:B:605:ILE:HD13	3:B:605:ILE:H	1.31	0.95
3:B:68:PRO:HB2	3:B:93:GLU:HB2	1.48	0.95
3:B:33:ASN:HA	3:B:53:ILE:HB	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:521:ILE:HD11	3:A:525:LEU:HB3	1.50	0.94
3:A:468:TYR:HE1	3:A:470:GLN:HB2	1.33	0.94
3:A:545:LEU:HD12	3:A:555:VAL:HG21	1.48	0.93
3:A:68:PRO:HB2	3:A:93:GLU:HB2	1.52	0.92
3:B:605:ILE:CD1	3:B:629:VAL:HG13	1.97	0.92
3:B:56:LEU:HD11	3:B:58:LEU:HG	1.49	0.91
3:B:33:ASN:HD22	3:B:33:ASN:N	1.65	0.91
3:B:90:LEU:HD11	3:B:94:LEU:HD22	1.52	0.91
3:A:133:ASN:H	3:A:157:ASN:ND2	1.70	0.90
3:A:577:ILE:HD13	3:A:605:ILE:HG21	1.53	0.90
3:A:31:ARG:HA	3:A:31:ARG:HE	1.34	0.90
3:A:605:ILE:CD1	3:A:629:VAL:HG13	2.02	0.90
3:B:521:ILE:HD11	3:B:525:LEU:HB3	1.55	0.89
3:B:450:GLN:CG	10:B:4241:NDG:H6C2	2.02	0.88
3:A:396:LEU:HB2	3:A:422:ILE:HD12	1.55	0.88
3:A:575:ASP:HA	3:A:597:ASN:O	1.73	0.88
3:B:599:ASN:HB3	3:B:621:LEU:O	1.74	0.87
3:A:536:ASP:CB	3:A:538:GLN:HE22	1.87	0.87
3:B:577:ILE:HD13	3:B:605:ILE:HG21	1.57	0.87
3:B:40:LEU:HB2	3:B:61:ASN:HD21	1.40	0.86
3:A:550:ASN:CB	3:A:551:PRO:HD2	2.05	0.86
3:B:269:SER:HA	3:B:296:TYR:CD1	2.11	0.86
1:C:41:G:O2'	1:C:42:C:H5'	1.76	0.86
3:B:488:ARG:HG3	3:B:514:SER:OG	1.75	0.86
3:A:605:ILE:HD13	3:A:605:ILE:H	1.40	0.85
3:B:654:ILE:HD13	3:B:655:SER:N	1.90	0.85
3:B:575:ASP:HA	3:B:597:ASN:O	1.76	0.85
3:B:33:ASN:HA	3:B:53:ILE:CB	2.06	0.85
3:A:488:ARG:HG3	3:A:514:SER:OG	1.76	0.84
3:B:396:LEU:HD12	3:B:422:ILE:HG12	1.59	0.84
3:B:334:THR:HG22	3:B:344:PRO:HB3	1.59	0.84
3:B:80:LEU:HD21	3:B:104:LEU:HD12	1.60	0.83
3:B:55:VAL:HG22	3:B:79:ILE:HG12	1.58	0.83
3:A:300:LEU:HD23	3:A:324:LEU:HD13	1.59	0.83
3:B:654:ILE:O	3:B:658:VAL:HG23	1.78	0.83
3:A:90:LEU:HD11	3:A:94:LEU:HD22	1.59	0.83
3:B:133:ASN:H	3:B:157:ASN:ND2	1.75	0.83
3:A:234:ASN:HB3	3:A:237:LEU:HD13	1.60	0.83
3:A:141:ASN:HB3	3:A:169:GLN:HE22	1.43	0.83
3:A:55:VAL:HG22	3:A:79:ILE:HG12	1.58	0.83
3:A:114:ILE:HD11	3:A:118:THR:HB	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:536:ASP:CB	3:B:538:GLN:HE22	1.92	0.82
3:B:482:LEU:HB2	3:B:505:LEU:HD22	1.61	0.81
3:B:141:ASN:HB3	3:B:169:GLN:HE22	1.43	0.81
3:A:461:ILE:HD12	3:A:482:LEU:HD11	1.61	0.81
3:A:47:ASP:HB2	3:A:73:ARG:HD3	1.61	0.81
3:A:609:GLN:H	3:A:609:GLN:NE2	1.77	0.81
3:A:37:CYS:HB3	3:A:40:LEU:HD21	1.63	0.81
3:B:500:SER:HB2	3:B:525:LEU:HA	1.62	0.80
3:B:42:LEU:H	3:B:61:ASN:HD22	1.28	0.80
3:A:40:LEU:HD22	3:A:42:LEU:HD12	1.63	0.80
3:B:49:LEU:HD22	3:B:73:ARG:HH21	1.47	0.80
3:B:561:LEU:H	3:B:561:LEU:HD12	1.47	0.80
3:A:578:PRO:HG2	3:A:581:VAL:HG11	1.64	0.80
3:A:561:LEU:HD12	3:A:561:LEU:H	1.45	0.79
3:A:35:ALA:HB3	3:A:56:LEU:HA	1.65	0.79
3:B:578:PRO:HG2	3:B:581:VAL:HG11	1.62	0.79
3:B:279:LEU:HB3	3:B:300:LEU:HD11	1.63	0.79
3:B:543:ALA:HB2	3:B:573:GLY:HA3	1.64	0.79
3:B:234:ASN:HB3	3:B:237:LEU:HD13	1.65	0.78
3:B:49:LEU:HD13	3:B:73:ARG:HH22	1.48	0.78
3:A:269:SER:HA	3:A:296:TYR:CD1	2.18	0.78
3:B:300:LEU:HD23	3:B:324:LEU:HD13	1.66	0.78
3:A:56:LEU:CD1	3:A:58:LEU:HG	2.11	0.78
3:A:80:LEU:HD21	3:A:104:LEU:HD12	1.64	0.78
3:B:268:PHE:HB3	3:B:271:LEU:HD23	1.66	0.78
3:B:49:LEU:HD13	3:B:73:ARG:NH2	2.00	0.77
3:B:367:ILE:HD12	3:B:367:ILE:H	1.49	0.77
3:A:133:ASN:H	3:A:157:ASN:HD21	1.32	0.77
3:A:63:LEU:HB2	3:A:85:ASN:HB3	1.67	0.77
3:B:398:ASN:ND2	6:B:3981:NAG:H62	1.99	0.77
3:A:393:LEU:HD21	3:A:396:LEU:HD23	1.65	0.77
3:A:279:LEU:HB3	3:A:300:LEU:HD11	1.66	0.77
3:B:150:ILE:CG2	3:B:174:GLN:HB2	2.13	0.77
11:B:5071:NDG:O3	11:B:5072:NAG:H61	1.85	0.76
3:B:90:LEU:HD11	3:B:94:LEU:CD2	2.15	0.76
3:A:268:PHE:HB3	3:A:271:LEU:HD23	1.66	0.76
3:B:609:GLN:H	3:B:609:GLN:NE2	1.83	0.76
3:B:31:ARG:C	3:B:32:TYR:HD1	1.89	0.76
3:A:599:ASN:HB3	3:A:621:LEU:O	1.85	0.76
3:A:482:LEU:HB2	3:A:505:LEU:HD22	1.68	0.76
3:B:127:GLU:HG3	3:B:151:LYS:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:38:SER:C	3:B:40:LEU:HD13	2.06	0.75
3:B:393:LEU:HD21	3:B:396:LEU:HD23	1.68	0.75
3:A:500:SER:HB2	3:A:525:LEU:HA	1.67	0.75
3:A:481:SER:HA	11:A:5071:NDG:H8C2	1.68	0.75
3:A:367:ILE:H	3:A:367:ILE:HD12	1.51	0.75
3:B:287:HIS:HA	3:B:309:ASN:O	1.86	0.75
3:B:605:ILE:HD11	3:B:629:VAL:CG1	2.02	0.74
3:A:598:LEU:HB2	3:A:620:ASN:HD22	1.51	0.74
3:B:147:LYS:HE2	3:B:147:LYS:HA	1.68	0.74
3:B:651:CYS:HB3	3:B:655:SER:OG	1.88	0.74
3:A:42:LEU:HB2	3:A:61:ASN:HD22	1.53	0.74
3:A:120:VAL:HA	3:A:145:ASN:ND2	2.03	0.74
10:A:4242:NDG:H4	10:A:4243:BMA:O2	1.88	0.74
3:A:90:LEU:HD11	3:A:94:LEU:CD2	2.18	0.74
3:A:550:ASN:HB2	3:A:551:PRO:HD2	1.68	0.74
3:A:115:SER:O	3:A:118:THR:HG22	1.87	0.74
3:A:104:LEU:HG	3:A:106:LEU:HD13	1.70	0.74
1:C:39:G:H2'	1:C:40:C:H6	1.51	0.74
3:A:398:ASN:ND2	6:A:3981:NAG:H61	2.03	0.74
3:B:578:PRO:HG2	3:B:581:VAL:CG1	2.17	0.73
3:A:67:PRO:HB3	4:A:724:NDG:H8C1	1.70	0.73
3:B:605:ILE:H	3:B:605:ILE:CD1	1.99	0.73
3:A:49:LEU:HB3	3:A:50:PRO:HD2	1.70	0.73
3:B:30:VAL:HA	3:B:35:ALA:HA	1.69	0.73
3:A:521:ILE:HD11	3:A:525:LEU:CB	2.19	0.73
3:B:63:LEU:HB2	3:B:85:ASN:HB3	1.69	0.73
3:B:521:ILE:HD11	3:B:525:LEU:CB	2.18	0.73
3:A:127:GLU:HG3	3:A:151:LYS:HB2	1.70	0.73
3:B:265:GLU:HA	3:B:293:SER:HA	1.70	0.73
3:A:40:LEU:N	3:A:40:LEU:HD12	2.03	0.73
3:A:168:VAL:HG13	3:A:195:GLY:H	1.52	0.73
3:B:120:VAL:HA	3:B:145:ASN:ND2	2.02	0.73
3:B:66:LEU:HB3	3:B:94:LEU:HD21	1.70	0.72
3:B:56:LEU:CD1	3:B:58:LEU:HG	2.17	0.72
3:A:396:LEU:HD12	3:A:422:ILE:CD1	2.19	0.72
3:A:419:ILE:CG2	3:A:422:ILE:HD11	2.19	0.72
3:A:334:THR:HG22	3:A:335:LYS:H	1.54	0.72
3:A:446:LYS:HB3	3:A:470:GLN:HB3	1.71	0.72
3:A:620:ASN:HB2	3:A:645:ASN:HD21	1.54	0.72
2:D:21:U:O2	3:A:541:ASN:ND2	2.22	0.72
3:B:605:ILE:N	3:B:605:ILE:HD13	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:CG2	3:A:174:GLN:HB2	2.18	0.71
3:A:246:SER:O	3:A:248:THR:HG23	1.90	0.71
3:B:620:ASN:HB2	3:B:645:ASN:HD21	1.54	0.71
3:B:300:LEU:HD21	3:B:303:LEU:HB2	1.70	0.71
3:A:605:ILE:CD1	3:A:605:ILE:H	2.04	0.71
3:B:262:ALA:CB	3:B:288:ASP:HB2	2.21	0.71
3:A:287:HIS:HA	3:A:309:ASN:O	1.91	0.71
3:A:654:ILE:O	3:A:658:VAL:HG23	1.89	0.71
3:A:49:LEU:HB3	3:A:50:PRO:CD	2.21	0.71
3:B:243:TRP:CD1	3:B:270:GLY:HA2	2.26	0.71
3:A:243:TRP:CD1	3:A:270:GLY:HA2	2.26	0.71
3:B:104:LEU:HG	3:B:106:LEU:HD13	1.71	0.71
3:A:605:ILE:HD13	3:A:605:ILE:N	2.06	0.70
6:A:2521:NAG:H2	6:A:2521:NAG:H61	1.73	0.70
3:A:265:GLU:HA	3:A:293:SER:HA	1.73	0.70
3:B:168:VAL:HG13	3:B:195:GLY:H	1.55	0.70
3:B:660:TRP:O	3:B:664:THR:HG22	1.91	0.70
3:A:300:LEU:HD21	3:A:303:LEU:HB2	1.73	0.70
3:B:446:LYS:HB3	3:B:470:GLN:HB3	1.74	0.70
3:A:42:LEU:HB2	3:A:61:ASN:ND2	2.05	0.70
3:B:313:LEU:HD12	3:B:346:ILE:HG21	1.72	0.70
3:A:150:ILE:HD13	3:A:172:ASN:O	1.92	0.70
3:B:201:LYS:HA	3:B:225:ALA:HB3	1.72	0.70
3:A:526:LEU:HD23	3:A:529:LEU:HD12	1.73	0.69
3:A:66:LEU:HB3	3:A:94:LEU:HD21	1.72	0.69
3:B:33:ASN:ND2	3:B:33:ASN:N	2.37	0.69
3:A:535:LEU:HD11	3:A:537:PHE:CE2	2.27	0.69
3:A:424:ASN:OD1	10:A:4241:NDG:H8C1	1.91	0.69
3:A:550:ASN:HB3	3:A:551:PRO:HD2	1.73	0.69
3:A:622:ILE:H	3:A:645:ASN:HD22	1.37	0.69
3:A:421:LYS:C	3:A:422:ILE:HD13	2.12	0.69
3:A:511:LEU:HD23	3:A:512:ASP:N	2.08	0.69
11:A:5071:NDG:O4	11:A:5072:NAG:H61	1.93	0.69
3:A:557:PHE:HD2	3:A:558:LEU:HG	1.57	0.68
3:A:430:LEU:HD23	3:A:433:LEU:HD22	1.75	0.68
3:B:313:LEU:HB2	3:B:346:ILE:HG22	1.75	0.68
8:A:2911:NAG:O3	8:A:2912:NAG:H2	1.93	0.68
3:B:38:SER:O	3:B:40:LEU:HD13	1.94	0.68
6:B:3981:NAG:O3	6:B:3982:NDG:H5	1.93	0.68
2:D:45:A:H2'	2:D:46:U:C6	2.28	0.68
3:B:215:GLY:HA2	3:B:218:GLN:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:461:ILE:HD12	3:B:482:LEU:HD11	1.76	0.68
3:B:93:GLU:O	3:B:97:ILE:HG12	1.94	0.68
3:B:526:LEU:HD23	3:B:529:LEU:HD12	1.76	0.68
3:A:34:VAL:HG12	3:A:55:VAL:HB	1.76	0.68
3:A:68:PRO:O	3:A:97:ILE:HG13	1.94	0.68
3:B:295:SER:HA	3:B:320:GLY:HA3	1.74	0.68
3:A:150:ILE:HG23	3:A:174:GLN:HB2	1.74	0.67
3:A:93:GLU:O	3:A:97:ILE:HG12	1.93	0.67
3:B:133:ASN:H	3:B:157:ASN:HD21	1.41	0.67
3:B:68:PRO:HA	3:B:94:LEU:HG	1.76	0.67
3:A:201:LYS:HA	3:A:225:ALA:HB3	1.74	0.67
3:B:34:VAL:HA	3:B:55:VAL:HB	1.74	0.67
3:B:546:TRP:HB3	3:B:578:PRO:HD3	1.77	0.67
3:B:116:ASP:HA	3:B:142:PRO:HA	1.77	0.67
3:B:150:ILE:HG23	3:B:174:GLN:HB2	1.73	0.67
3:A:147:LYS:HE2	3:A:147:LYS:HA	1.75	0.67
3:B:542:LEU:H	3:B:572:ASN:ND2	1.92	0.67
3:B:49:LEU:HD22	3:B:73:ARG:NH2	2.09	0.67
3:B:598:LEU:HB2	3:B:620:ASN:HD22	1.60	0.67
3:B:34:VAL:O	3:B:34:VAL:HG23	1.94	0.67
3:B:607:ASP:N	3:B:609:GLN:HE22	1.92	0.67
3:A:536:ASP:HB3	3:A:538:GLN:NE2	2.02	0.66
3:B:68:PRO:O	3:B:97:ILE:HG13	1.95	0.66
3:B:68:PRO:CB	3:B:93:GLU:HB2	2.24	0.66
3:A:578:PRO:HG2	3:A:581:VAL:CG1	2.25	0.66
3:A:313:LEU:HB2	3:A:346:ILE:HG22	1.77	0.66
3:A:541:ASN:OD1	3:A:541:ASN:O	2.13	0.66
3:A:40:LEU:HD13	3:A:61:ASN:HD21	1.60	0.66
3:A:624:SER:HB3	3:A:653:SER:HB3	1.75	0.66
3:B:291:ASN:OD1	3:B:316:ARG:HB3	1.95	0.66
3:B:593:LEU:HB2	3:B:617:LEU:HD23	1.75	0.66
3:B:622:ILE:H	3:B:645:ASN:HD22	1.44	0.66
3:B:557:PHE:HD2	3:B:558:LEU:HG	1.61	0.66
3:A:295:SER:HA	3:A:320:GLY:HA3	1.78	0.66
3:A:275:ASN:HD21	7:A:2751:NAG:C6	2.10	0.65
3:B:325:ARG:C	3:B:357:LEU:HD12	2.15	0.65
3:B:180:LYS:HA	3:B:206:SER:HB2	1.76	0.65
3:B:115:SER:O	3:B:118:THR:HG22	1.96	0.65
3:A:215:GLY:HA2	3:A:218:GLN:HG2	1.77	0.65
3:B:624:SER:HB3	3:B:653:SER:HB3	1.77	0.65
3:B:33:ASN:CA	3:B:53:ILE:HB	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:419:ILE:HG21	3:A:422:ILE:HD11	1.76	0.65
3:B:275:ASN:ND2	12:B:2751:NAG:H61	2.11	0.65
3:A:660:TRP:O	3:A:664:THR:HG22	1.95	0.65
3:B:325:ARG:HA	3:B:357:LEU:HA	1.79	0.65
3:A:607:ASP:N	3:A:609:GLN:HE22	1.94	0.65
3:A:596:ASN:O	3:A:620:ASN:HA	1.96	0.65
3:A:180:LYS:HA	3:A:206:SER:HB2	1.77	0.65
3:A:568:ASN:O	3:A:569:LEU:HD12	1.96	0.65
3:B:187:ARG:O	3:B:191:LEU:HD23	1.97	0.65
3:B:55:VAL:HG13	3:B:79:ILE:HG13	1.79	0.65
3:A:511:LEU:HD21	3:A:513:LEU:HG	1.78	0.65
3:A:468:TYR:OH	3:A:493:LYS:HD3	1.97	0.65
3:B:624:SER:HB3	3:B:653:SER:CB	2.27	0.65
1:C:12:U:H2'	1:C:13:A:H8	1.61	0.65
3:B:185:ALA:C	3:B:186:LEU:HD12	2.17	0.65
3:A:68:PRO:CB	3:A:93:GLU:HB2	2.26	0.64
3:B:150:ILE:O	3:B:173:LEU:HD12	1.97	0.64
3:B:231:ALA:HB3	3:B:233:LEU:HD11	1.79	0.64
3:B:533:GLU:HB2	3:B:534:ILE:HD12	1.79	0.64
3:B:596:ASN:O	3:B:620:ASN:HA	1.97	0.64
3:B:94:LEU:H	3:B:94:LEU:HD12	1.62	0.64
3:A:624:SER:HB3	3:A:653:SER:CB	2.27	0.64
3:B:297:LEU:HD13	3:B:300:LEU:HD13	1.80	0.64
3:B:252:ASN:HD22	6:B:2521:NAG:H61	1.60	0.64
3:A:94:LEU:HD12	3:A:94:LEU:H	1.62	0.64
3:B:545:LEU:O	3:B:546:TRP:HD1	1.80	0.64
3:B:654:ILE:HD11	3:B:691:PHE:CE1	2.33	0.64
3:A:68:PRO:HA	3:A:94:LEU:HG	1.79	0.64
3:A:187:ARG:O	3:A:191:LEU:HD23	1.98	0.64
3:A:533:GLU:HA	3:A:564:LEU:HA	1.80	0.64
3:A:107:GLN:HB2	3:A:131:MET:HB3	1.78	0.64
3:A:97:ILE:HB	3:A:98:LEU:HD22	1.79	0.64
3:B:483:GLN:O	3:B:508:LEU:HD12	1.98	0.64
3:A:55:VAL:HG13	3:A:79:ILE:HG13	1.78	0.63
3:B:45:ILE:HG23	3:B:45:ILE:O	1.96	0.63
3:A:484:ARG:HG2	3:A:510:ILE:HB	1.79	0.63
6:A:3981:NAG:H83	6:A:3981:NAG:O3	1.97	0.63
3:A:150:ILE:O	3:A:173:LEU:HD12	1.99	0.63
3:A:511:LEU:CD2	3:A:513:LEU:HG	2.28	0.63
3:B:102:LYS:O	3:B:125:LEU:HD12	1.98	0.63
3:A:538:GLN:NE2	3:A:538:GLN:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:LEU:HB3	3:A:197:SER:HB2	1.78	0.63
3:B:198:SER:OG	3:B:222:LYS:HB2	1.98	0.63
1:C:27:G:H4'	3:A:519:ALA:HB1	1.81	0.63
3:B:286:LEU:HD21	3:B:289:VAL:HG22	1.81	0.63
3:B:53:ILE:O	3:B:76:GLN:HB3	1.98	0.63
3:A:33:ASN:O	3:A:53:ILE:HB	1.99	0.63
3:B:541:ASN:O	3:B:541:ASN:OD1	2.15	0.63
3:A:42:LEU:H	3:A:61:ASN:HD22	1.47	0.63
3:B:246:SER:O	3:B:248:THR:HG23	1.99	0.63
3:A:59:THR:HG22	3:A:60:HIS:CD2	2.34	0.63
3:A:561:LEU:HD22	3:A:564:LEU:HD12	1.79	0.63
3:A:550:ASN:CB	3:A:551:PRO:CD	2.76	0.63
3:A:300:LEU:CD2	3:A:324:LEU:HD13	2.28	0.63
3:A:185:ALA:C	3:A:186:LEU:HD12	2.19	0.63
3:B:568:ASN:O	3:B:569:LEU:HD12	1.99	0.63
3:B:97:ILE:HB	3:B:98:LEU:HD22	1.81	0.62
3:A:545:LEU:HD12	3:A:555:VAL:CG2	2.25	0.62
3:B:500:SER:OG	3:B:525:LEU:HD12	1.98	0.62
3:B:443:ILE:H	3:B:466:ASN:HD22	1.45	0.62
3:A:231:ALA:HB3	3:A:233:LEU:HD11	1.79	0.62
3:B:696:CYS:O	3:B:697:LYS:HG2	1.99	0.62
3:A:577:ILE:HD11	3:A:601:LEU:CD1	2.29	0.62
3:A:607:ASP:H	3:A:609:GLN:HE22	1.46	0.62
3:B:138:ILE:HD12	3:B:159:LEU:HD11	1.79	0.62
3:B:68:PRO:HB2	3:B:93:GLU:CB	2.27	0.62
3:A:535:LEU:HD11	3:A:537:PHE:HE2	1.62	0.62
3:A:143:PHE:C	3:A:145:ASN:H	1.99	0.62
3:A:44:HIS:O	3:A:46:PRO:HD3	1.98	0.62
3:A:589:LYS:O	3:A:612:LEU:HD12	1.99	0.62
3:B:50:PRO:O	3:B:53:ILE:HD12	2.00	0.62
3:B:37:CYS:HB3	3:B:40:LEU:HD22	1.80	0.62
3:B:509:THR:O	3:B:532:LEU:HD22	1.99	0.62
3:A:116:ASP:HA	3:A:142:PRO:HA	1.81	0.62
3:A:458:ILE:HD11	3:A:461:ILE:HG13	1.81	0.62
3:B:607:ASP:H	3:B:609:GLN:HE22	1.48	0.62
3:A:262:ALA:CB	3:A:288:ASP:HB2	2.30	0.62
3:B:577:ILE:HD11	3:B:601:LEU:CD1	2.29	0.61
3:A:533:GLU:HB2	3:A:534:ILE:HD12	1.82	0.61
3:B:300:LEU:HD22	3:B:321:LEU:HD22	1.81	0.61
1:C:39:G:H2'	1:C:40:C:C6	2.33	0.61
3:A:32:TYR:HD1	3:A:32:TYR:H	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:194:LEU:HB3	3:B:197:SER:HB2	1.82	0.61
3:B:242:CYS:HA	3:B:245:LEU:HD12	1.81	0.61
3:B:262:ALA:HB1	3:B:288:ASP:HB2	1.82	0.61
3:A:612:LEU:HD21	3:A:615:LEU:HD13	1.83	0.61
3:A:325:ARG:HA	3:A:357:LEU:HA	1.81	0.61
3:B:570:GLU:HB2	3:B:592:ASN:ND2	2.15	0.61
3:A:114:ILE:HG12	3:A:118:THR:HG21	1.83	0.61
3:B:314:SER:HB2	3:B:315:PRO:HD2	1.82	0.61
3:B:37:CYS:HB3	3:B:40:LEU:CD2	2.30	0.61
3:B:536:ASP:HB3	3:B:538:GLN:NE2	2.06	0.61
3:A:521:ILE:HG13	3:A:525:LEU:HD22	1.82	0.61
3:B:484:ARG:HG2	3:B:510:ILE:HB	1.83	0.61
3:B:675:TYR:O	3:B:688:LEU:HB2	2.01	0.61
3:B:535:LEU:HD11	3:B:537:PHE:CE2	2.35	0.61
3:B:468:TYR:OH	3:B:493:LYS:HD3	2.01	0.61
3:B:561:LEU:HD22	3:B:564:LEU:HD12	1.82	0.61
3:A:212:PHE:H	3:A:240:LYS:NZ	1.99	0.61
3:B:153:ASP:HA	3:B:177:LEU:HB2	1.83	0.60
3:B:215:GLY:HA2	3:B:218:GLN:CG	2.30	0.60
3:A:313:LEU:HD12	3:A:346:ILE:HG21	1.83	0.60
3:B:521:ILE:HG13	3:B:525:LEU:HD22	1.83	0.60
3:A:242:CYS:HA	3:A:245:LEU:HD12	1.83	0.60
3:B:279:LEU:CB	3:B:300:LEU:HD11	2.31	0.60
3:B:107:GLN:HB2	3:B:131:MET:HB3	1.83	0.60
3:B:538:GLN:NE2	3:B:538:GLN:H	2.00	0.60
3:A:63:LEU:HB3	3:A:87:ILE:HD11	1.84	0.60
3:B:31:ARG:C	3:B:32:TYR:CD1	2.72	0.60
3:B:630:PHE:HB3	3:B:634:PHE:CE1	2.37	0.60
3:B:212:PHE:H	3:B:240:LYS:NZ	1.99	0.60
3:A:494:ASN:O	3:A:497:ILE:HD12	2.00	0.60
3:B:334:THR:O	3:B:344:PRO:HG3	2.00	0.60
3:B:535:LEU:HD11	3:B:537:PHE:HE2	1.67	0.60
3:A:675:TYR:O	3:A:688:LEU:HB2	2.02	0.60
3:A:68:PRO:HB2	3:A:93:GLU:CB	2.30	0.60
3:A:458:ILE:HD13	3:A:459:PHE:N	2.16	0.60
3:B:511:LEU:HD23	3:B:512:ASP:N	2.15	0.60
2:D:23:C:OP1	3:A:539:HIS:HB3	2.01	0.60
3:A:102:LYS:O	3:A:125:LEU:HD12	2.02	0.60
3:B:65:ARG:O	3:B:67:PRO:HD3	2.02	0.60
3:B:36:ASP:HA	3:B:57:ASN:HB3	1.83	0.60
3:A:640:LEU:HG	3:A:641:ASP:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:64:ARG:HG2	3:B:65:ARG:HD2	1.83	0.60
3:B:577:ILE:O	3:B:577:ILE:HD12	2.02	0.59
3:A:42:LEU:HD11	3:A:46:PRO:HG3	1.84	0.59
3:B:329:LEU:HD13	3:B:333:PHE:CZ	2.37	0.59
3:A:365:ASN:HB3	3:A:367:ILE:HD12	1.83	0.59
3:B:61:ASN:O	3:B:85:ASN:OD1	2.21	0.59
3:B:430:LEU:HD23	3:B:433:LEU:HD22	1.83	0.59
3:A:325:ARG:C	3:A:357:LEU:HD12	2.23	0.59
3:B:468:TYR:CE1	3:B:470:GLN:HB2	2.21	0.59
3:A:321:LEU:HD13	3:A:324:LEU:HD22	1.85	0.59
3:B:511:LEU:HD21	3:B:513:LEU:HG	1.83	0.59
3:B:640:LEU:HG	3:B:641:ASP:N	2.17	0.59
3:B:63:LEU:O	3:B:86:SER:O	2.19	0.59
3:B:597:ASN:HA	3:B:621:LEU:HD13	1.85	0.59
3:B:49:LEU:O	3:B:51:SER:N	2.34	0.59
3:B:252:ASN:ND2	6:B:2521:NAG:H61	2.18	0.59
1:C:16:U:H4'	9:A:4135:MAN:O2	2.02	0.59
3:A:520:ASN:HB3	3:A:544:ARG:HH12	1.66	0.59
3:B:143:PHE:C	3:B:145:ASN:H	2.06	0.59
1:C:12:U:H2'	1:C:13:A:C8	2.38	0.59
3:A:396:LEU:HD12	3:A:422:ILE:HD12	1.84	0.59
3:B:334:THR:CG2	3:B:344:PRO:HB3	2.32	0.59
3:A:103:VAL:HG22	3:A:127:GLU:HB3	1.83	0.59
3:A:458:ILE:HD13	3:A:458:ILE:C	2.23	0.59
3:B:178:LEU:O	3:B:204:LEU:HA	2.02	0.59
3:B:107:GLN:HA	3:B:131:MET:H	1.67	0.58
3:A:599:ASN:OD1	3:A:600:LYS:HG3	2.04	0.58
3:A:488:ARG:O	3:A:490:VAL:HG13	2.04	0.58
3:A:63:LEU:O	3:A:86:SER:O	2.20	0.58
3:A:520:ASN:HB3	3:A:544:ARG:NH1	2.19	0.58
3:A:314:SER:HB2	3:A:315:PRO:HD2	1.85	0.58
3:A:393:LEU:O	3:A:393:LEU:HD23	2.03	0.58
3:A:509:THR:O	3:A:532:LEU:HD22	2.03	0.58
3:A:215:GLY:HA2	3:A:218:GLN:CG	2.33	0.58
3:A:45:ILE:O	3:A:45:ILE:HG23	2.03	0.58
3:A:53:ILE:O	3:A:76:GLN:HB3	2.03	0.58
3:B:152:LEU:HD13	3:B:152:LEU:O	2.03	0.58
3:A:71:PHE:HE2	3:A:94:LEU:HD23	1.69	0.58
3:B:34:VAL:HG12	3:B:55:VAL:HB	1.86	0.58
3:B:488:ARG:O	3:B:490:VAL:HG13	2.03	0.58
3:A:79:ILE:HB	3:A:103:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:336:GLN:HG3	3:B:343:HIS:HB3	1.86	0.58
3:A:153:ASP:HA	3:A:177:LEU:HB2	1.85	0.58
3:A:56:LEU:HD11	3:A:58:LEU:CG	2.25	0.58
3:A:315:PRO:HA	3:A:350:SER:HA	1.85	0.58
6:A:3982:NDG:H6C2	6:A:3982:NDG:H2	1.85	0.58
3:A:71:PHE:O	3:A:97:ILE:HG22	2.04	0.58
3:A:396:LEU:CB	3:A:422:ILE:HD12	2.32	0.58
3:A:79:ILE:CG2	3:A:103:VAL:HB	2.34	0.58
3:B:313:LEU:HD12	3:B:346:ILE:CG2	2.34	0.58
3:A:521:ILE:HD13	3:A:522:ASN:O	2.04	0.57
3:A:300:LEU:HD22	3:A:321:LEU:HD22	1.86	0.57
3:A:598:LEU:HB2	3:A:620:ASN:ND2	2.18	0.57
3:B:511:LEU:CD2	3:B:513:LEU:HG	2.34	0.57
3:B:459:PHE:CE1	3:B:483:GLN:HG3	2.39	0.57
3:A:640:LEU:HD21	3:A:642:MET:CE	2.34	0.57
3:A:306:GLU:HG2	3:A:330:LYS:HB3	1.86	0.57
3:A:297:LEU:HD13	3:A:300:LEU:HD13	1.87	0.57
3:B:315:PRO:HA	3:B:350:SER:HA	1.84	0.57
1:C:21:A:C1'	3:B:541:ASN:HB2	2.34	0.57
3:B:577:ILE:CD1	3:B:605:ILE:HG21	2.33	0.57
3:A:534:ILE:HG23	3:A:566:ILE:HG23	1.86	0.57
3:A:481:SER:HA	11:A:5071:NDG:C8	2.34	0.57
3:B:329:LEU:HD13	3:B:333:PHE:HZ	1.70	0.57
3:A:80:LEU:HD23	3:A:80:LEU:H	1.69	0.57
3:A:107:GLN:HA	3:A:131:MET:H	1.69	0.57
3:B:520:ASN:HB3	3:B:544:ARG:NH1	2.20	0.57
3:B:79:ILE:HB	3:B:103:VAL:HB	1.85	0.57
3:B:114:ILE:HD11	3:B:118:THR:CB	2.35	0.57
3:A:306:GLU:HB3	3:A:307:TYR:HD1	1.70	0.57
3:B:520:ASN:HB3	3:B:544:ARG:HH12	1.69	0.57
3:B:108:HIS:H	3:B:132:SER:H	1.52	0.57
3:B:482:LEU:HB2	3:B:505:LEU:CD2	2.33	0.57
3:B:422:ILE:H	3:B:445:GLN:NE2	2.03	0.57
3:A:483:GLN:O	3:A:508:LEU:HD12	2.04	0.57
3:B:343:HIS:ND1	3:B:343:HIS:O	2.38	0.57
3:A:65:ARG:O	3:A:67:PRO:HD3	2.05	0.57
1:C:24:G:N2	2:D:24:C:C2	2.73	0.57
3:B:563:HIS:HA	3:B:587:GLU:OE2	2.05	0.57
3:B:109:ASN:O	3:B:132:SER:O	2.23	0.56
3:A:109:ASN:O	3:A:132:SER:O	2.23	0.56
3:A:545:LEU:O	3:A:546:TRP:HD1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:101:LEU:HD22	3:B:125:LEU:HD13	1.85	0.56
3:A:108:HIS:H	3:A:132:SER:H	1.51	0.56
3:A:597:ASN:HA	3:A:621:LEU:HD13	1.87	0.56
3:B:109:ASN:O	3:B:133:ASN:HA	2.06	0.56
3:B:103:VAL:HG22	3:B:127:GLU:HB3	1.85	0.56
3:A:564:LEU:HD23	3:A:564:LEU:C	2.26	0.56
3:A:250:ILE:C	3:A:250:ILE:HD13	2.26	0.56
1:C:1:A:N6	2:D:45:A:N6	2.52	0.56
3:B:126:THR:HA	3:B:149:LEU:HA	1.86	0.56
3:A:511:LEU:HD23	3:A:511:LEU:C	2.25	0.56
3:A:388:LYS:HA	3:A:416:LYS:O	2.06	0.56
3:B:388:LYS:HA	3:B:416:LYS:O	2.05	0.56
3:B:522:ASN:C	3:B:522:ASN:HD22	2.08	0.56
3:A:421:LYS:HG2	3:A:445:GLN:NE2	2.21	0.56
3:B:365:ASN:HB3	3:B:367:ILE:HD12	1.86	0.56
3:A:168:VAL:HG13	3:A:195:GLY:N	2.20	0.56
3:A:485:LEU:HG	3:A:487:LEU:CD2	2.36	0.56
3:A:335:LYS:HZ2	3:A:335:LYS:N	2.03	0.56
3:B:233:LEU:HD13	3:B:258:ASN:OD1	2.04	0.56
3:B:570:GLU:HB2	3:B:592:ASN:HD21	1.70	0.56
3:A:178:LEU:O	3:A:204:LEU:HA	2.06	0.56
3:B:306:GLU:HG2	3:B:330:LYS:HB3	1.87	0.56
3:A:500:SER:OG	3:A:525:LEU:HD12	2.06	0.56
3:A:443:ILE:H	3:A:466:ASN:HD22	1.53	0.56
3:A:126:THR:HA	3:A:148:ASN:O	2.06	0.56
3:B:521:ILE:HD13	3:B:522:ASN:O	2.05	0.56
3:A:140:SER:C	3:A:142:PRO:HD3	2.27	0.56
3:A:577:ILE:O	3:A:577:ILE:HD12	2.06	0.55
3:A:630:PHE:HB3	3:A:634:PHE:CE1	2.40	0.55
3:A:63:LEU:HB3	3:A:87:ILE:CD1	2.36	0.55
3:B:321:LEU:HD13	3:B:324:LEU:HD22	1.88	0.55
3:A:37:CYS:HB3	3:A:40:LEU:HD11	1.87	0.55
3:A:643:ARG:O	3:A:644:PHE:HB2	2.07	0.55
3:B:79:ILE:CG2	3:B:103:VAL:HB	2.36	0.55
3:B:589:LYS:O	3:B:612:LEU:HD12	2.06	0.55
3:A:550:ASN:HB3	3:A:551:PRO:CD	2.35	0.55
3:B:393:LEU:HD23	3:B:393:LEU:O	2.06	0.55
3:B:577:ILE:HD11	3:B:601:LEU:HD12	1.86	0.55
3:A:497:ILE:HD11	3:A:501:PRO:HD3	1.88	0.55
3:B:252:ASN:HD22	6:B:2521:NAG:C6	2.19	0.55
3:A:603:PRO:O	3:A:604:PHE:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:276:LEU:O	3:B:300:LEU:HA	2.06	0.55
3:B:484:ARG:HG3	3:B:484:ARG:HH11	1.70	0.55
3:B:32:TYR:CD1	3:B:32:TYR:N	2.73	0.55
3:A:593:LEU:HB2	3:A:617:LEU:HD23	1.89	0.55
3:A:141:ASN:CB	3:A:169:GLN:HE22	2.16	0.55
3:A:64:ARG:HG2	3:A:65:ARG:HD2	1.89	0.55
3:B:275:ASN:ND2	12:B:2751:NAG:C6	2.69	0.55
3:A:696:CYS:O	3:A:697:LYS:HB3	2.07	0.55
3:B:114:ILE:HG12	3:B:118:THR:HG21	1.88	0.54
3:A:126:THR:HA	3:A:149:LEU:HA	1.89	0.54
3:A:109:ASN:O	3:A:133:ASN:HA	2.06	0.54
3:A:334:THR:C	3:A:335:LYS:HD3	2.27	0.54
3:A:313:LEU:HD13	3:A:318:PHE:HE1	1.72	0.54
3:A:101:LEU:HD22	3:A:125:LEU:HD13	1.88	0.54
3:A:538:GLN:HG3	3:A:568:ASN:OD1	2.07	0.54
3:B:239:GLU:HA	3:B:267:THR:O	2.07	0.54
3:A:180:LYS:H	3:A:206:SER:HB2	1.72	0.54
3:B:131:MET:O	3:B:155:SER:O	2.24	0.54
3:A:233:LEU:HD13	3:A:258:ASN:OD1	2.07	0.54
3:B:33:ASN:O	3:B:55:VAL:N	2.39	0.54
8:A:2911:NAG:H5	8:A:2916:FUC:O5	2.06	0.54
3:B:486:MET:C	3:B:487:LEU:HD22	2.28	0.54
3:B:603:PRO:O	3:B:604:PHE:HB2	2.06	0.54
3:A:187:ARG:HD3	3:A:189:GLU:OE1	2.07	0.54
3:A:462:TYR:HD1	3:A:486:MET:HG3	1.72	0.54
1:C:43:C:H2'	1:C:44:A:C8	2.43	0.54
3:A:484:ARG:HG3	3:A:484:ARG:HH11	1.73	0.54
3:A:198:SER:OG	3:A:222:LYS:HB2	2.07	0.54
3:B:168:VAL:HG13	3:B:195:GLY:N	2.22	0.54
3:A:36:ASP:HA	3:A:57:ASN:HB3	1.90	0.54
3:B:643:ARG:O	3:B:644:PHE:HB2	2.08	0.54
3:A:449:GLY:HA2	3:A:475:SER:O	2.08	0.54
3:B:641:ASP:OD2	3:B:643:ARG:HG2	2.08	0.53
3:A:689:LYS:HG3	3:A:690:LEU:N	2.23	0.53
3:B:82:ALA:O	3:B:105:ASN:O	2.26	0.53
3:A:262:ALA:HB1	3:A:288:ASP:HB2	1.90	0.53
3:B:464:SER:O	3:B:465:TYR:HB2	2.08	0.53
3:B:443:ILE:N	3:B:466:ASN:HD22	2.06	0.53
3:B:126:THR:HA	3:B:148:ASN:O	2.07	0.53
3:A:577:ILE:HD11	3:A:601:LEU:HD13	1.89	0.53
3:A:80:LEU:HD21	3:A:104:LEU:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:163:LYS:HB2	3:A:190:GLU:HB2	1.89	0.53
3:B:68:PRO:HB3	3:B:94:LEU:CD1	2.38	0.53
3:A:276:LEU:O	3:A:300:LEU:HA	2.08	0.53
3:A:609:GLN:N	3:A:609:GLN:NE2	2.54	0.53
3:B:295:SER:HA	3:B:320:GLY:CA	2.38	0.53
3:B:212:PHE:CD2	3:B:241:LEU:HB2	2.43	0.53
3:B:435:ILE:HG13	3:B:460:GLU:HG2	1.91	0.53
1:C:16:U:H2'	1:C:17:G:H8	1.72	0.53
3:A:180:LYS:HA	3:A:206:SER:CB	2.38	0.53
3:B:566:ILE:HD13	3:B:566:ILE:C	2.29	0.53
3:A:291:ASN:OD1	3:A:316:ARG:HB3	2.09	0.53
3:B:80:LEU:H	3:B:80:LEU:HD23	1.74	0.53
3:A:615:LEU:HB3	3:A:640:LEU:HD12	1.90	0.53
3:A:451:GLU:CD	3:A:451:GLU:H	2.10	0.53
3:B:33:ASN:C	3:B:53:ILE:HB	2.29	0.53
3:B:59:THR:HG22	3:B:60:HIS:CD2	2.43	0.53
3:A:279:LEU:CB	3:A:300:LEU:HD11	2.37	0.53
3:B:212:PHE:CE2	3:B:241:LEU:HB2	2.44	0.53
3:B:612:LEU:HD21	3:B:615:LEU:HD13	1.90	0.53
3:B:370:THR:OG1	3:B:400:THR:HG23	2.08	0.53
3:B:56:LEU:HD11	3:B:58:LEU:CG	2.32	0.53
3:A:151:LYS:HG2	3:A:175:GLU:OE1	2.08	0.53
3:A:410:LEU:N	3:A:410:LEU:HD12	2.24	0.53
3:B:163:LYS:HB2	3:B:190:GLU:HB2	1.91	0.53
3:A:534:ILE:HG13	3:A:566:ILE:CG2	2.38	0.52
3:B:180:LYS:H	3:B:206:SER:HB2	1.74	0.52
3:B:485:LEU:HG	3:B:487:LEU:CD2	2.39	0.52
3:A:436:LEU:HD21	3:A:438:LEU:HG	1.92	0.52
3:B:689:LYS:HG3	3:B:690:LEU:N	2.25	0.52
3:B:331:ARG:NH2	3:B:335:LYS:HE2	2.24	0.52
3:B:421:LYS:HG2	3:B:445:GLN:NE2	2.24	0.52
3:A:80:LEU:HD23	3:A:80:LEU:N	2.25	0.52
3:A:114:ILE:CG1	3:A:118:THR:HG21	2.39	0.52
3:B:73:ARG:HG3	3:B:73:ARG:HH11	1.75	0.52
3:B:205:SER:OG	3:B:229:ASN:HB2	2.09	0.52
3:B:654:ILE:C	3:B:654:ILE:HD13	2.28	0.52
3:B:449:GLY:H	3:B:475:SER:HA	1.75	0.52
3:A:534:ILE:HG13	3:A:566:ILE:HG22	1.92	0.52
3:B:511:LEU:HD23	3:B:511:LEU:C	2.29	0.52
3:B:40:LEU:HB2	3:B:61:ASN:ND2	2.19	0.52
3:A:234:ASN:CB	3:A:237:LEU:HD13	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:61:ASN:O	3:A:85:ASN:OD1	2.28	0.52
3:A:275:ASN:ND2	7:A:2751:NAG:H61	2.24	0.52
9:A:4131:NDG:C6	9:A:4132:NAG:HN2	2.23	0.52
3:A:522:ASN:C	3:A:522:ASN:HD22	2.12	0.52
3:A:555:VAL:O	3:A:557:PHE:N	2.41	0.52
3:A:602:GLU:O	3:A:605:ILE:HG23	2.09	0.52
3:B:35:ALA:O	3:B:56:LEU:HA	2.10	0.52
3:A:582:PHE:HB3	3:A:609:GLN:OE1	2.10	0.52
3:B:534:ILE:HD12	3:B:534:ILE:N	2.25	0.52
3:B:502:PHE:CD2	3:B:525:LEU:HD11	2.45	0.52
3:A:422:ILE:H	3:A:445:GLN:NE2	2.07	0.52
3:A:458:ILE:CD1	3:A:461:ILE:HG13	2.39	0.52
1:C:22:A:H5"	3:B:539:HIS:HB3	1.92	0.52
3:B:71:PHE:O	3:B:97:ILE:HG22	2.10	0.51
3:B:151:LYS:HG2	3:B:175:GLU:OE1	2.10	0.51
3:B:39:HIS:HA	3:B:60:HIS:O	2.10	0.51
3:A:40:LEU:CD1	3:A:40:LEU:N	2.72	0.51
3:B:80:LEU:HD21	3:B:104:LEU:CD1	2.36	0.51
3:A:525:LEU:O	3:A:526:LEU:HB2	2.08	0.51
3:B:521:ILE:HD12	3:B:557:PHE:CE1	2.45	0.51
3:B:336:GLN:N	3:B:366:ASN:OD1	2.43	0.51
3:B:180:LYS:HA	3:B:206:SER:CB	2.40	0.51
3:B:241:LEU:HD12	3:B:241:LEU:O	2.10	0.51
3:B:477:ALA:HA	3:B:504:PRO:HG3	1.92	0.51
3:A:398:ASN:ND2	6:A:3981:NAG:C6	2.71	0.51
3:A:150:ILE:HD12	3:A:174:GLN:HE21	1.75	0.51
3:B:180:LYS:CA	3:B:206:SER:HB2	2.39	0.51
3:A:180:LYS:CA	3:A:206:SER:HB2	2.39	0.51
3:B:534:ILE:HG13	3:B:566:ILE:CG2	2.40	0.51
3:B:654:ILE:H	3:B:654:ILE:HD12	1.76	0.51
3:A:550:ASN:O	3:A:551:PRO:C	2.49	0.51
3:B:436:LEU:HD21	3:B:438:LEU:HG	1.92	0.51
3:B:337:SER:OG	3:B:342:SER:HB2	2.10	0.51
3:A:32:TYR:O	3:A:33:ASN:HB3	2.10	0.51
3:A:53:ILE:HG12	3:A:77:LEU:HD23	1.92	0.51
3:B:92:PRO:HB3	3:B:117:GLN:O	2.10	0.51
3:B:588:LEU:C	3:B:588:LEU:HD23	2.31	0.51
3:A:105:ASN:HA	3:A:129:ASP:HB3	1.92	0.51
3:B:138:ILE:CD1	3:B:159:LEU:HD11	2.41	0.51
3:A:570:GLU:HB2	3:A:592:ASN:ND2	2.25	0.51
3:A:286:LEU:HD21	3:A:289:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:577:ILE:HD11	3:A:601:LEU:HD12	1.92	0.51
3:A:410:LEU:CD1	3:A:410:LEU:N	2.74	0.51
1:C:16:U:H2'	1:C:17:G:C8	2.46	0.51
1:C:3:U:H2'	1:C:4:C:H6	1.76	0.51
3:B:526:LEU:HA	3:B:529:LEU:CD1	2.40	0.51
3:A:250:ILE:HD12	3:A:276:LEU:HD21	1.93	0.51
3:A:143:PHE:C	3:A:145:ASN:N	2.64	0.51
3:B:449:GLY:HA2	3:B:475:SER:O	2.11	0.51
3:B:126:THR:HG22	3:B:148:ASN:HB3	1.92	0.50
3:B:671:LEU:HA	3:B:675:TYR:CD1	2.46	0.50
3:B:450:GLN:HG3	10:B:4241:NDG:C6	2.21	0.50
3:B:35:ALA:N	3:B:55:VAL:O	2.38	0.50
3:A:534:ILE:N	3:A:534:ILE:HD12	2.26	0.50
3:A:421:LYS:O	3:A:422:ILE:HD13	2.10	0.50
3:A:540:ASN:O	3:A:541:ASN:C	2.50	0.50
3:A:275:ASN:ND2	7:A:2751:NAG:C6	2.73	0.50
3:B:489:ARG:HA	3:B:515:ASN:O	2.11	0.50
3:A:601:LEU:N	3:A:601:LEU:HD22	2.26	0.50
3:A:641:ASP:OD2	3:A:643:ARG:HG2	2.11	0.50
3:A:640:LEU:HD21	3:A:642:MET:HE3	1.92	0.50
3:A:558:LEU:CA	3:A:561:LEU:HD11	2.41	0.50
3:A:489:ARG:HA	3:A:515:ASN:O	2.11	0.50
3:B:521:ILE:HG21	3:B:557:PHE:HE1	1.76	0.50
3:B:266:SER:HA	3:B:269:SER:HB3	1.93	0.50
3:A:111:LEU:O	3:A:135:ILE:HG12	2.12	0.50
3:B:147:LYS:NZ	3:B:171:GLU:HG2	2.26	0.50
3:A:295:SER:HA	3:A:320:GLY:CA	2.41	0.50
1:C:16:U:H4'	9:A:4135:MAN:O3	2.12	0.50
3:A:331:ARG:HA	3:A:364:ASP:O	2.10	0.50
3:B:651:CYS:HB3	3:B:655:SER:HG	1.74	0.50
3:B:33:ASN:CB	3:B:53:ILE:HA	2.41	0.50
3:A:424:ASN:CG	10:A:4241:NDG:N2	2.65	0.50
2:D:7:G:H2'	2:D:8:C:H6	1.77	0.50
3:A:30:VAL:O	3:A:30:VAL:HG12	2.12	0.50
3:A:468:TYR:CE1	3:A:470:GLN:HB2	2.26	0.50
3:A:393:LEU:HD21	3:A:396:LEU:CD2	2.38	0.50
3:A:266:SER:HA	3:A:269:SER:HB3	1.93	0.50
3:B:510:ILE:HG12	3:B:534:ILE:HD13	1.93	0.50
3:A:231:ALA:HB3	3:A:233:LEU:CD1	2.42	0.50
3:A:177:LEU:N	3:A:177:LEU:HD12	2.26	0.50
3:B:306:GLU:HB3	3:B:307:TYR:HD1	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:87:ILE:HD12	3:B:109:ASN:ND2	2.26	0.50
3:B:111:LEU:O	3:B:135:ILE:HG12	2.11	0.50
3:B:239:GLU:HG3	3:B:266:SER:O	2.12	0.50
3:A:131:MET:O	3:A:155:SER:O	2.28	0.50
3:B:615:LEU:HB3	3:B:640:LEU:HD12	1.93	0.50
3:A:92:PRO:HB3	3:A:117:GLN:O	2.12	0.50
3:B:599:ASN:OD1	3:B:600:LYS:HG3	2.12	0.49
3:A:563:HIS:HA	3:A:587:GLU:OE2	2.12	0.49
3:B:359:TYR:C	3:B:359:TYR:CD2	2.85	0.49
3:A:526:LEU:HD23	3:A:529:LEU:CD1	2.39	0.49
3:B:557:PHE:CD2	3:B:558:LEU:HG	2.45	0.49
3:B:300:LEU:CD2	3:B:324:LEU:HD13	2.37	0.49
3:B:324:LEU:HD21	3:B:327:LEU:HD13	1.93	0.49
3:A:152:LEU:HD13	3:A:152:LEU:O	2.12	0.49
3:B:500:SER:CB	3:B:525:LEU:HA	2.37	0.49
3:B:564:LEU:HD23	3:B:564:LEU:C	2.33	0.49
5:B:724:NAG:O3	5:B:724:NAG:H83	2.11	0.49
3:B:269:SER:HA	3:B:296:TYR:CE1	2.47	0.49
3:A:147:LYS:NZ	3:A:171:GLU:HG2	2.27	0.49
3:B:231:ALA:HB3	3:B:233:LEU:CD1	2.43	0.49
3:B:258:ASN:HB2	3:B:284:ASN:OD1	2.12	0.49
3:A:437:ASP:OD2	3:A:462:TYR:HD2	1.94	0.49
3:B:532:LEU:HD11	3:B:535:LEU:HB2	1.94	0.49
3:A:47:ASP:O	3:A:47:ASP:OD1	2.31	0.49
3:B:234:ASN:ND2	3:B:236:HIS:H	2.09	0.49
3:B:484:ARG:NH1	3:B:484:ARG:HG3	2.26	0.49
3:B:138:ILE:HD13	3:B:164:LEU:CD2	2.42	0.49
3:B:177:LEU:N	3:B:177:LEU:HD12	2.28	0.49
1:C:8:G:H2'	1:C:9:G:H8	1.77	0.49
3:A:477:ALA:HA	3:A:504:PRO:HG3	1.94	0.49
3:A:417:ASN:O	3:A:418:HIS:HB2	2.11	0.49
1:C:7:C:OP1	3:A:39:HIS:HB3	2.12	0.49
3:B:114:ILE:HD11	3:B:118:THR:OG1	2.12	0.49
3:B:187:ARG:HA	3:B:213:SER:HB3	1.95	0.49
3:A:66:LEU:O	3:A:68:PRO:HD3	2.13	0.49
3:B:412:LEU:HD22	3:B:430:LEU:HD21	1.93	0.49
3:B:140:SER:C	3:B:142:PRO:HD3	2.33	0.49
3:A:67:PRO:HB2	3:A:70:ASN:HB2	1.95	0.49
3:B:45:ILE:O	3:B:45:ILE:CG2	2.61	0.49
3:B:451:GLU:H	3:B:451:GLU:CD	2.13	0.49
3:B:577:ILE:HD11	3:B:601:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:141:ASN:CB	3:B:169:GLN:HE22	2.20	0.49
6:B:3981:NAG:H3	6:B:3982:NDG:O	2.12	0.49
3:B:80:LEU:HD21	3:B:104:LEU:HA	1.95	0.49
3:B:53:ILE:HG12	3:B:77:LEU:HD23	1.94	0.49
3:A:94:LEU:O	3:A:98:LEU:HD23	2.12	0.49
3:B:526:LEU:HA	3:B:529:LEU:HD11	1.94	0.49
3:B:252:ASN:ND2	6:B:2521:NAG:C6	2.76	0.49
3:A:189:GLU:O	3:A:192:GLU:HG2	2.13	0.49
3:B:331:ARG:HA	3:B:364:ASP:O	2.11	0.49
3:B:383:TYR:HD2	3:B:411:THR:OG1	1.96	0.49
3:A:484:ARG:HG3	3:A:484:ARG:NH1	2.28	0.48
3:A:537:PHE:CZ	3:A:557:PHE:HZ	2.31	0.48
3:B:526:LEU:HD23	3:B:529:LEU:CD1	2.41	0.48
3:B:251:GLN:O	3:B:276:LEU:HD13	2.12	0.48
3:A:443:ILE:N	3:A:466:ASN:HD22	2.11	0.48
3:B:437:ASP:OD2	3:B:462:TYR:HD2	1.96	0.48
3:A:464:SER:O	3:A:465:TYR:HB2	2.12	0.48
3:B:649:CYS:HB2	3:B:683:TYR:HB3	1.94	0.48
3:B:77:LEU:O	3:B:100:LEU:O	2.31	0.48
3:A:334:THR:O	3:A:335:LYS:HD3	2.13	0.48
3:B:243:TRP:CD1	3:B:270:GLY:CA	2.96	0.48
3:B:114:ILE:CD1	3:B:118:THR:HG21	2.42	0.48
3:A:77:LEU:O	3:A:100:LEU:O	2.32	0.48
3:A:37:CYS:HB3	3:A:40:LEU:CD2	2.40	0.48
3:B:187:ARG:HG3	3:B:187:ARG:HH11	1.78	0.48
3:A:486:MET:C	3:A:487:LEU:HD22	2.33	0.48
1:C:43:C:H2'	1:C:44:A:H8	1.79	0.48
3:B:578:PRO:CG	3:B:581:VAL:HG11	2.40	0.48
3:A:239:GLU:HA	3:A:267:THR:O	2.13	0.48
3:A:226:LEU:HD12	3:A:227:LEU:H	1.78	0.48
3:B:190:GLU:HG3	3:B:191:LEU:HD22	1.95	0.48
3:B:179:ALA:HB1	3:B:205:SER:HB2	1.95	0.48
3:B:105:ASN:O	3:B:106:LEU:HD12	2.13	0.48
3:A:79:ILE:CB	3:A:103:VAL:HB	2.43	0.48
3:A:53:ILE:HG12	3:A:77:LEU:CD2	2.44	0.48
2:D:5:G:H2'	2:D:6:C:O4'	2.12	0.48
6:A:2521:NAG:H61	6:A:2521:NAG:C2	2.42	0.48
3:B:390:PHE:CD2	3:B:393:LEU:HD13	2.49	0.48
3:B:169:GLN:HG3	3:B:170:LEU:CD2	2.43	0.48
3:A:150:ILE:HD12	3:A:174:GLN:NE2	2.28	0.48
1:C:31:U:H2'	1:C:32:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:68:PRO:HB3	3:B:94:LEU:HD12	1.96	0.48
3:B:53:ILE:HG12	3:B:77:LEU:CD2	2.44	0.48
3:A:297:LEU:C	3:A:299:SER:H	2.16	0.48
3:A:73:ARG:HH11	3:A:73:ARG:HG3	1.78	0.48
3:B:640:LEU:HD21	3:B:642:MET:CE	2.44	0.48
3:B:331:ARG:HH22	3:B:335:LYS:CE	2.26	0.48
3:B:393:LEU:HD21	3:B:396:LEU:CD2	2.42	0.48
3:B:31:ARG:HA	3:B:31:ARG:HD3	1.72	0.48
3:B:542:LEU:H	3:B:572:ASN:HD22	1.60	0.48
3:A:169:GLN:HG3	3:A:170:LEU:CD2	2.44	0.48
3:A:243:TRP:CD1	3:A:270:GLY:CA	2.95	0.48
3:B:550:ASN:N	3:B:551:PRO:CD	2.77	0.48
3:A:396:LEU:HB3	3:A:426:THR:HG21	1.96	0.47
3:A:459:PHE:CE1	3:A:483:GLN:HG3	2.48	0.47
3:A:187:ARG:HA	3:A:213:SER:HB3	1.95	0.47
3:A:359:TYR:C	3:A:359:TYR:CD2	2.88	0.47
3:A:196:ASN:HD22	5:A:1961:NAG:H4	1.79	0.47
3:A:510:ILE:HG12	3:A:534:ILE:HD13	1.96	0.47
3:B:558:LEU:CA	3:B:561:LEU:HD11	2.44	0.47
3:A:250:ILE:HD13	3:A:251:GLN:N	2.29	0.47
3:A:306:GLU:HB3	3:A:307:TYR:CD1	2.47	0.47
3:A:447:LEU:HD23	3:A:451:GLU:HG3	1.96	0.47
2:D:13:G:O2'	2:D:14:U:H5'	2.13	0.47
3:A:530:GLU:HG3	3:A:530:GLU:O	2.13	0.47
3:A:479:VAL:O	3:A:479:VAL:HG23	2.15	0.47
3:A:234:ASN:ND2	3:A:236:HIS:H	2.13	0.47
3:B:534:ILE:HG23	3:B:566:ILE:HG23	1.96	0.47
3:B:441:ASN:O	3:B:466:ASN:HA	2.14	0.47
3:A:500:SER:CB	3:A:525:LEU:HA	2.43	0.47
2:D:6:C:N3	2:D:7:G:N7	2.61	0.47
3:A:217:PHE:HB2	3:A:244:GLU:O	2.14	0.47
3:A:446:LYS:HD3	3:A:470:GLN:NE2	2.29	0.47
3:B:593:LEU:HB2	3:B:617:LEU:CD2	2.45	0.47
1:C:21:A:O4'	3:B:541:ASN:HB2	2.13	0.47
3:A:570:GLU:HB2	3:A:592:ASN:HD21	1.80	0.47
3:B:459:PHE:CE2	3:B:484:ARG:NH1	2.83	0.47
3:A:59:THR:HG22	3:A:60:HIS:CG	2.50	0.47
3:A:347:ASP:HA	3:A:371:LYS:NZ	2.29	0.47
3:B:80:LEU:N	3:B:80:LEU:HD23	2.30	0.47
3:A:561:LEU:HB2	3:A:564:LEU:HB2	1.97	0.47
3:A:68:PRO:HB3	3:A:94:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:227:LEU:HD23	3:A:254:SER:HB3	1.97	0.47
3:A:126:THR:HG22	3:A:148:ASN:HB3	1.96	0.47
3:B:485:LEU:HG	3:B:487:LEU:HD21	1.97	0.47
3:A:205:SER:OG	3:A:229:ASN:HB2	2.14	0.47
3:B:105:ASN:HA	3:B:129:ASP:HB3	1.96	0.47
3:A:82:ALA:O	3:A:105:ASN:O	2.33	0.47
1:C:22:A:OP1	3:B:539:HIS:HB3	2.15	0.47
2:D:28:G:H4'	3:B:519:ALA:HB1	1.97	0.47
3:A:324:LEU:HD21	3:A:327:LEU:HD13	1.96	0.47
3:A:42:LEU:HD23	3:A:43:THR:H	1.80	0.47
3:A:239:GLU:HG3	3:A:266:SER:O	2.15	0.47
3:B:226:LEU:HD12	3:B:227:LEU:H	1.79	0.47
3:A:206:SER:HA	3:A:230:ASN:O	2.15	0.47
3:A:640:LEU:HD21	3:A:642:MET:HE2	1.97	0.47
3:B:417:ASN:O	3:B:418:HIS:HB2	2.14	0.47
3:B:654:ILE:CD1	3:B:655:SER:N	2.73	0.47
3:A:180:LYS:N	3:A:206:SER:HB2	2.30	0.47
3:A:671:LEU:HA	3:A:675:TYR:CD1	2.50	0.47
3:B:383:TYR:HD2	3:B:411:THR:HG1	1.63	0.47
3:B:67:PRO:HB2	3:B:70:ASN:HB2	1.97	0.46
3:A:365:ASN:HB3	3:A:367:ILE:CD1	2.45	0.46
3:B:357:LEU:O	3:B:380:SER:HB2	2.15	0.46
3:A:190:GLU:HG3	3:A:191:LEU:HD22	1.95	0.46
3:A:603:PRO:O	3:A:604:PHE:CB	2.63	0.46
3:B:92:PRO:HG2	3:B:117:GLN:HB3	1.97	0.46
3:A:458:ILE:HD12	3:A:482:LEU:HD21	1.98	0.46
10:A:4241:NDG:C7	10:A:4241:NDG:O3	2.62	0.46
2:D:20:C:O2'	2:D:21:U:H5'	2.14	0.46
3:A:412:LEU:HD22	3:A:430:LEU:HD21	1.97	0.46
3:A:53:ILE:HD11	3:A:74:TYR:CD2	2.50	0.46
3:B:217:PHE:HB2	3:B:244:GLU:O	2.16	0.46
3:B:79:ILE:CB	3:B:103:VAL:HB	2.45	0.46
3:A:557:PHE:CD2	3:A:558:LEU:HG	2.46	0.46
3:B:410:LEU:HD12	3:B:410:LEU:N	2.31	0.46
3:A:80:LEU:CD2	3:A:104:LEU:HA	2.45	0.46
3:A:309:ASN:OD1	3:A:334:THR:HG23	2.15	0.46
3:B:313:LEU:CB	3:B:346:ILE:HG22	2.43	0.46
8:A:2911:NAG:O3	8:A:2911:NAG:H83	2.16	0.46
3:A:275:ASN:HD21	7:A:2751:NAG:H61	1.78	0.46
3:A:696:CYS:O	3:A:697:LYS:CB	2.63	0.46
3:A:92:PRO:HG2	3:A:117:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:G:C2'	1:C:42:C:H5'	2.44	0.46
3:A:80:LEU:HD21	3:A:104:LEU:CD1	2.39	0.46
3:A:31:ARG:CA	3:A:31:ARG:HE	2.15	0.46
3:A:40:LEU:HD13	3:A:61:ASN:ND2	2.29	0.46
10:B:4241:NDG:O4	10:B:4242:NDG:H8C1	2.15	0.46
3:B:409:LEU:O	3:B:433:LEU:HA	2.16	0.46
3:A:301:ARG:O	3:A:324:LEU:HD12	2.16	0.46
3:B:169:GLN:HG3	3:B:170:LEU:HD23	1.97	0.46
2:D:24:C:H2'	2:D:25:U:H6	1.81	0.46
1:C:3:U:H2'	1:C:4:C:C6	2.50	0.46
3:A:179:ALA:HB1	3:A:205:SER:HB2	1.98	0.46
3:B:347:ASP:HA	3:B:371:LYS:NZ	2.31	0.46
1:C:6:G:O2'	1:C:7:C:H5'	2.16	0.46
3:B:212:PHE:H	3:B:240:LYS:HZ2	1.64	0.46
3:B:525:LEU:O	3:B:526:LEU:HB2	2.15	0.46
3:B:409:LEU:C	3:B:410:LEU:HD12	2.37	0.46
3:A:105:ASN:O	3:A:106:LEU:HD12	2.16	0.46
3:B:297:LEU:C	3:B:299:SER:H	2.18	0.46
2:D:18:U:H2'	2:D:19:G:C8	2.51	0.46
3:A:382:LYS:HA	3:A:408:PRO:O	2.15	0.46
3:A:651:CYS:HA	3:A:655:SER:OG	2.15	0.46
3:A:277:THR:HG21	6:A:2521:NAG:C8	2.25	0.46
3:A:532:LEU:HD11	3:A:535:LEU:HB2	1.98	0.46
3:A:357:LEU:O	3:A:380:SER:HB2	2.15	0.46
3:A:521:ILE:CD1	3:A:522:ASN:O	2.64	0.46
3:A:458:ILE:HD12	3:A:482:LEU:CD2	2.46	0.46
3:A:73:ARG:NH1	3:A:73:ARG:HG3	2.31	0.46
3:B:227:LEU:HD23	3:B:254:SER:HB3	1.97	0.46
3:B:180:LYS:N	3:B:206:SER:HB2	2.31	0.45
3:B:534:ILE:HG13	3:B:566:ILE:HG22	1.97	0.45
3:B:540:ASN:O	3:B:541:ASN:C	2.54	0.45
3:B:154:LEU:O	3:B:178:LEU:HD23	2.16	0.45
3:B:462:TYR:HD1	3:B:486:MET:HG3	1.81	0.45
3:B:183:ILE:O	3:B:209:LEU:HD23	2.16	0.45
2:D:31:A:O2'	2:D:32:A:H5'	2.15	0.45
3:B:545:LEU:HD12	3:B:555:VAL:HG21	1.99	0.45
3:B:73:ARG:HG3	3:B:73:ARG:NH1	2.31	0.45
3:B:484:ARG:HG2	3:B:510:ILE:HD12	1.97	0.45
3:B:277:THR:HG22	3:B:278:GLN:N	2.31	0.45
3:B:578:PRO:HG2	3:B:581:VAL:HG13	1.98	0.45
3:B:410:LEU:CD1	3:B:410:LEU:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:47:ASP:O	3:B:73:ARG:HD3	2.17	0.45
3:B:366:ASN:O	3:B:367:ILE:C	2.53	0.45
3:B:306:GLU:HB3	3:B:307:TYR:CD1	2.51	0.45
3:A:577:ILE:CD1	3:A:605:ILE:HG21	2.35	0.45
3:B:561:LEU:HB2	3:B:564:LEU:HB2	1.97	0.45
3:A:301:ARG:C	3:A:324:LEU:HD12	2.37	0.45
3:A:114:ILE:HD11	3:A:118:THR:CB	2.40	0.45
3:B:49:LEU:HA	3:B:73:ARG:NH2	2.31	0.45
3:B:543:ALA:HB2	3:B:573:GLY:CA	2.42	0.45
2:D:7:G:H2'	2:D:8:C:C6	2.51	0.45
3:A:614:SER:HA	3:A:637:LEU:HD11	1.98	0.45
3:A:183:ILE:O	3:A:209:LEU:HD23	2.17	0.45
3:A:568:ASN:C	3:A:569:LEU:HD12	2.36	0.45
3:A:558:LEU:C	3:A:561:LEU:HD11	2.36	0.45
10:B:4242:NDG:H4	10:B:4243:BMA:O2	2.16	0.45
3:B:106:LEU:HD23	3:B:111:LEU:HD11	1.98	0.45
3:A:497:ILE:N	3:A:497:ILE:HD13	2.32	0.45
3:B:239:GLU:HG3	3:B:267:THR:HA	1.98	0.45
3:B:396:LEU:HB3	3:B:426:THR:HG21	1.97	0.45
3:A:79:ILE:HG22	3:A:103:VAL:HB	1.99	0.45
3:A:201:LYS:NZ	3:A:227:LEU:HD11	2.32	0.45
3:B:187:ARG:HD3	3:B:189:GLU:OE1	2.17	0.45
2:D:22:U:H2'	2:D:23:C:C6	2.51	0.45
3:A:263:THR:HG23	3:A:286:LEU:HD11	1.98	0.45
3:B:352:GLN:HA	3:B:377:GLY:HA3	1.98	0.45
3:B:302:TYR:CE2	6:B:2522:NDG:H8C3	2.52	0.45
3:A:526:LEU:HA	3:A:529:LEU:HD11	1.97	0.45
3:A:532:LEU:HD13	3:A:532:LEU:C	2.37	0.45
3:A:34:VAL:HG12	3:A:55:VAL:CB	2.45	0.45
3:B:530:GLU:HG3	3:B:530:GLU:O	2.16	0.45
3:B:71:PHE:HE2	3:B:94:LEU:HD23	1.81	0.45
3:A:497:ILE:H	3:A:497:ILE:CD1	2.29	0.45
3:A:37:CYS:CB	3:A:40:LEU:HD11	2.47	0.45
3:B:434:ARG:O	3:B:459:PHE:N	2.46	0.45
3:A:154:LEU:O	3:A:178:LEU:HD23	2.17	0.45
3:A:449:GLY:H	3:A:475:SER:HA	1.81	0.45
3:B:614:SER:HA	3:B:637:LEU:HD11	1.98	0.45
3:A:444:GLU:HG2	3:A:444:GLU:O	2.16	0.45
3:A:409:LEU:O	3:A:433:LEU:HA	2.17	0.45
12:B:2751:NAG:H83	12:B:2751:NAG:H3	1.99	0.45
2:D:7:G:O2'	2:D:8:C:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:G:O2'	1:C:10:A:H5'	2.16	0.45
2:D:15:C:H2'	2:D:16:A:H8	1.82	0.45
3:A:625:VAL:HB	3:A:657:PHE:HB2	1.97	0.45
3:A:526:LEU:HA	3:A:529:LEU:CD1	2.46	0.45
3:B:150:ILE:HG23	3:B:174:GLN:CB	2.44	0.45
3:A:212:PHE:CE2	3:A:241:LEU:HB2	2.53	0.45
2:D:18:U:H2'	2:D:19:G:H8	1.82	0.44
3:B:263:THR:HG23	3:B:286:LEU:HD11	2.00	0.44
3:A:212:PHE:CD2	3:A:241:LEU:HB2	2.53	0.44
3:A:461:ILE:HG22	3:A:461:ILE:O	2.16	0.44
2:D:17:A:C6	2:D:18:U:C4	3.05	0.44
3:B:601:LEU:HD22	3:B:601:LEU:N	2.32	0.44
3:A:390:PHE:CD2	3:A:393:LEU:HD13	2.52	0.44
3:A:169:GLN:HG3	3:A:170:LEU:HD23	1.99	0.44
3:B:321:LEU:O	3:B:354:LEU:HD23	2.17	0.44
3:B:434:ARG:O	3:B:458:ILE:HD12	2.17	0.44
2:D:30:C:H2'	2:D:31:A:H8	1.82	0.44
3:A:140:SER:OG	3:A:141:ASN:N	2.50	0.44
3:B:301:ARG:O	3:B:324:LEU:HD12	2.16	0.44
3:A:313:LEU:HD12	3:A:346:ILE:CG2	2.46	0.44
3:A:212:PHE:H	3:A:240:LYS:HZ2	1.64	0.44
13:B:2912:NAG:O7	13:B:2916:FUL:H63	2.17	0.44
3:A:383:TYR:HD2	3:A:411:THR:OG1	2.00	0.44
3:A:56:LEU:HD13	3:A:56:LEU:C	2.38	0.44
3:B:603:PRO:O	3:B:604:PHE:CB	2.65	0.44
3:A:409:LEU:C	3:A:410:LEU:HD12	2.38	0.44
7:A:2751:NAG:H4	7:A:2752:NAG:N2	2.32	0.44
3:A:241:LEU:O	3:A:241:LEU:HD12	2.17	0.44
2:D:23:C:H2'	2:D:24:C:C6	2.52	0.44
3:B:217:PHE:HD1	3:B:220:ILE:HD12	1.82	0.44
3:B:384:LEU:O	3:B:412:LEU:HA	2.17	0.44
3:A:40:LEU:CD1	3:A:61:ASN:HD21	2.28	0.44
3:B:609:GLN:N	3:B:609:GLN:NE2	2.59	0.44
2:D:23:C:H5"	3:A:539:HIS:HB3	1.99	0.44
3:A:497:ILE:HD13	3:A:497:ILE:H	1.83	0.44
3:A:422:ILE:HD13	3:A:422:ILE:N	2.30	0.44
3:A:80:LEU:HD23	3:A:103:VAL:O	2.17	0.44
3:B:114:ILE:CG1	3:B:118:THR:HG21	2.47	0.44
11:B:5072:NAG:H83	11:B:5072:NAG:O3	2.17	0.44
3:A:313:LEU:CB	3:A:346:ILE:HG22	2.47	0.44
3:A:194:LEU:HD12	3:A:220:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:613:ARG:C	3:A:637:LEU:HD12	2.38	0.44
3:A:588:LEU:HD23	3:A:588:LEU:C	2.38	0.44
3:A:31:ARG:HA	3:A:31:ARG:NE	2.17	0.44
1:C:21:A:H1'	3:B:541:ASN:HB2	1.99	0.44
3:B:345:ASN:HD21	3:B:371:LYS:HZ1	1.66	0.44
3:A:649:CYS:HB2	3:A:683:TYR:HB3	1.99	0.44
3:B:33:ASN:HA	3:B:53:ILE:CG2	2.48	0.43
3:B:212:PHE:H	3:B:240:LYS:HZ1	1.66	0.43
3:A:126:THR:HG22	3:A:148:ASN:O	2.18	0.43
3:B:80:LEU:CD2	3:B:104:LEU:HA	2.48	0.43
3:A:625:VAL:HG11	3:A:657:PHE:CD1	2.53	0.43
3:A:605:ILE:HD11	3:A:629:VAL:CG1	2.14	0.43
3:B:135:ILE:N	3:B:157:ASN:O	2.51	0.43
3:B:599:ASN:O	3:B:601:LEU:HD22	2.18	0.43
3:B:55:VAL:HG12	3:B:56:LEU:N	2.34	0.43
3:A:482:LEU:HB2	3:A:505:LEU:CD2	2.41	0.43
3:B:331:ARG:NH2	3:B:335:LYS:CE	2.81	0.43
3:B:602:GLU:O	3:B:603:PRO:C	2.55	0.43
3:B:33:ASN:O	3:B:54:THR:N	2.39	0.43
3:B:50:PRO:O	3:B:53:ILE:HG23	2.18	0.43
3:A:419:ILE:HG22	3:A:422:ILE:HD11	2.00	0.43
3:B:301:ARG:C	3:B:324:LEU:HD12	2.39	0.43
3:B:333:PHE:CD2	3:B:367:ILE:HD11	2.53	0.43
3:A:194:LEU:HD12	3:A:220:ILE:CD1	2.48	0.43
3:B:359:TYR:HD2	3:B:359:TYR:O	2.01	0.43
3:A:39:HIS:C	3:A:40:LEU:HD12	2.39	0.43
3:B:233:LEU:HD12	3:B:233:LEU:N	2.32	0.43
3:A:485:LEU:HG	3:A:487:LEU:HD21	2.00	0.43
3:B:555:VAL:O	3:B:557:PHE:N	2.42	0.43
3:B:558:LEU:C	3:B:561:LEU:HD11	2.39	0.43
3:A:114:ILE:HG13	3:A:115:SER:N	2.34	0.43
3:A:42:LEU:HD22	3:A:44:HIS:O	2.19	0.43
3:B:313:LEU:HD13	3:B:318:PHE:HE1	1.83	0.43
3:A:187:ARG:C	3:A:189:GLU:H	2.21	0.43
3:A:187:ARG:HG3	3:A:187:ARG:HH11	1.83	0.43
2:D:24:C:O2'	2:D:25:U:H5'	2.19	0.43
9:A:4131:NDG:H6C2	9:A:4132:NAG:HN2	1.83	0.43
3:B:651:CYS:HA	3:B:655:SER:OG	2.19	0.43
3:A:366:ASN:O	3:A:367:ILE:C	2.56	0.43
3:B:262:ALA:HB2	3:B:288:ASP:HB2	1.98	0.43
3:B:571:SER:HA	3:B:595:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:134:SER:HB2	3:A:136:HIS:CE1	2.53	0.43
3:B:410:LEU:O	3:B:433:LEU:HD12	2.19	0.43
3:A:450:GLN:HG3	10:A:4241:NDG:H5	1.99	0.43
3:B:143:PHE:C	3:B:145:ASN:N	2.69	0.43
3:B:230:ASN:HA	3:B:257:ASN:O	2.19	0.43
3:B:187:ARG:C	3:B:189:GLU:H	2.22	0.43
3:B:263:THR:HG23	3:B:286:LEU:CD1	2.49	0.43
2:D:14:U:O2'	2:D:15:C:H5'	2.18	0.43
3:B:345:ASN:ND2	3:B:371:LYS:NZ	2.67	0.43
3:A:45:ILE:CG2	3:A:45:ILE:O	2.64	0.43
2:D:40:G:H2'	2:D:41:C:C6	2.54	0.43
3:A:652:GLU:OE1	3:B:681:HIS:HB3	2.19	0.43
10:B:4241:NDG:H5	10:B:4242:NDG:H8C1	2.00	0.43
3:B:602:GLU:O	3:B:605:ILE:HG23	2.19	0.43
3:B:59:THR:HG22	3:B:60:HIS:CG	2.54	0.43
3:B:582:PHE:HA	3:B:585:LEU:HD12	2.01	0.43
3:B:613:ARG:C	3:B:637:LEU:HD12	2.40	0.43
3:B:651:CYS:O	3:B:655:SER:HB2	2.18	0.42
3:A:575:ASP:OD2	3:A:576:GLU:N	2.52	0.42
3:A:90:LEU:HG	3:A:94:LEU:HD13	2.00	0.42
3:B:630:PHE:O	3:B:634:PHE:CD1	2.72	0.42
3:A:544:ARG:HG3	3:A:544:ARG:H	1.51	0.42
3:B:527:GLU:HG3	3:B:559:LYS:NZ	2.33	0.42
3:B:382:LYS:HA	3:B:408:PRO:O	2.19	0.42
3:B:126:THR:HG22	3:B:148:ASN:O	2.18	0.42
3:A:441:ASN:O	3:A:466:ASN:HA	2.19	0.42
9:A:4131:NDG:H6C1	9:A:4132:NAG:HN2	1.83	0.42
2:D:3:U:H2'	2:D:4:G:O4'	2.19	0.42
3:A:599:ASN:OD1	3:A:600:LYS:N	2.52	0.42
3:A:536:ASP:CA	3:A:538:GLN:HE22	2.32	0.42
3:A:133:ASN:O	3:A:134:SER:C	2.57	0.42
3:B:575:ASP:OD2	3:B:576:GLU:N	2.53	0.42
3:B:66:LEU:O	3:B:68:PRO:HD3	2.19	0.42
3:B:365:ASN:HB3	3:B:367:ILE:CD1	2.48	0.42
3:B:661:ILE:CG2	3:B:671:LEU:HD21	2.49	0.42
3:B:42:LEU:O	3:B:62:GLN:O	2.37	0.42
3:B:169:GLN:O	3:B:170:LEU:HB2	2.20	0.42
3:A:384:LEU:O	3:A:412:LEU:HA	2.20	0.42
3:A:497:ILE:CD1	3:A:501:PRO:HD3	2.49	0.42
3:A:535:LEU:HD11	3:A:537:PHE:CD2	2.53	0.42
3:A:396:LEU:CG	3:A:422:ILE:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:234:ASN:HD22	3:B:236:HIS:H	1.67	0.42
7:A:2751:NAG:H4	7:A:2752:NAG:HN2	1.85	0.42
3:A:53:ILE:HD11	3:A:74:TYR:HD2	1.85	0.42
2:D:27:U:H2'	2:D:28:G:C8	2.55	0.42
3:B:502:PHE:CE2	3:B:525:LEU:HD11	2.54	0.42
3:B:537:PHE:CZ	3:B:557:PHE:HZ	2.38	0.42
3:B:382:LYS:HB2	3:B:410:LEU:HD13	2.00	0.42
3:B:427:PHE:CZ	3:B:436:LEU:HD11	2.55	0.42
3:A:609:GLN:H	3:A:609:GLN:HE21	1.61	0.42
3:B:243:TRP:O	3:B:246:SER:HB2	2.20	0.42
3:B:201:LYS:NZ	3:B:227:LEU:HD11	2.34	0.42
3:B:206:SER:HA	3:B:230:ASN:O	2.20	0.42
3:B:449:GLY:N	3:B:475:SER:HA	2.34	0.42
3:B:479:VAL:O	3:B:479:VAL:HG23	2.20	0.42
3:B:91:GLU:HB3	3:B:93:GLU:HG2	2.02	0.42
3:A:598:LEU:O	3:A:622:ILE:HG12	2.20	0.42
3:A:169:GLN:O	3:A:170:LEU:HB2	2.20	0.42
3:A:643:ARG:NH1	3:A:670:GLU:OE1	2.53	0.42
3:B:96:GLN:HB3	3:B:121:PHE:CG	2.55	0.42
3:A:116:ASP:O	3:A:120:VAL:HG23	2.19	0.42
3:A:246:SER:O	3:A:248:THR:N	2.53	0.42
3:A:370:THR:OG1	3:A:400:THR:HG23	2.20	0.42
1:C:16:U:C4'	9:A:4135:MAN:O3	2.67	0.42
3:A:599:ASN:O	3:A:601:LEU:HD22	2.20	0.41
3:B:575:ASP:OD2	3:B:575:ASP:C	2.59	0.41
3:B:433:LEU:HD21	3:B:436:LEU:HB2	2.01	0.41
3:A:140:SER:O	3:A:142:PRO:HD3	2.19	0.41
3:A:106:LEU:HD23	3:A:111:LEU:HD11	2.01	0.41
3:B:297:LEU:HB3	3:B:300:LEU:HB2	2.01	0.41
3:A:382:LYS:HB2	3:A:410:LEU:HD13	2.02	0.41
3:A:643:ARG:HG3	3:A:644:PHE:CD2	2.55	0.41
6:A:3982:NDG:H6C2	6:A:3982:NDG:C2	2.50	0.41
3:B:598:LEU:HB2	3:B:620:ASN:ND2	2.30	0.41
3:B:116:ASP:CA	3:B:142:PRO:HA	2.48	0.41
3:A:38:SER:O	3:A:60:HIS:HB2	2.20	0.41
3:B:658:VAL:O	3:B:661:ILE:HB	2.20	0.41
3:B:67:PRO:HA	3:B:68:PRO:HD2	1.91	0.41
3:A:239:GLU:HG3	3:A:267:THR:HA	2.02	0.41
8:A:2912:NAG:H82	8:A:2912:NAG:H3	2.01	0.41
3:A:177:LEU:N	3:A:177:LEU:CD1	2.83	0.41
3:B:128:LEU:N	3:B:149:LEU:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:689:LYS:CG	3:A:690:LEU:N	2.83	0.41
3:A:436:LEU:HD23	3:A:436:LEU:C	2.40	0.41
3:B:133:ASN:O	3:B:134:SER:C	2.57	0.41
3:B:234:ASN:CB	3:B:237:LEU:HD13	2.42	0.41
3:A:546:TRP:HB3	3:A:578:PRO:HD3	2.02	0.41
3:A:645:ASN:HA	3:A:646:PRO:HD3	1.90	0.41
2:D:17:A:H4'	14:B:4135:MAN:H62	2.03	0.41
3:A:246:SER:C	3:A:248:THR:N	2.74	0.41
3:A:478:LEU:O	3:A:478:LEU:HD23	2.20	0.41
3:B:584:ASN:HA	3:B:586:PHE:CE2	2.55	0.41
3:B:654:ILE:CD1	3:B:654:ILE:C	2.89	0.41
3:B:33:ASN:HB3	3:B:53:ILE:HA	2.03	0.41
3:B:612:LEU:HD23	3:B:633:PRO:HB2	2.03	0.41
2:D:12:U:H2'	2:D:13:G:H8	1.85	0.41
3:B:521:ILE:CD1	3:B:522:ASN:O	2.68	0.41
3:A:234:ASN:HD22	3:A:236:HIS:H	1.69	0.41
3:B:39:HIS:O	3:B:40:LEU:HD12	2.20	0.41
3:A:620:ASN:HB2	3:A:645:ASN:ND2	2.29	0.41
3:B:147:LYS:HZ2	3:B:171:GLU:HG2	1.85	0.41
3:B:369:SER:OG	3:B:370:THR:N	2.54	0.41
3:B:337:SER:HB3	3:B:340:LEU:HB2	2.01	0.41
3:A:435:ILE:HG12	3:A:460:GLU:HG2	2.03	0.41
3:A:602:GLU:HA	3:A:602:GLU:OE2	2.19	0.41
3:A:68:PRO:HB3	3:A:94:LEU:HD12	2.03	0.41
3:B:37:CYS:HB2	3:B:57:ASN:O	2.20	0.41
3:A:37:CYS:C	3:A:40:LEU:HD11	2.41	0.41
10:A:4241:NDG:O3	10:A:4242:NDG:C1	2.69	0.41
2:D:20:C:H2'	2:D:21:U:H6	1.86	0.41
3:B:233:LEU:CD1	3:B:233:LEU:N	2.83	0.41
3:A:661:ILE:CG2	3:A:671:LEU:HD21	2.50	0.41
3:B:486:MET:O	3:B:487:LEU:HD22	2.20	0.41
1:C:31:U:H2'	1:C:32:G:H8	1.86	0.41
3:B:625:VAL:HB	3:B:657:PHE:HB2	2.03	0.41
3:A:83:GLY:O	3:A:84:PHE:HB2	2.20	0.41
3:A:389:THR:HG22	3:A:389:THR:O	2.20	0.41
3:B:620:ASN:HB3	3:B:621:LEU:H	1.76	0.41
3:B:79:ILE:HG22	3:B:103:VAL:HB	2.03	0.41
3:B:40:LEU:CB	3:B:61:ASN:HD21	2.21	0.41
3:B:582:PHE:HB3	3:B:609:GLN:OE1	2.21	0.41
3:B:131:MET:O	3:B:156:HIS:HB3	2.21	0.41
2:D:30:C:H2'	2:D:31:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:96:GLN:HB3	3:B:121:PHE:CD2	2.56	0.41
3:B:521:ILE:HD12	3:B:557:PHE:HE1	1.86	0.40
3:B:140:SER:OG	3:B:141:ASN:N	2.50	0.40
3:A:294:PHE:C	3:A:296:TYR:N	2.74	0.40
3:A:309:ASN:OD1	3:A:334:THR:HA	2.21	0.40
3:B:189:GLU:O	3:B:192:GLU:HG2	2.21	0.40
3:B:331:ARG:HH22	3:B:335:LYS:HD3	1.86	0.40
3:B:92:PRO:HG3	3:B:117:GLN:C	2.41	0.40
3:A:263:THR:HG23	3:A:286:LEU:CD1	2.50	0.40
3:B:66:LEU:HA	3:B:66:LEU:HD23	1.92	0.40
3:B:94:LEU:O	3:B:98:LEU:HD23	2.21	0.40
3:A:493:LYS:O	3:A:494:ASN:HB2	2.21	0.40
3:A:168:VAL:HG11	3:A:195:GLY:HA3	2.02	0.40
2:D:19:G:H2'	2:D:20:C:C6	2.55	0.40
3:B:187:ARG:HB2	3:B:190:GLU:HG2	2.03	0.40
3:A:212:PHE:H	3:A:240:LYS:HZ1	1.67	0.40
3:B:447:LEU:HD23	3:B:451:GLU:HG3	2.02	0.40
3:A:564:LEU:O	3:A:588:LEU:HA	2.21	0.40
3:A:396:LEU:CD1	3:A:422:ILE:HD12	2.50	0.40
6:B:3981:NAG:H83	6:B:3981:NAG:H3	2.03	0.40
3:A:230:ASN:HA	3:A:257:ASN:O	2.21	0.40
3:B:187:ARG:C	3:B:189:GLU:N	2.75	0.40
3:A:197:SER:O	3:A:221:GLY:HA3	2.21	0.40
3:B:648:ASP:O	3:B:654:ILE:HG23	2.22	0.40
3:B:422:ILE:CD1	3:B:438:LEU:HD13	2.52	0.40
3:A:458:ILE:CD1	3:A:458:ILE:C	2.88	0.40
3:A:410:LEU:O	3:A:433:LEU:HD12	2.22	0.40
3:A:297:LEU:HB3	3:A:300:LEU:HB2	2.03	0.40
3:B:114:ILE:HD11	3:B:118:THR:HG21	2.02	0.40
3:A:591:ILE:HB	3:A:615:LEU:HD12	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
3	A	655/697 (94%)	527 (80%)	117 (18%)	11 (2%)	11 52
3	B	664/697 (95%)	537 (81%)	113 (17%)	14 (2%)	9 48
All	All	1319/1394 (95%)	1064 (81%)	230 (17%)	25 (2%)	10 50

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	551	PRO
3	A	247	ASN
3	A	290	GLY
3	A	38	SER
3	A	267	THR
3	A	465	TYR
3	A	556	ASN
3	B	38	SER
3	B	247	ASN
3	B	465	TYR
3	B	556	ASN
3	B	604	PHE
3	A	555	VAL
3	A	604	PHE
3	B	30	VAL
3	B	49	LEU
3	B	267	THR
3	B	635	GLN
3	B	603	PRO
3	A	368	PRO
3	B	290	GLY
3	B	67	PRO
3	B	368	PRO
3	A	631	GLY
3	B	449	GLY

5.3.2 Protein sidechains (i)

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
3	A	619/651 (95%)	564 (91%)	55 (9%)	12 47
3	B	625/651 (96%)	574 (92%)	51 (8%)	14 51
All	All	1244/1302 (96%)	1138 (92%)	106 (8%)	13 49

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	31	ARG
3	A	40	LEU
3	A	42	LEU
3	A	45	ILE
3	A	50	PRO
3	A	53	ILE
3	A	65	ARG
3	A	76	GLN
3	A	81	ASP
3	A	89	LYS
3	A	116	ASP
3	A	154	LEU
3	A	189	GLU
3	A	218	GLN
3	A	250	ILE
3	A	273	TRP
3	A	276	LEU
3	A	312	ARG
3	A	323	ASN
3	A	335	LYS
3	A	345	ASN
3	A	347	ASP
3	A	355	LYS
3	A	359	TYR
3	A	381	LEU
3	A	394	GLN
3	A	407	SER
3	A	409	LEU
3	A	410	LEU
3	A	411	THR
3	A	442	GLU
3	A	445	GLN
3	A	446	LYS
3	A	458	ILE

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Mol	Chain	Res	Type
3	A	478	LEU
3	A	481	SER
3	A	483	GLN
3	A	497	ILE
3	A	521	ILE
3	A	522	ASN
3	A	544	ARG
3	A	551	PRO
3	A	561	LEU
3	A	572	ASN
3	A	574	LEU
3	A	577	ILE
3	A	605	ILE
3	A	608	ASP
3	A	609	GLN
3	A	628	ASP
3	A	638	ASN
3	A	672	SER
3	A	673	THR
3	A	679	THR
3	A	686	PHE
3	B	32	TYR
3	B	33	ASN
3	B	45	ILE
3	B	53	ILE
3	B	65	ARG
3	B	76	GLN
3	B	81	ASP
3	B	89	LYS
3	B	98	LEU
3	B	116	ASP
3	B	154	LEU
3	B	189	GLU
3	B	218	GLN
3	B	273	TRP
3	B	276	LEU
3	B	288	ASP
3	B	301	ARG
3	B	312	ARG
3	B	323	ASN
3	B	345	ASN
3	B	347	ASP

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Mol	Chain	Res	Type
3	B	355	LYS
3	B	359	TYR
3	B	381	LEU
3	B	409	LEU
3	B	410	LEU
3	B	411	THR
3	B	442	GLU
3	B	446	LYS
3	B	478	LEU
3	B	481	SER
3	B	521	ILE
3	B	522	ASN
3	B	544	ARG
3	B	556	ASN
3	B	561	LEU
3	B	566	ILE
3	B	572	ASN
3	B	574	LEU
3	B	577	ILE
3	B	605	ILE
3	B	608	ASP
3	B	609	GLN
3	B	628	ASP
3	B	638	ASN
3	B	651	CYS
3	B	654	ILE
3	B	672	SER
3	B	673	THR
3	B	679	THR
3	B	686	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	61	ASN
3	A	76	GLN
3	A	85	ASN
3	A	108	HIS
3	A	113	GLN
3	A	145	ASN
3	A	157	ASN
3	A	169	GLN

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Mol	Chain	Res	Type
3	A	174	GLN
3	A	218	GLN
3	A	230	ASN
3	A	234	ASN
3	A	345	ASN
3	A	445	GLN
3	A	450	GLN
3	A	466	ASN
3	A	470	GLN
3	A	483	GLN
3	A	494	ASN
3	A	517	ASN
3	A	522	ASN
3	A	538	GLN
3	A	541	ASN
3	A	556	ASN
3	A	572	ASN
3	A	609	GLN
3	A	620	ASN
3	A	638	ASN
3	A	645	ASN
3	A	674	HIS
3	B	33	ASN
3	B	61	ASN
3	B	76	GLN
3	B	85	ASN
3	B	107	GLN
3	B	108	HIS
3	B	113	GLN
3	B	145	ASN
3	B	146	GLN
3	B	157	ASN
3	B	169	GLN
3	B	218	GLN
3	B	230	ASN
3	B	234	ASN
3	B	336	GLN
3	B	345	ASN
3	B	445	GLN
3	B	450	GLN
3	B	466	ASN
3	B	470	GLN

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Mol	Chain	Res	Type
3	B	483	GLN
3	B	494	ASN
3	B	517	ASN
3	B	522	ASN
3	B	538	GLN
3	B	539	HIS
3	B	541	ASN
3	B	556	ASN
3	B	572	ASN
3	B	609	GLN
3	B	618	GLN
3	B	620	ASN
3	B	638	ASN
3	B	645	ASN
3	B	674	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	45/46 (97%)	0	0
2	D	45/46 (97%)	0	0
All	All	90/92 (97%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

40 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	$\#\|Z\| > 2$
6	NAG	A	2521	3,6	14,14,15	0.99	1 (7%)	15,19,21	0.81	0
6	NDG	A	2522	6	14,14,15	0.91	1 (7%)	15,19,21	1.01	2 (13%)
7	NAG	A	2751	3,7	14,14,15	0.85	0	15,19,21	1.05	2 (13%)
7	NAG	A	2752	7	14,14,15	0.81	1 (7%)	15,19,21	0.67	0
7	MAN	A	2753	7	11,11,12	0.87	0	14,15,17	0.86	2 (14%)
8	NAG	A	2911	8,3	14,14,15	0.91	0	15,19,21	0.72	0
8	NAG	A	2912	8	14,14,15	0.88	1 (7%)	15,19,21	0.56	0
8	FUC	A	2916	8	10,10,11	0.81	0	14,14,16	0.68	0
6	NAG	A	3981	3,6	14,14,15	1.09	1 (7%)	15,19,21	0.90	0
6	NDG	A	3982	6	14,14,15	0.98	1 (7%)	15,19,21	0.97	1 (6%)
9	NDG	A	4131	9,3	14,14,15	0.50	0	15,19,21	1.32	2 (13%)
9	NAG	A	4132	9	14,14,15	0.77	0	15,19,21	0.81	0
9	MAN	A	4133	9	11,11,12	1.15	1 (9%)	14,15,17	0.95	1 (7%)
9	MAN	A	4134	9	11,11,12	0.89	0	14,15,17	0.84	1 (7%)
9	MAN	A	4135	9	11,11,12	0.89	0	14,15,17	1.17	1 (7%)
10	NDG	A	4241	10,3	14,14,15	1.01	1 (7%)	15,19,21	0.87	0
10	NDG	A	4242	10	14,14,15	0.80	0	15,19,21	0.82	0
10	BMA	A	4243	10	11,11,12	0.68	0	14,15,17	0.41	0
11	NDG	A	5071	11,3	14,14,15	0.55	0	15,19,21	1.17	2 (13%)
11	NAG	A	5072	11	14,14,15	0.82	1 (7%)	15,19,21	0.88	1 (6%)
6	NAG	B	2521	3,6	14,14,15	1.09	1 (7%)	15,19,21	1.17	2 (13%)
6	NDG	B	2522	6	14,14,15	1.02	1 (7%)	15,19,21	0.87	0
12	NAG	B	2751	3,12	14,14,15	1.04	0	15,19,21	1.27	2 (13%)
12	NAG	B	2752	12	14,14,15	0.81	0	15,19,21	0.62	0
12	BMA	B	2753	12	11,11,12	0.96	1 (9%)	14,15,17	0.96	1 (7%)
13	NAG	B	2911	3,13	14,14,15	0.98	1 (7%)	15,19,21	0.74	0
13	NAG	B	2912	13	14,14,15	0.90	0	15,19,21	1.04	1 (6%)
13	FUL	B	2916	13	10,10,11	0.71	0	14,14,16	0.78	0
6	NAG	B	3981	3,6	14,14,15	0.80	0	15,19,21	0.85	0
6	NDG	B	3982	6	14,14,15	0.90	0	15,19,21	1.01	1 (6%)
14	NDG	B	4131	3,14	14,14,15	0.70	0	15,19,21	1.13	1 (6%)
14	NDG	B	4132	14	14,14,15	1.07	0	15,19,21	1.27	2 (13%)
14	MAN	B	4133	14	11,11,12	1.26	1 (9%)	14,15,17	1.14	1 (7%)
14	MAN	B	4134	14	11,11,12	0.83	0	14,15,17	0.92	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	MAN	B	4135	14	11,11,12	0.87	0	14,15,17	1.17	2 (14%)
10	NDG	B	4241	10,3	14,14,15	0.94	0	15,19,21	0.97	1 (6%)
10	NDG	B	4242	10	14,14,15	1.07	1 (7%)	15,19,21	0.72	0
10	BMA	B	4243	10	11,11,12	0.89	0	14,15,17	0.35	0
11	NDG	B	5071	11,3	14,14,15	1.27	1 (7%)	15,19,21	0.86	0
11	NAG	B	5072	11	14,14,15	1.16	1 (7%)	15,19,21	1.20	1 (6%)

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
6	NAG	A	2521	3,6	-	0/6/23/26	0/1/1/1
6	NDG	A	2522	6	-	1/6/23/26	0/1/1/1
7	NAG	A	2751	3,7	-	1/6/23/26	0/1/1/1
7	NAG	A	2752	7	-	0/6/23/26	0/1/1/1
7	MAN	A	2753	7	-	0/2/19/22	1/1/1/1
8	NAG	A	2911	8,3	-	0/6/23/26	0/1/1/1
8	NAG	A	2912	8	-	0/6/23/26	0/1/1/1
8	FUC	A	2916	8	-	0/0/17/20	0/1/1/1
6	NAG	A	3981	3,6	-	0/6/23/26	0/1/1/1
6	NDG	A	3982	6	-	0/6/23/26	0/1/1/1
9	NDG	A	4131	9,3	-	0/6/23/26	0/1/1/1
9	NAG	A	4132	9	-	0/6/23/26	0/1/1/1
9	MAN	A	4133	9	-	0/2/19/22	0/1/1/1
9	MAN	A	4134	9	-	0/2/19/22	0/1/1/1
9	MAN	A	4135	9	-	0/2/19/22	0/1/1/1
10	NDG	A	4241	10,3	-	0/6/23/26	0/1/1/1
10	NDG	A	4242	10	-	0/6/23/26	0/1/1/1
10	BMA	A	4243	10	-	0/2/19/22	0/1/1/1
11	NDG	A	5071	11,3	-	2/6/23/26	0/1/1/1
11	NAG	A	5072	11	-	1/6/23/26	0/1/1/1
6	NAG	B	2521	3,6	-	1/6/23/26	0/1/1/1
6	NDG	B	2522	6	-	1/6/23/26	0/1/1/1
12	NAG	B	2751	3,12	-	0/6/23/26	0/1/1/1
12	NAG	B	2752	12	-	0/6/23/26	0/1/1/1
12	BMA	B	2753	12	-	0/2/19/22	0/1/1/1
13	NAG	B	2911	3,13	-	0/6/23/26	0/1/1/1
13	NAG	B	2912	13	-	0/6/23/26	0/1/1/1
13	FUL	B	2916	13	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	3981	3,6	-	0/6/23/26	0/1/1/1
6	NDG	B	3982	6	-	0/6/23/26	0/1/1/1
14	NDG	B	4131	3,14	-	0/6/23/26	0/1/1/1
14	NDG	B	4132	14	-	0/6/23/26	0/1/1/1
14	MAN	B	4133	14	-	0/2/19/22	0/1/1/1
14	MAN	B	4134	14	-	0/2/19/22	1/1/1/1
14	MAN	B	4135	14	-	0/2/19/22	0/1/1/1
10	NDG	B	4241	10,3	-	0/6/23/26	0/1/1/1
10	NDG	B	4242	10	-	1/6/23/26	0/1/1/1
10	BMA	B	4243	10	-	0/2/19/22	0/1/1/1
11	NDG	B	5071	11,3	-	0/6/23/26	0/1/1/1
11	NAG	B	5072	11	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	5072	NAG	C1-C2	2.03	1.55	1.52
7	A	2752	NAG	C1-C2	2.07	1.55	1.52
12	B	2753	BMA	C2-C3	2.10	1.55	1.52
6	A	2521	NAG	C1-C2	2.15	1.55	1.52
6	A	3982	NDG	C1-C2	2.22	1.55	1.52
6	A	2522	NDG	C1-C2	2.26	1.55	1.52
8	A	2912	NAG	C1-C2	2.27	1.55	1.52
6	B	2521	NAG	C1-C2	2.50	1.55	1.52
14	B	4133	MAN	C2-C3	2.51	1.56	1.52
10	B	4242	NDG	C1-C2	2.58	1.56	1.52
6	B	2522	NDG	C1-C2	2.63	1.56	1.52
11	B	5071	NDG	C1-C2	2.65	1.56	1.52
9	A	4133	MAN	C2-C3	2.76	1.56	1.52
13	B	2911	NAG	C1-C2	2.83	1.56	1.52
6	A	3981	NAG	C1-C2	2.90	1.56	1.52
10	A	4241	NDG	C1-C2	3.03	1.56	1.52
11	B	5072	NAG	C1-C2	3.09	1.56	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	4131	NDG	C2-N2-C7	-3.62	118.38	123.04
14	B	4132	NDG	C2-N2-C7	-3.42	118.65	123.04
9	A	4131	NDG	C2-N2-C7	-3.02	119.15	123.04
9	A	4131	NDG	C4-C3-C2	-2.98	106.60	111.23
11	A	5071	NDG	C2-N2-C7	-2.82	119.41	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	4241	NDG	C2-N2-C7	-2.75	119.51	123.04
14	B	4132	NDG	C4-C3-C2	-2.73	106.98	111.23
11	A	5071	NDG	C4-C3-C2	-2.72	106.99	111.23
6	A	2522	NDG	C2-N2-C7	-2.14	120.29	123.04
11	A	5072	NAG	C2-N2-C7	-2.09	120.35	123.04
7	A	2751	NAG	C2-N2-C7	-2.09	120.35	123.04
6	B	2521	NAG	C2-N2-C7	-2.04	120.42	123.04
12	B	2751	NAG	C4-C3-C2	2.02	114.37	111.23
7	A	2753	MAN	C1-C2-C3	2.02	111.93	109.54
9	A	4133	MAN	C3-C4-C5	2.03	113.73	110.20
6	A	2522	NDG	C1-O-C5	2.11	114.93	112.25
9	A	4134	MAN	C1-O5-C5	2.28	115.14	112.25
7	A	2753	MAN	C1-O5-C5	2.31	115.19	112.25
6	B	2521	NAG	C4-C3-C2	2.36	114.89	111.23
7	A	2751	NAG	C3-C4-C5	2.40	114.38	110.20
14	B	4134	MAN	C1-O5-C5	2.52	115.44	112.25
14	B	4135	MAN	C1-O5-C5	2.59	115.53	112.25
6	A	3982	NDG	C1-O-C5	2.60	115.55	112.25
13	B	2912	NAG	C4-C3-C2	2.77	115.54	111.23
6	B	3982	NDG	C1-O-C5	2.92	115.95	112.25
12	B	2753	BMA	C1-C2-C3	3.02	113.11	109.54
14	B	4135	MAN	C1-C2-C3	3.19	113.32	109.54
12	B	2751	NAG	C3-C4-C5	3.38	116.09	110.20
14	B	4133	MAN	C1-C2-C3	3.55	113.74	109.54
11	B	5072	NAG	C1-O5-C5	3.66	116.89	112.25
9	A	4135	MAN	C1-O5-C5	3.68	116.92	112.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2521	NAG	O7-C7-N2-C2
10	B	4242	NDG	O7-C7-N2-C2
6	A	2522	NDG	O7-C7-N2-C2
6	B	2522	NDG	O7-C7-N2-C2
11	A	5071	NDG	C8-C7-N2-C2
7	A	2751	NAG	O7-C7-N2-C2
11	A	5072	NAG	O7-C7-N2-C2
11	A	5071	NDG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2753	MAN	C1-C2-C3-C4-C5-O5
14	B	4134	MAN	C1-C2-C3-C4-C5-O5

29 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2521	NAG	4	0
7	A	2751	NAG	6	0
7	A	2752	NAG	2	0
8	A	2911	NAG	3	0
8	A	2912	NAG	2	0
8	A	2916	FUC	1	0
6	A	3981	NAG	3	0
6	A	3982	NDG	2	0
9	A	4131	NDG	3	0
9	A	4132	NAG	3	0
9	A	4135	MAN	3	0
10	A	4241	NDG	5	0
10	A	4242	NDG	2	0
10	A	4243	BMA	1	0
11	A	5071	NDG	3	0
11	A	5072	NAG	1	0
6	B	2521	NAG	4	0
6	B	2522	NDG	1	0
12	B	2751	NAG	3	0
13	B	2912	NAG	1	0
13	B	2916	FUL	1	0
6	B	3981	NAG	4	0
6	B	3982	NDG	2	0
14	B	4135	MAN	1	0
10	B	4241	NDG	5	0
10	B	4242	NDG	3	0
10	B	4243	BMA	1	0
11	B	5071	NDG	1	0
11	B	5072	NAG	2	0

5.6 Ligand geometry (i)

4 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	1961	3	14,14,15	0.96	0	15,19,21	0.99	1 (6%)
4	NDG	A	724	3	14,14,15	0.88	1 (7%)	15,19,21	0.91	0
5	NAG	B	1961	3	14,14,15	1.20	1 (7%)	15,19,21	0.90	1 (6%)
5	NAG	B	724	3	14,14,15	0.84	1 (7%)	15,19,21	0.67	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	1961	3	-	1/6/23/26	0/1/1/1
4	NDG	A	724	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1961	3	-	2/6/23/26	0/1/1/1
5	NAG	B	724	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	724	NDG	C1-C2	2.22	1.55	1.52
5	B	724	NAG	C1-C2	2.38	1.55	1.52
5	B	1961	NAG	C1-C2	3.47	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1961	NAG	C1-O5-C5	2.41	115.31	112.25
5	A	1961	NAG	C1-O5-C5	2.85	115.87	112.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1961	NAG	O7-C7-N2-C2
5	B	1961	NAG	C8-C7-N2-C2
5	B	1961	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1961	NAG	1	0
4	A	724	NDG	1	0
5	B	724	NAG	1	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

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, 95^{th} 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	C	46/46 (100%)	0.25	0 100 100	167, 194, 197, 197	0
2	D	46/46 (100%)	0.22	0 100 100	164, 193, 197, 197	0
3	A	661/697 (94%)	0.36	28 (4%) 40 35	108, 144, 182, 191	0
3	B	668/697 (95%)	0.33	40 (5%) 25 22	109, 144, 179, 189	0
All	All	1421/1486 (95%)	0.34	68 (4%) 34 30	108, 145, 188, 197	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	62	GLN	7.0
3	B	663	GLN	5.9
3	B	302	TYR	5.4
3	A	41	LYS	4.4
3	B	42	LEU	4.2
3	B	217	PHE	4.1
3	B	223	LEU	4.0
3	A	138	ILE	3.7
3	A	683	TYR	3.6
3	A	56	LEU	3.6
3	B	636	ASN	3.6
3	B	41	LYS	3.5
3	B	62	GLN	3.3
3	B	688	LEU	3.3
3	B	640	LEU	3.2
3	B	139	LYS	3.1
3	B	45	ILE	3.0
3	B	46	PRO	3.0
3	B	138	ILE	3.0
3	B	326	TYR	2.9
3	A	80	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	B	693	THR	2.9
3	B	689	LYS	2.9
3	B	327	LEU	2.9
3	B	682	HIS	2.8
3	A	28	CYS	2.8
3	A	82	ALA	2.8
3	A	519	ALA	2.8
3	A	344	PRO	2.8
3	A	75	SER	2.7
3	A	199	LEU	2.7
3	B	318	PHE	2.7
3	A	674	HIS	2.6
3	B	279	LEU	2.5
3	A	636	ASN	2.5
3	A	58	LEU	2.5
3	B	39	HIS	2.5
3	A	65	ARG	2.4
3	B	58	LEU	2.4
3	B	106	LEU	2.4
3	A	321	LEU	2.4
3	A	76	GLN	2.4
3	A	612	LEU	2.3
3	B	63	LEU	2.3
3	A	77	LEU	2.3
3	A	43	THR	2.3
3	B	32	TYR	2.3
3	A	652	GLU	2.3
3	B	40	LEU	2.3
3	B	657	PHE	2.3
3	B	90	LEU	2.3
3	B	526	LEU	2.3
3	B	690	LEU	2.2
3	B	250	ILE	2.2
3	B	253	LEU	2.2
3	B	529	LEU	2.2
3	B	64	ARG	2.2
3	A	106	LEU	2.1
3	A	223	LEU	2.1
3	A	615	LEU	2.1
3	B	303	LEU	2.1
3	A	188	SER	2.1
3	A	54	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	683	TYR	2.1
3	B	200	ARG	2.1
3	B	35	ALA	2.0
3	A	40	LEU	2.0
3	B	268	PHE	2.0

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)

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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
8	FUC	A	2916	10/11	0.77	0.32	1.28	189,190,191,191	0
14	NDG	B	4131	14/15	0.91	0.24	0.18	141,144,149,155	0
9	NDG	A	4131	14/15	0.97	0.23	-0.18	140,145,147,152	0
6	NAG	A	2521	14/15	0.90	0.16	-0.99	171,175,177,179	0
9	MAN	A	4134	11/12	0.63	0.50	-	188,190,191,192	0
6	NDG	A	3982	14/15	0.83	0.30	-	184,185,187,188	0
6	NDG	A	2522	14/15	0.80	0.29	-	181,182,182,183	0
14	NDG	B	4132	14/15	0.88	0.19	-	158,165,169,175	0
11	NDG	A	5071	14/15	0.94	0.15	-	160,164,165,168	0
13	FUL	B	2916	10/11	0.85	0.23	-	191,192,192,192	0
6	NDG	B	2522	14/15	0.76	1.02	-	186,188,188,188	0
10	NDG	B	4242	14/15	0.91	0.22	-	177,181,184,188	0
9	MAN	A	4135	11/12	0.55	0.23	-	186,187,187,188	0
10	BMA	B	4243	11/12	0.67	0.25	-	190,191,192,192	0
11	NAG	A	5072	14/15	0.83	0.23	-	170,172,174,174	0
10	NDG	B	4241	14/15	0.84	0.18	-	168,171,174,177	0
6	NAG	B	2521	14/15	0.74	0.41	-	173,177,179,183	0
8	NAG	A	2912	14/15	0.85	0.20	-	179,180,180,180	0
13	NAG	B	2912	14/15	0.90	0.38	-	176,179,180,180	0
12	NAG	B	2751	14/15	0.91	0.23	-	173,176,179,182	0
9	MAN	A	4133	11/12	0.87	0.24	-	177,180,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	NAG	B	2752	14/15	0.90	0.20	-	183,184,188,190	0
11	NAG	B	5072	14/15	0.63	0.43	-	197,197,197,197	0
12	BMA	B	2753	11/12	0.81	0.37	-	191,193,193,194	0
11	NDG	B	5071	14/15	0.88	0.34	-	160,162,163,163	0
10	BMA	A	4243	11/12	0.66	0.23	-	186,187,187,187	0
9	NAG	A	4132	14/15	0.90	0.22	-	159,162,167,172	0
7	NAG	A	2751	14/15	0.91	0.27	-	167,172,176,180	0
6	NDG	B	3982	14/15	0.86	0.24	-	172,175,177,177	0
8	NAG	A	2911	14/15	0.78	0.20	-	172,176,178,178	0
6	NAG	B	3981	14/15	0.94	0.14	-	163,167,168,171	0
14	MAN	B	4134	11/12	0.76	0.28	-	188,189,190,190	0
10	NDG	A	4241	14/15	0.87	0.17	-	169,173,174,176	0
10	NDG	A	4242	14/15	0.82	0.44	-	180,182,184,186	0
13	NAG	B	2911	14/15	0.85	0.24	-	169,171,173,176	0
6	NAG	A	3981	14/15	0.93	0.22	-	168,171,176,180	0
7	MAN	A	2753	11/12	0.88	0.15	-	192,195,196,197	0
7	NAG	A	2752	14/15	0.93	0.26	-	183,185,188,191	0
14	MAN	B	4135	11/12	0.65	0.32	-	185,187,187,188	0
14	MAN	B	4133	11/12	0.61	0.29	-	180,182,186,187	0

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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	NDG	A	724	14/15	0.77	0.26	1.15	196,197,197,197	0
5	NAG	B	724	14/15	0.78	0.31	-0.05	189,190,190,190	0
5	NAG	B	1961	14/15	0.85	0.20	-	181,183,184,184	0
5	NAG	A	1961	14/15	0.68	0.30	-	182,186,187,187	0

6.5 Other polymers

There are no such residues in this entry.