



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:46 PM GMT

PDB ID : 2GD4  
Title : Crystal Structure of the Antithrombin-S195A Factor Xa-Pentasaccharide Complex  
Authors : Johnson, D.J.; Li, W.; Adams, T.E.; Huntington, J.A.  
Deposited on : 2006-03-15  
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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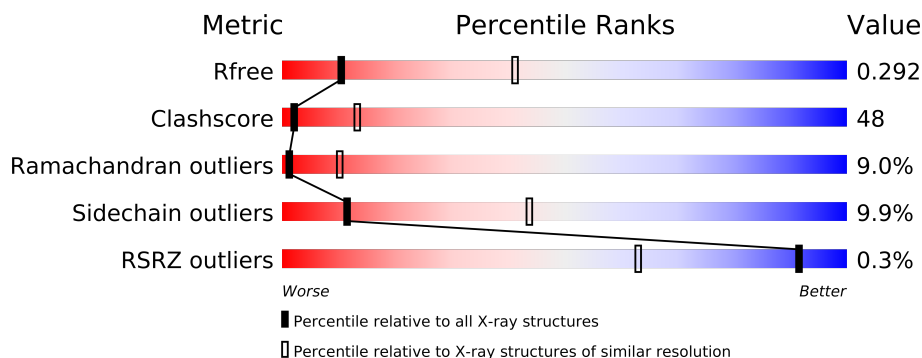
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	58	
1	L	58	
2	B	241	
2	H	241	
3	C	443	
3	I	443	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11165 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 Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	54	Total	C	N	O	S	0	0	0
			366	219	67	73	7			
1	A	52	Total	C	N	O	S	6	0	0
			349	209	62	71	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	85	MET	-	CLONING ARTIFACT	UNP P00742
A	85	MET	-	CLONING ARTIFACT	UNP P00742

- Molecule 2 is a protein called Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	234	Total	C	N	O	S	0	0	0
			1811	1143	312	342	14			
2	B	239	Total	C	N	O	S	3	0	0
			1840	1162	319	345	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	ALA	SER	ENGINEERED	UNP P00742
B	104	ALA	SER	ENGINEERED	UNP P00742

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	417	Total	C	N	O	S	14	0	0
			3197	2045	537	599	16			

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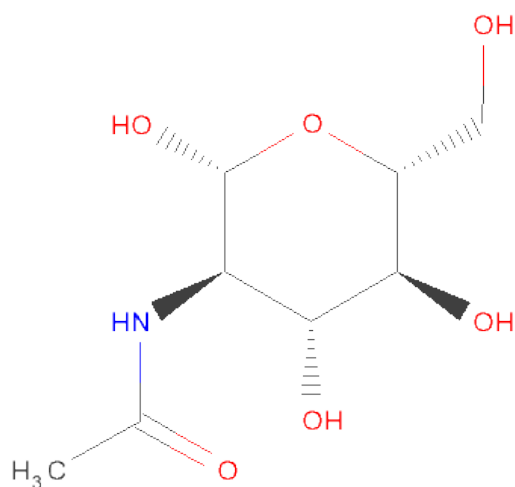
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	418	Total	C	N	O	S	20	0	0
			3200	2048	538	597	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008
I	347	ALA	GLU	ENGINEERED	UNP P01008
I	348	ALA	LYS	ENGINEERED	UNP P01008
I	350	ALA	LYS	ENGINEERED	UNP P01008
C	137	ALA	SER	ENGINEERED	UNP P01008
C	347	ALA	GLU	ENGINEERED	UNP P01008
C	348	ALA	LYS	ENGINEERED	UNP P01008
C	350	ALA	LYS	ENGINEERED	UNP P01008

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



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

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	6	Total	C	N	O	0	0
			71	40	2	29		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008
I	347	ALA	GLU	ENGINEERED	UNP P01008
I	348	ALA	LYS	ENGINEERED	UNP P01008
I	350	ALA	LYS	ENGINEERED	UNP P01008

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

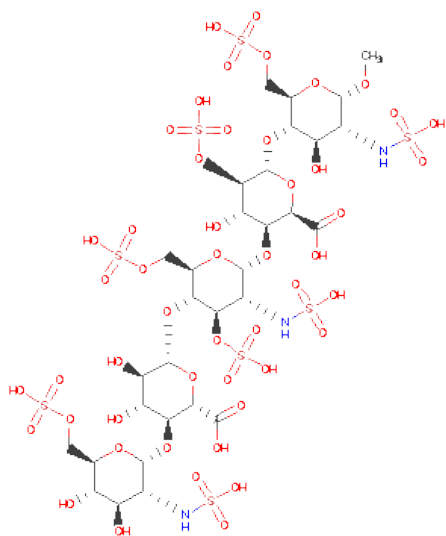
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	ALA	SER	ENGINEERED	UNP P01008
C	347	ALA	GLU	ENGINEERED	UNP P01008
C	348	ALA	LYS	ENGINEERED	UNP P01008
C	350	ALA	LYS	ENGINEERED	UNP P01008

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TRISULFOAMINO HEPARIN PENTASACCHARIDE (three-letter code: NTO) (formula: C<sub>31</sub>H<sub>53</sub>N<sub>3</sub>O<sub>49</sub>S<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	I	1	Total	C	N	O	S	0	0
			91	31	3	49	8		
8	C	1	Total	C	N	O	S	0	0
			91	31	3	49	8		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	O	0	0
			2	2		
9	B	9	Total	O	0	0
			9	9		
9	C	17	Total	O	0	0
			17	17		
9	H	10	Total	O	0	0
			10	10		
9	I	22	Total	O	0	0
			22	22		
9	L	3	Total	O	0	0
			3	3		

### 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: Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain L: 



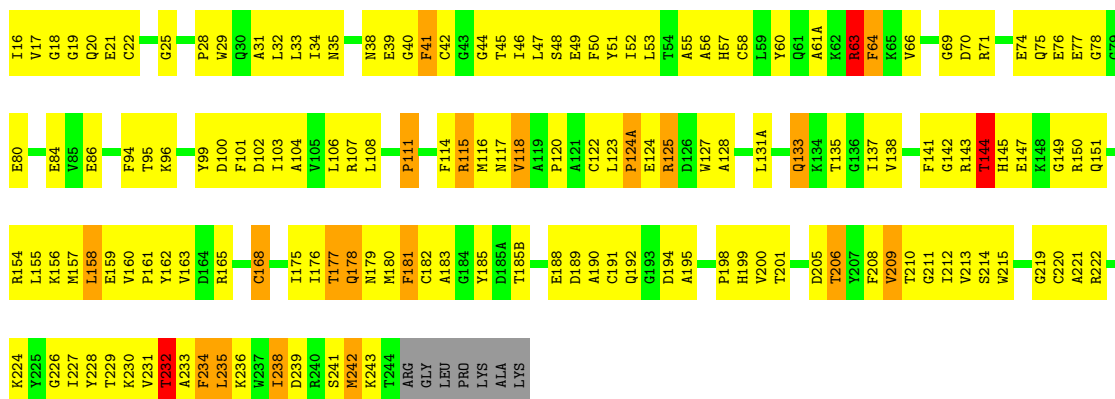
- Molecule 1: Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain A: 



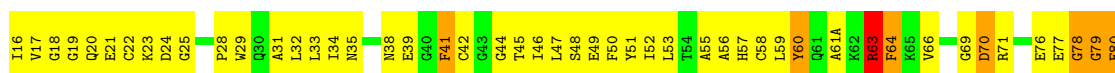
- Molecule 2: Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

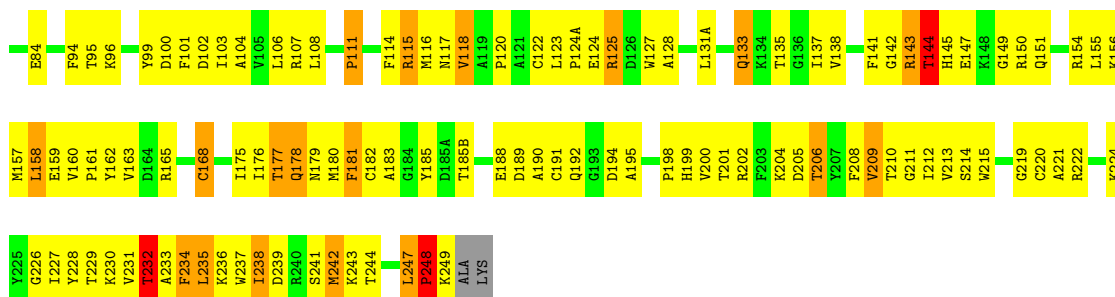
Chain H: 



- Molecule 2: Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

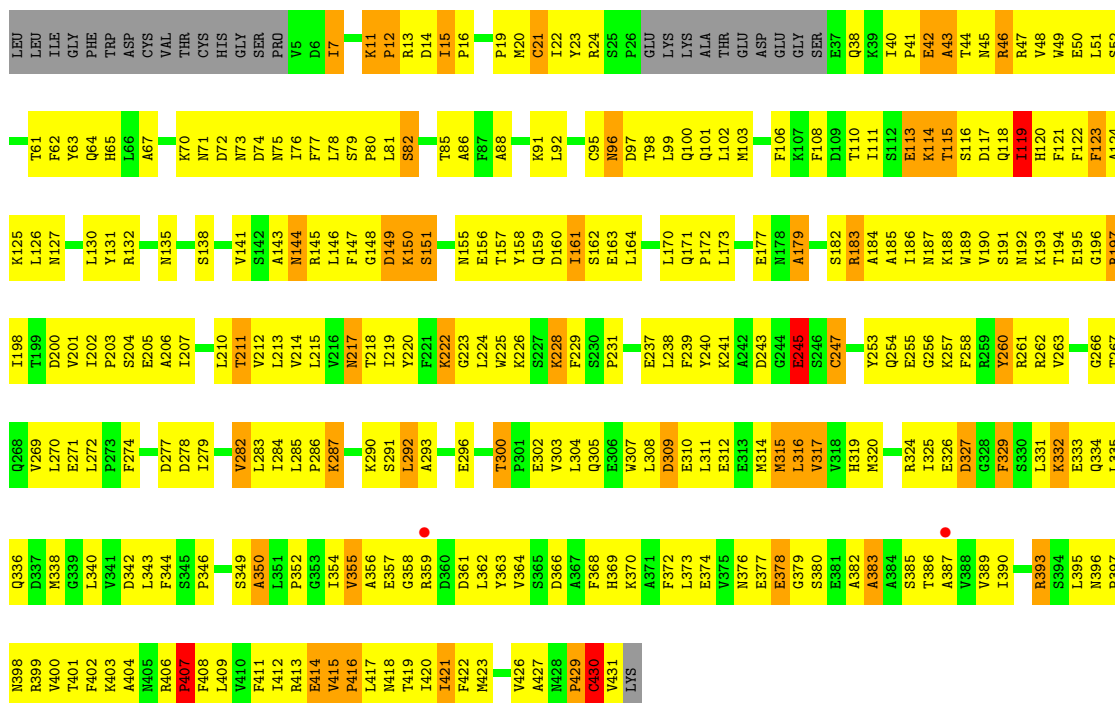
Chain B: 





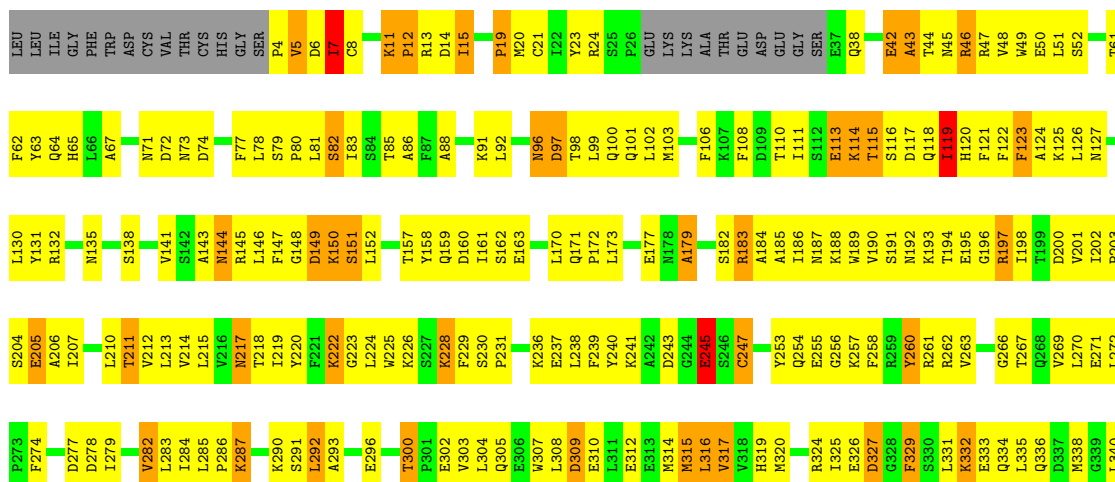
### • Molecule 3: Antithrombin-III

Chain I:

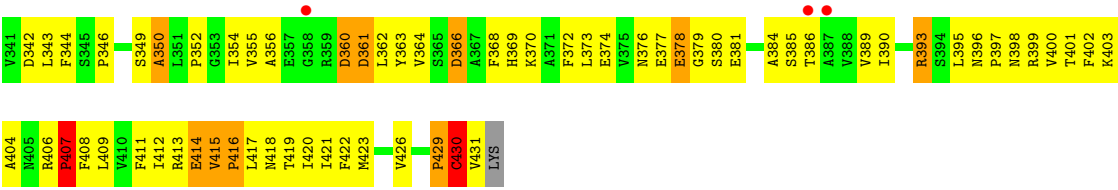


### • Molecule 3: Antithrombin-III

Chain C:







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.26Å 60.59Å 156.17Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	36.90 – 3.30 36.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (36.90-3.30) 93.7 (36.92-3.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.247 , 0.298 0.248 , 0.292	Depositor DCC
$R_{free}$ test set	1202 reflections (4.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 29814 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	11165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: CA, BMA, NAG, NTO, 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	0.31	0/355	0.61	0/484
1	L	0.31	0/372	0.65	0/506
2	B	0.50	0/1879	0.78	1/2541 (0.0%)
2	H	0.50	0/1849	0.76	1/2500 (0.0%)
3	C	0.43	0/3267	0.72	0/4440
3	I	0.44	0/3263	0.71	0/4435
All	All	0.45	0/10985	0.73	2/14906 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	168	CYS	CA-CB-SG	5.41	123.75	114.00
2	B	168	CYS	CA-CB-SG	5.26	123.47	114.00

There are no chirality outliers.

There are no planarity outliers.

### 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	349	0	279	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	366	0	296	31	0
2	B	1840	0	1752	183	0
2	H	1811	0	1727	176	0
3	C	3200	0	3073	317	0
3	I	3197	0	3072	323	0
4	C	28	0	26	1	0
4	I	28	0	26	1	0
5	I	71	0	59	9	0
6	C	28	0	25	8	0
7	B	1	0	0	0	0
7	H	1	0	0	0	0
8	C	91	0	51	3	0
8	I	91	0	51	3	0
9	A	2	0	0	1	0
9	B	9	0	0	0	0
9	C	17	0	0	2	0
9	H	10	0	0	1	0
9	I	22	0	0	0	0
9	L	3	0	0	0	0
All	All	11165	0	10437	1035	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 48.

All (1035) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:I:601:NAG:H61	5:I:602:NAG:N2	1.59	1.17
2:B:235:LEU:H	2:B:235:LEU:HD22	1.03	1.14
6:C:601:NAG:H61	6:C:602:NAG:N2	1.59	1.13
2:H:235:LEU:HD22	2:H:235:LEU:H	1.02	1.12
2:B:237:TRP:HD1	2:B:248:PRO:HG2	1.19	1.05
6:C:601:NAG:C6	6:C:602:NAG:HN2	1.71	1.03
5:I:601:NAG:C6	5:I:602:NAG:HN2	1.70	1.03
5:I:603:BMA:H2	5:I:605:MAN:H5	1.42	1.01
3:I:144:ASN:HB3	3:I:217:ASN:HA	1.45	0.98
3:C:144:ASN:HB3	3:C:217:ASN:HA	1.46	0.96
3:C:340:LEU:HD21	3:C:343:LEU:HD23	1.49	0.95
3:I:340:LEU:HD21	3:I:343:LEU:HD23	1.48	0.95
1:A:130:TYR:HE1	2:B:115:ARG:HA	1.32	0.94
2:B:237:TRP:CD1	2:B:248:PRO:HG2	2.06	0.91
3:I:308:LEU:HD13	3:I:413:ARG:NH1	1.85	0.90
3:C:308:LEU:HD13	3:C:413:ARG:NH1	1.86	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:389:VAL:HG12	3:I:390:ILE:H	1.37	0.90
3:I:326:GLU:HB3	3:I:372:PHE:HD2	1.37	0.89
3:C:326:GLU:HB3	3:C:372:PHE:HD2	1.36	0.89
2:H:235:LEU:H	2:H:235:LEU:CD2	1.85	0.89
3:C:326:GLU:HB3	3:C:372:PHE:CD2	2.08	0.89
3:I:326:GLU:HB3	3:I:372:PHE:CD2	2.08	0.89
3:C:389:VAL:HG12	3:C:390:ILE:H	1.37	0.88
2:B:235:LEU:HD22	2:B:235:LEU:N	1.88	0.88
2:H:235:LEU:HD22	2:H:235:LEU:N	1.87	0.88
2:B:235:LEU:CD2	2:B:235:LEU:H	1.86	0.88
3:I:144:ASN:HD22	3:I:144:ASN:N	1.73	0.86
3:I:98:THR:HB	3:I:350:ALA:HB3	1.58	0.86
3:I:355:VAL:HG23	3:I:356:ALA:H	1.38	0.86
3:I:144:ASN:HD22	3:I:144:ASN:H	1.22	0.85
3:C:98:THR:HB	3:C:350:ALA:HB3	1.57	0.85
1:L:130:TYR:HE1	2:H:115:ARG:HA	1.39	0.85
3:I:224:LEU:CD1	3:I:379:GLY:HA2	2.07	0.84
2:B:70:ASP:HB2	2:B:80:GLU:HB3	1.59	0.84
3:C:144:ASN:HD22	3:C:144:ASN:N	1.74	0.84
3:C:224:LEU:CD1	3:C:379:GLY:HA2	2.08	0.84
3:C:144:ASN:HD22	3:C:144:ASN:H	1.23	0.83
1:L:134:LYS:HE2	2:H:206:THR:HG23	1.59	0.83
3:I:183:ARG:HH21	3:I:204:SER:HA	1.44	0.82
3:I:23:TYR:HE2	3:I:100:GLN:HG3	1.44	0.82
2:B:219:GLY:HA3	2:B:222:ARG:HE	1.46	0.81
5:I:603:BMA:H2	5:I:605:MAN:C5	2.12	0.80
3:C:183:ARG:HH21	3:C:204:SER:HA	1.44	0.80
2:H:219:GLY:HA3	2:H:222:ARG:HE	1.46	0.80
3:I:267:THR:HG23	3:I:286:PRO:HA	1.64	0.79
3:I:224:LEU:HD12	3:I:379:GLY:HA2	1.65	0.79
3:C:267:THR:HG23	3:C:286:PRO:HA	1.65	0.79
3:C:319:HIS:HB2	3:C:403:LYS:HA	1.65	0.79
3:I:183:ARG:NH2	3:I:204:SER:HA	1.98	0.78
3:C:183:ARG:NH2	3:C:204:SER:HA	1.98	0.78
2:B:38:ASN:O	2:B:39:GLU:HG2	1.83	0.78
3:C:20:MET:HB3	6:C:602:NAG:H5	1.66	0.77
2:H:38:ASN:O	2:H:39:GLU:HG2	1.83	0.77
3:C:218:THR:HG22	3:C:370:LYS:HB3	1.66	0.77
3:I:319:HIS:HB2	3:I:403:LYS:HA	1.65	0.77
3:C:332:LYS:HG2	3:C:366:ASP:OD1	1.85	0.77
3:C:50:GLU:HG2	3:C:111:ILE:HG22	1.66	0.77
3:I:50:GLU:HG2	3:I:111:ILE:HG22	1.66	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:TYR:CE1	2:B:115:ARG:HA	2.19	0.77
2:B:183:ALA:HB3	2:B:228:TYR:CE1	2.20	0.76
3:I:141:VAL:HG11	3:I:194:THR:HA	1.67	0.76
2:H:183:ALA:HB3	2:H:228:TYR:CE1	2.21	0.76
3:I:218:THR:HG22	3:I:370:LYS:HB3	1.67	0.76
3:C:224:LEU:HD12	3:C:379:GLY:HA2	1.65	0.76
3:C:141:VAL:HG11	3:C:194:THR:HA	1.68	0.75
2:H:232:THR:C	2:H:235:LEU:HD21	2.07	0.75
3:I:63:TYR:HE1	3:I:296:GLU:HG2	1.52	0.75
2:H:195:ALA:HA	2:H:213:VAL:HG12	1.68	0.75
1:A:115:TYR:CE1	1:A:131:PRO:HB2	2.22	0.74
1:A:130:TYR:HE1	2:B:115:ARG:CA	1.99	0.74
3:C:407:PRO:HB2	9:C:907:HOH:O	1.86	0.74
3:C:63:TYR:HE1	3:C:296:GLU:HG2	1.52	0.74
2:B:239:ASP:HA	2:B:242:MET:HB2	1.70	0.74
2:B:232:THR:C	2:B:235:LEU:HD21	2.07	0.74
3:I:326:GLU:CB	3:I:372:PHE:HD2	2.01	0.74
1:L:115:TYR:CE1	1:L:131:PRO:HB2	2.22	0.74
3:C:396:ASN:O	3:C:399:ARG:HG3	1.88	0.74
3:C:229:PHE:CE2	3:C:254:GLN:HG2	2.23	0.73
3:I:23:TYR:CE2	3:I:100:GLN:HG3	2.23	0.73
3:I:229:PHE:CE2	3:I:254:GLN:HG2	2.24	0.73
3:C:412:ILE:HB	3:C:422:PHE:HB2	1.70	0.73
2:B:195:ALA:HA	2:B:213:VAL:HG12	1.68	0.73
3:C:326:GLU:CB	3:C:372:PHE:HD2	2.00	0.73
2:H:19:GLY:HA3	2:H:158:LEU:HB2	1.71	0.73
3:I:12:PRO:HG3	3:I:121:PHE:CD2	2.24	0.73
2:B:124(A):PRO:HB2	2:B:128:ALA:HB2	1.70	0.73
3:C:285:LEU:HD22	3:C:404:ALA:HA	1.71	0.72
1:A:134:LYS:HE2	2:B:206:THR:HG23	1.69	0.72
2:B:78:GLY:O	2:B:80:GLU:N	2.22	0.72
2:H:239:ASP:HA	2:H:242:MET:HB2	1.70	0.72
3:I:49:TRP:HA	3:I:417:LEU:HD11	1.71	0.72
2:B:19:GLY:HA3	2:B:158:LEU:HB2	1.71	0.72
3:I:396:ASN:O	3:I:399:ARG:HG3	1.88	0.72
3:I:170:LEU:HD23	3:I:171:GLN:N	2.05	0.72
1:L:129:PRO:O	1:L:131:PRO:HD3	1.90	0.72
3:I:412:ILE:HB	3:I:422:PHE:HB2	1.71	0.72
3:C:49:TRP:HA	3:C:417:LEU:HD11	1.71	0.72
2:H:124(A):PRO:HB2	2:H:128:ALA:HB2	1.71	0.72
2:B:45:THR:HB	2:B:53:LEU:HB3	1.72	0.71
1:A:129:PRO:O	1:A:131:PRO:HD3	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:189:ASP:CG	2:H:190:ALA:H	1.94	0.71
3:I:285:LEU:HD22	3:I:404:ALA:HA	1.72	0.71
2:H:45:THR:HB	2:H:53:LEU:HB3	1.72	0.71
3:I:344:PHE:HD1	3:I:364:VAL:HB	1.55	0.71
3:I:308:LEU:HD13	3:I:413:ARG:HH11	1.55	0.71
2:B:189:ASP:CG	2:B:190:ALA:H	1.93	0.71
3:C:236:LYS:N	3:C:236:LYS:HD2	2.06	0.71
2:H:56:ALA:HB2	2:H:103:ILE:H	1.54	0.70
3:C:170:LEU:HD23	3:C:171:GLN:N	2.05	0.70
2:B:56:ALA:HB2	2:B:103:ILE:H	1.55	0.70
3:C:344:PHE:HD1	3:C:364:VAL:HB	1.55	0.70
2:B:209:VAL:HG22	2:B:231:VAL:HG21	1.73	0.70
3:I:271:GLU:OE2	3:I:413:ARG:NH2	2.24	0.70
3:C:308:LEU:HD13	3:C:413:ARG:HH11	1.55	0.70
3:I:207:ILE:HG23	3:I:211:THR:HG21	1.73	0.70
2:B:128:ALA:HA	2:B:131(A):LEU:HD23	1.73	0.69
2:H:161:PRO:HD3	2:H:185:TYR:CZ	2.27	0.69
2:B:150:ARG:HG2	3:C:253:TYR:CD1	2.28	0.69
3:I:144:ASN:CB	3:I:217:ASN:HA	2.21	0.69
3:C:271:GLU:OE2	3:C:413:ARG:NH2	2.26	0.69
3:C:207:ILE:HG23	3:C:211:THR:HG21	1.73	0.69
3:C:144:ASN:CB	3:C:217:ASN:HA	2.22	0.69
3:C:257:LYS:HA	3:C:314:MET:O	1.93	0.69
2:B:161:PRO:HD3	2:B:185:TYR:CZ	2.27	0.69
3:C:135:ASN:HA	3:C:138:SER:O	1.92	0.69
3:C:47:ARG:HD3	3:C:115:THR:HG23	1.75	0.69
2:H:209:VAL:HG22	2:H:231:VAL:HG21	1.73	0.68
2:H:150:ARG:HG2	3:I:253:TYR:CD1	2.28	0.68
3:C:415:VAL:HG12	3:C:416:PRO:CD	2.23	0.68
5:I:603:BMA:C2	5:I:605:MAN:H5	2.21	0.68
2:H:128:ALA:HA	2:H:131(A):LEU:HD23	1.74	0.68
2:B:28:PRO:HG2	2:B:29:TRP:CE3	2.28	0.68
3:I:135:ASN:HA	3:I:138:SER:O	1.93	0.68
3:I:415:VAL:HG12	3:I:416:PRO:CD	2.23	0.68
2:H:33:LEU:HD23	2:H:66:VAL:HG22	1.74	0.67
2:H:33:LEU:HD12	2:H:42:CYS:CB	2.25	0.67
3:C:148:GLY:O	3:C:172:PRO:HA	1.94	0.67
3:C:218:THR:CG2	3:C:370:LYS:HB3	2.25	0.67
3:C:429:PRO:HG2	3:C:430:CYS:H	1.60	0.67
2:B:32:LEU:HD22	2:B:141:PHE:CE2	2.30	0.67
3:I:47:ARG:HD3	3:I:115:THR:HG23	1.76	0.67
2:B:33:LEU:HD23	2:B:66:VAL:HG22	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:28:PRO:HG2	2:H:29:TRP:CE3	2.29	0.67
1:L:130:TYR:HE1	2:H:115:ARG:CA	2.07	0.67
3:I:257:LYS:HA	3:I:314:MET:O	1.94	0.67
2:H:234:PHE:H	2:H:235:LEU:HD22	1.59	0.67
3:I:389:VAL:HG12	3:I:390:ILE:N	2.09	0.67
2:B:33:LEU:HD12	2:B:42:CYS:CB	2.24	0.67
3:I:148:GLY:O	3:I:172:PRO:HA	1.94	0.67
3:I:102:LEU:HD21	3:I:343:LEU:HD22	1.77	0.67
3:C:327:ASP:O	3:C:370:LYS:HD2	1.95	0.67
3:I:144:ASN:ND2	3:I:144:ASN:N	2.41	0.67
3:I:340:LEU:HD21	3:I:343:LEU:CD2	2.23	0.67
2:H:32:LEU:HD22	2:H:141:PHE:CE2	2.30	0.67
3:C:81:LEU:HD21	3:C:127:ASN:OD1	1.95	0.66
2:B:50:PHE:HE1	2:B:111:PRO:HD3	1.60	0.66
3:I:218:THR:CG2	3:I:370:LYS:HB3	2.25	0.66
3:I:81:LEU:HD21	3:I:127:ASN:OD1	1.95	0.66
3:I:327:ASP:O	3:I:370:LYS:HD2	1.95	0.66
2:B:103:ILE:HG12	2:B:104:ALA:N	2.10	0.66
3:C:159:GLN:HE22	3:C:170:LEU:H	1.42	0.66
3:C:145:ARG:CZ	3:C:171:GLN:HB2	2.25	0.66
3:I:145:ARG:CZ	3:I:171:GLN:HB2	2.26	0.66
2:B:47:LEU:HD22	2:B:123:LEU:HD11	1.75	0.66
3:I:85:THR:O	3:I:88:ALA:HB3	1.96	0.66
3:I:159:GLN:HE22	3:I:170:LEU:H	1.42	0.66
2:B:94:PHE:HB2	2:B:101:PHE:O	1.94	0.66
2:H:47:LEU:HD22	2:H:123:LEU:HD11	1.76	0.66
2:H:94:PHE:HB2	2:H:101:PHE:O	1.96	0.66
3:I:429:PRO:HG2	3:I:430:CYS:H	1.60	0.65
2:B:234:PHE:H	2:B:235:LEU:HD22	1.60	0.65
3:I:304:LEU:HD21	3:I:420:ILE:HD11	1.78	0.65
3:I:379:GLY:O	3:I:380:SER:HB2	1.97	0.65
3:I:159:GLN:NE2	3:I:170:LEU:H	1.95	0.65
3:I:266:GLY:HA3	3:I:287:LYS:HE2	1.78	0.65
3:C:85:THR:O	3:C:88:ALA:HB3	1.96	0.65
3:C:102:LEU:HD21	3:C:343:LEU:HD22	1.78	0.65
3:I:414:GLU:OE1	3:I:417:LEU:N	2.30	0.65
2:H:214:SER:HG	2:H:215:TRP:HD1	1.44	0.65
3:C:266:GLY:HA3	3:C:287:LYS:HE2	1.77	0.65
3:I:222:LYS:NZ	3:I:374:GLU:HG2	2.12	0.65
3:C:340:LEU:HD21	3:C:343:LEU:CD2	2.24	0.65
3:C:159:GLN:NE2	3:C:170:LEU:H	1.95	0.65
3:C:12:PRO:HG3	3:C:121:PHE:CD2	2.32	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:56:ALA:N	2:B:102:ASP:OD1	2.29	0.64
3:C:415:VAL:HG12	3:C:416:PRO:N	2.11	0.64
2:H:103:ILE:HG12	2:H:104:ALA:N	2.11	0.64
3:I:344:PHE:CD1	3:I:364:VAL:HB	2.33	0.64
3:I:415:VAL:HG12	3:I:416:PRO:N	2.11	0.64
2:B:50:PHE:CE1	2:B:111:PRO:HD3	2.32	0.64
2:H:232:THR:O	2:H:235:LEU:HD21	1.98	0.64
3:C:304:LEU:HD21	3:C:420:ILE:HD11	1.79	0.64
3:C:23:TYR:HE2	3:C:100:GLN:HG3	1.63	0.64
3:C:77:PHE:O	3:C:78:LEU:HB3	1.98	0.64
2:B:232:THR:O	2:B:235:LEU:HD21	1.98	0.63
3:I:77:PHE:O	3:I:78:LEU:HB3	1.98	0.63
3:C:204:SER:O	3:C:205:GLU:HB3	1.99	0.63
3:C:332:LYS:HG3	3:C:333:GLU:N	2.13	0.63
2:B:122:CYS:HB2	2:B:208:PHE:CD1	2.33	0.63
3:C:344:PHE:CD1	3:C:364:VAL:HB	2.33	0.63
3:C:414:GLU:OE1	3:C:417:LEU:N	2.30	0.63
2:H:50:PHE:HE1	2:H:111:PRO:HD3	1.62	0.63
3:C:226:LYS:HD2	3:C:277:ASP:OD1	1.98	0.63
1:L:130:TYR:CE1	2:H:115:ARG:HA	2.28	0.63
3:I:47:ARG:HD2	3:I:122:PHE:CZ	2.34	0.63
2:H:56:ALA:N	2:H:102:ASP:OD1	2.30	0.63
2:B:33:LEU:HD12	2:B:42:CYS:HB3	1.81	0.63
3:I:204:SER:O	3:I:205:GLU:HB3	1.99	0.63
3:C:47:ARG:HD2	3:C:122:PHE:CZ	2.34	0.63
3:C:379:GLY:O	3:C:380:SER:HB2	1.99	0.63
2:B:158:LEU:HD21	2:B:160:VAL:HG13	1.81	0.63
3:I:226:LYS:HD2	3:I:277:ASP:OD1	1.99	0.63
3:I:305:GLN:HE21	3:I:309:ASP:CG	2.02	0.63
1:A:131:PRO:HG2	1:A:134:LYS:HG3	1.81	0.62
2:H:158:LEU:HD21	2:H:160:VAL:CG1	2.29	0.62
2:H:158:LEU:HD21	2:H:160:VAL:HG13	1.79	0.62
2:H:231:VAL:O	2:H:233:ALA:N	2.32	0.62
2:H:56:ALA:HB3	2:H:102:ASP:HA	1.81	0.62
1:L:129:PRO:HG2	1:L:130:TYR:H	1.65	0.62
2:B:77:GLU:HG2	2:B:77:GLU:O	1.98	0.62
2:H:122:CYS:HB2	2:H:208:PHE:CD1	2.34	0.62
2:B:56:ALA:HB3	2:B:102:ASP:HA	1.81	0.62
3:C:222:LYS:NZ	3:C:374:GLU:HG2	2.13	0.62
2:H:143:ARG:O	2:H:144:THR:HG23	1.99	0.62
3:I:115:THR:C	3:I:117:ASP:H	2.03	0.62
2:B:158:LEU:HD21	2:B:160:VAL:CG1	2.30	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:115:THR:C	3:C:117:ASP:H	2.03	0.62
3:I:141:VAL:CG1	3:I:194:THR:HA	2.30	0.62
2:H:50:PHE:CE1	2:H:111:PRO:HD3	2.33	0.62
2:B:143:ARG:O	2:B:144:THR:HG23	2.00	0.62
2:H:33:LEU:HD12	2:H:42:CYS:HB3	1.81	0.62
2:B:231:VAL:O	2:B:233:ALA:N	2.33	0.61
3:C:305:GLN:HE21	3:C:309:ASP:CG	2.02	0.61
3:I:406:ARG:HB2	3:I:407:PRO:HD2	1.83	0.61
3:I:414:GLU:OE1	3:I:416:PRO:HD2	2.01	0.61
2:H:201:THR:OG1	2:H:210:THR:HG21	2.00	0.61
3:C:144:ASN:ND2	3:C:144:ASN:N	2.42	0.61
3:I:163:GLU:HB3	3:I:164:LEU:HD12	1.82	0.61
3:C:300:THR:H	3:C:303:VAL:HG12	1.66	0.61
3:I:349:SER:O	3:I:350:ALA:HB2	2.00	0.61
3:C:243:ASP:OD1	3:C:245:GLU:HB2	2.01	0.61
3:I:240:TYR:CD2	3:I:240:TYR:N	2.67	0.61
2:B:201:THR:OG1	2:B:210:THR:HG21	2.00	0.61
1:A:129:PRO:HG2	1:A:130:TYR:H	1.64	0.61
1:L:97:ASP:HB2	1:L:123:ALA:HA	1.83	0.61
3:C:240:TYR:N	3:C:240:TYR:CD2	2.67	0.61
3:C:349:SER:O	3:C:350:ALA:HB2	1.99	0.61
3:C:141:VAL:CG1	3:C:194:THR:HA	2.31	0.61
3:C:414:GLU:OE1	3:C:416:PRO:HD2	2.00	0.61
1:A:97:ASP:HB2	1:A:123:ALA:HA	1.82	0.61
3:I:225:TRP:HB2	3:I:379:GLY:HA3	1.82	0.60
3:C:225:TRP:HB2	3:C:379:GLY:HA3	1.83	0.60
3:C:406:ARG:HB2	3:C:407:PRO:HD2	1.83	0.60
2:B:143:ARG:HD3	2:B:149:GLY:O	2.01	0.60
3:I:115:THR:O	3:I:117:ASP:N	2.35	0.60
3:I:270:LEU:HD21	3:I:272:LEU:HD21	1.84	0.60
1:L:131:PRO:HG2	1:L:134:LYS:HG3	1.81	0.60
3:I:282:VAL:HG13	3:I:411:PHE:HB2	1.84	0.60
3:I:287:LYS:HG3	3:I:290:LYS:HB2	1.83	0.60
2:H:143:ARG:HD3	2:H:149:GLY:O	2.01	0.60
3:I:243:ASP:OD1	3:I:245:GLU:HB2	2.01	0.60
3:C:269:VAL:HG11	3:C:307:TRP:O	2.02	0.60
2:H:212:ILE:HB	2:H:229:THR:HB	1.84	0.60
3:I:210:LEU:O	3:I:212:VAL:HG13	2.02	0.60
3:C:157:THR:O	3:C:160:ASP:N	2.35	0.60
3:I:222:LYS:HD3	3:I:374:GLU:CG	2.32	0.60
1:L:134:LYS:CE	2:H:206:THR:HG23	2.31	0.60
3:C:115:THR:O	3:C:117:ASP:N	2.35	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:287:LYS:HG3	3:C:290:LYS:HB2	1.83	0.60
2:B:138:VAL:HG11	2:B:228:TYR:CE2	2.36	0.59
2:B:212:ILE:HB	2:B:229:THR:HB	1.84	0.59
3:C:270:LEU:O	3:C:282:VAL:HA	2.02	0.59
3:C:270:LEU:HD21	3:C:272:LEU:HD21	1.84	0.59
3:C:389:VAL:HG12	3:C:390:ILE:N	2.14	0.59
2:H:35:ASN:OD1	2:H:38:ASN:N	2.35	0.59
2:H:78:GLY:C	2:H:80:GLU:H	2.05	0.59
3:C:258:PHE:HB2	3:C:316:LEU:HD11	1.84	0.59
3:C:282:VAL:HG13	3:C:411:PHE:HB2	1.83	0.59
3:I:77:PHE:CE2	3:I:373:LEU:HB2	2.37	0.59
5:I:601:NAG:O7	5:I:601:NAG:O3	2.18	0.59
2:H:138:VAL:HG11	2:H:228:TYR:CE2	2.37	0.59
3:C:182:SER:O	3:C:185:ALA:HB3	2.03	0.59
3:I:239:PHE:CD2	3:I:429:PRO:HG3	2.38	0.59
3:C:80:PRO:HD2	3:C:421:ILE:O	2.03	0.59
3:C:239:PHE:CE1	3:C:406:ARG:HA	2.38	0.59
3:I:300:THR:H	3:I:303:VAL:HG12	1.67	0.59
3:I:355:VAL:HG23	3:I:356:ALA:N	2.13	0.59
2:B:211:GLY:HA2	2:B:229:THR:O	2.03	0.59
3:I:270:LEU:O	3:I:282:VAL:HA	2.03	0.59
3:C:77:PHE:CE2	3:C:373:LEU:HB2	2.38	0.59
3:C:210:LEU:O	3:C:212:VAL:HG13	2.02	0.59
2:H:31:ALA:HB3	2:H:44:GLY:HA3	1.85	0.59
2:H:158:LEU:CD2	2:H:160:VAL:HG13	2.33	0.59
2:B:69:GLY:HA3	2:B:118:VAL:HG22	1.83	0.59
3:C:222:LYS:CE	3:C:374:GLU:HG2	2.33	0.58
3:C:222:LYS:HD3	3:C:374:GLU:CG	2.32	0.58
3:C:239:PHE:CD2	3:C:429:PRO:HG3	2.37	0.58
2:H:69:GLY:HA3	2:H:118:VAL:HG22	1.84	0.58
3:I:157:THR:O	3:I:160:ASP:N	2.35	0.58
3:I:269:VAL:HG11	3:I:307:TRP:O	2.02	0.58
3:I:98:THR:CB	3:I:350:ALA:HB3	2.31	0.58
2:B:35:ASN:OD1	2:B:38:ASN:N	2.36	0.58
2:H:18:GLY:HA3	2:H:188:GLU:OE2	2.03	0.58
2:B:189:ASP:CG	2:B:190:ALA:N	2.56	0.58
6:C:601:NAG:H61	6:C:602:NAG:HN2	0.74	0.58
3:I:96:ASN:O	3:I:98:THR:N	2.37	0.58
3:I:182:SER:O	3:I:185:ALA:HB3	2.03	0.58
3:I:80:PRO:HD2	3:I:421:ILE:O	2.04	0.58
3:I:12:PRO:HG3	3:I:121:PHE:CE2	2.37	0.58
3:I:164:LEU:HD12	3:I:164:LEU:H	1.67	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:222:LYS:CE	3:I:374:GLU:HG2	2.32	0.58
2:H:189:ASP:CG	2:H:190:ALA:N	2.57	0.58
2:B:19:GLY:CA	2:B:158:LEU:HB2	2.34	0.58
3:C:12:PRO:HG3	3:C:121:PHE:CE2	2.38	0.58
2:B:100:ASP:OD1	2:B:177:THR:HG21	2.05	0.57
2:B:128:ALA:HA	2:B:131(A):LEU:CD2	2.33	0.57
3:C:202:ILE:HD13	3:C:207:ILE:HD11	1.86	0.57
2:H:19:GLY:CA	2:H:158:LEU:HB2	2.34	0.57
2:H:128:ALA:HA	2:H:131(A):LEU:CD2	2.34	0.57
2:H:211:GLY:HA2	2:H:229:THR:O	2.04	0.57
3:C:23:TYR:CE2	3:C:100:GLN:HG3	2.39	0.57
3:I:258:PHE:HB2	3:I:316:LEU:HD11	1.85	0.57
3:C:98:THR:CB	3:C:350:ALA:HB3	2.31	0.57
3:I:239:PHE:CE1	3:I:406:ARG:HA	2.39	0.57
2:B:64:PHE:N	2:B:64:PHE:CD1	2.72	0.57
3:C:19:PRO:HA	6:C:602:NAG:O7	2.04	0.57
2:H:100:ASP:OD1	2:H:177:THR:HG21	2.04	0.57
2:B:195:ALA:HA	2:B:213:VAL:CG1	2.35	0.57
3:I:179:ALA:O	3:I:182:SER:N	2.37	0.57
3:I:267:THR:HG23	3:I:286:PRO:CA	2.32	0.57
2:B:34:ILE:HA	2:B:39:GLU:O	2.05	0.57
3:C:15:ILE:H	3:C:15:ILE:HD13	1.69	0.57
3:I:22:ILE:O	3:I:22:ILE:HD12	2.04	0.57
2:H:151:GLN:CD	3:I:399:ARG:HH12	2.07	0.57
2:H:44:GLY:O	2:H:198:PRO:HD3	2.05	0.57
2:B:76:GLU:HA	2:B:80:GLU:OE1	2.05	0.57
2:H:33:LEU:HD12	2:H:42:CYS:HB2	1.87	0.57
2:B:44:GLY:O	2:B:198:PRO:HD3	2.05	0.57
3:C:147:PHE:HB2	3:C:214:VAL:HG23	1.87	0.57
5:I:601:NAG:H61	5:I:602:NAG:HN2	0.74	0.56
3:C:71:ASN:HB3	3:C:74:ASP:OD2	2.05	0.56
3:I:220:TYR:CD1	3:I:372:PHE:HD1	2.23	0.56
3:I:24:ARG:CZ	3:I:113:GLU:OE1	2.52	0.56
2:B:158:LEU:CD2	2:B:160:VAL:HG13	2.34	0.56
2:B:18:GLY:HA3	2:B:188:GLU:OE2	2.04	0.56
2:H:125:ARG:O	2:H:128:ALA:HB3	2.05	0.56
3:I:202:ILE:HD13	3:I:207:ILE:HD11	1.86	0.56
3:I:164:LEU:N	3:I:164:LEU:HD12	2.20	0.56
2:H:77:GLU:N	2:H:77:GLU:OE1	2.39	0.56
2:B:31:ALA:HB3	2:B:44:GLY:HA3	1.86	0.56
2:B:133:GLN:O	2:B:162:TYR:HD2	1.89	0.56
3:I:382:ALA:O	3:I:383:ALA:C	2.43	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:219:ILE:HG22	3:I:220:TYR:N	2.21	0.56
3:C:332:LYS:HG3	3:C:333:GLU:H	1.70	0.56
3:I:7:ILE:HD13	3:I:7:ILE:N	2.20	0.56
2:H:103:ILE:HG13	2:H:212:ILE:CD1	2.35	0.56
3:C:267:THR:HG23	3:C:286:PRO:CA	2.33	0.56
2:B:125:ARG:O	2:B:128:ALA:HB3	2.05	0.56
2:H:195:ALA:HA	2:H:213:VAL:CG1	2.34	0.56
3:C:228:LYS:O	3:C:254:GLN:NE2	2.39	0.56
3:I:71:ASN:HB3	3:I:74:ASP:OD2	2.04	0.56
3:C:91:LYS:HG2	3:C:99:LEU:HD11	1.88	0.56
2:H:34:ILE:HA	2:H:39:GLU:O	2.05	0.56
2:B:22:CYS:SG	2:B:157:MET:HB3	2.46	0.56
2:H:64:PHE:N	2:H:64:PHE:CD1	2.73	0.56
2:B:33:LEU:HD12	2:B:42:CYS:HB2	1.87	0.56
2:H:158:LEU:CD1	2:H:188:GLU:HB3	2.36	0.56
3:I:207:ILE:HG23	3:I:211:THR:CG2	2.36	0.56
2:H:77:GLU:HG2	2:H:77:GLU:O	2.05	0.56
3:I:91:LYS:HG2	3:I:99:LEU:HD11	1.88	0.56
2:H:211:GLY:HA2	2:H:231:VAL:HG23	1.88	0.55
1:A:116:THR:HG23	1:A:127:THR:OG1	2.07	0.55
3:I:222:LYS:HD3	3:I:374:GLU:HG2	1.88	0.55
3:C:421:ILE:HG22	3:C:422:PHE:CD2	2.41	0.55
3:I:331:LEU:HD11	3:I:369:HIS:HB2	1.88	0.55
3:I:147:PHE:HB2	3:I:214:VAL:HG23	1.88	0.55
2:B:47:LEU:HD13	2:B:123:LEU:HD21	1.88	0.55
3:C:224:LEU:O	3:C:274:PHE:HA	2.07	0.55
3:I:213:LEU:HB3	3:I:363:TYR:O	2.07	0.55
2:B:158:LEU:CD1	2:B:188:GLU:HB3	2.36	0.55
2:B:16:ILE:HG22	2:B:17:VAL:N	2.22	0.55
2:B:103:ILE:HG13	2:B:212:ILE:CD1	2.36	0.55
3:C:222:LYS:HD3	3:C:374:GLU:HG2	1.89	0.55
3:I:421:ILE:HG22	3:I:422:PHE:CD2	2.41	0.55
3:C:213:LEU:HB3	3:C:363:TYR:O	2.06	0.55
1:L:116:THR:HG23	1:L:127:THR:OG1	2.07	0.55
2:B:84:GLU:O	2:B:108:LEU:HD23	2.07	0.55
3:C:77:PHE:CZ	3:C:373:LEU:HB2	2.42	0.55
2:H:133:GLN:O	2:H:162:TYR:HD2	1.89	0.55
3:C:331:LEU:HD11	3:C:369:HIS:HB2	1.89	0.55
2:H:181:PHE:CE2	2:H:228:TYR:HB2	2.42	0.55
3:I:327:ASP:O	3:I:370:LYS:HA	2.07	0.55
2:B:123:LEU:HD12	2:B:123:LEU:N	2.22	0.55
3:I:159:GLN:HE22	3:I:170:LEU:N	2.05	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:123:LEU:HD12	2:H:123:LEU:N	2.22	0.54
3:C:236:LYS:H	3:C:236:LYS:HD2	1.70	0.54
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.88	0.54
3:C:47:ARG:O	3:C:50:GLU:HB3	2.08	0.54
3:I:63:TYR:HB2	3:I:423:MET:SD	2.47	0.54
3:I:228:LYS:O	3:I:254:GLN:NE2	2.41	0.54
3:I:15:ILE:HD13	3:I:15:ILE:H	1.71	0.54
3:I:261:ARG:HD2	3:I:262:ARG:N	2.22	0.54
3:C:220:TYR:CD1	3:C:372:PHE:HD1	2.24	0.54
2:H:47:LEU:HD13	2:H:123:LEU:HD21	1.89	0.54
2:H:51:TYR:CE1	2:H:107:ARG:HG3	2.43	0.54
3:C:11:LYS:CE	3:C:11:LYS:H	2.19	0.54
3:I:340:LEU:CD2	3:I:343:LEU:HD23	2.32	0.54
3:C:327:ASP:O	3:C:370:LYS:HA	2.07	0.54
2:H:16:ILE:HG22	2:H:17:VAL:N	2.22	0.54
3:I:352:PRO:O	3:I:356:ALA:HB2	2.07	0.54
3:I:96:ASN:OD1	4:I:501:NAG:H61	2.08	0.54
3:C:179:ALA:O	3:C:182:SER:N	2.37	0.54
3:I:77:PHE:CZ	3:I:373:LEU:HB2	2.42	0.54
3:C:219:ILE:HG22	3:C:220:TYR:N	2.21	0.54
3:C:147:PHE:CZ	3:C:186:ILE:HG23	2.43	0.54
3:C:285:LEU:CD2	3:C:404:ALA:HA	2.36	0.54
3:C:63:TYR:HB2	3:C:423:MET:SD	2.47	0.54
2:B:51:TYR:HA	2:B:106:LEU:O	2.08	0.54
3:C:207:ILE:HG23	3:C:211:THR:CG2	2.37	0.54
3:C:261:ARG:HD2	3:C:262:ARG:N	2.22	0.54
2:B:181:PHE:CE2	2:B:228:TYR:HB2	2.42	0.54
2:B:46:ILE:HA	2:B:52:ILE:HD13	1.90	0.54
2:H:56:ALA:HB2	2:H:103:ILE:N	2.23	0.54
2:H:200:VAL:HG12	2:H:209:VAL:HA	1.89	0.54
3:I:147:PHE:CZ	3:I:186:ILE:HG23	2.43	0.54
3:C:4:PRO:O	3:C:5:VAL:HB	2.08	0.54
3:I:186:ILE:O	3:I:189:TRP:HB3	2.08	0.54
3:I:171:GLN:HG3	3:I:173:LEU:CD2	2.37	0.54
2:H:22:CYS:SG	2:H:157:MET:HB3	2.47	0.54
3:I:70:LYS:HD2	3:I:76:ILE:CD1	2.38	0.54
3:I:224:LEU:O	3:I:274:PHE:HA	2.07	0.53
3:C:205:GLU:HG2	3:C:205:GLU:O	2.07	0.53
2:H:51:TYR:HA	2:H:106:LEU:O	2.08	0.53
3:C:231:PRO:HA	3:C:377:GLU:OE2	2.08	0.53
2:H:84:GLU:O	2:H:108:LEU:HD23	2.08	0.53
3:C:260:TYR:CE2	3:C:400:VAL:HG11	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:64:GLN:O	3:I:67:ALA:HB3	2.08	0.53
3:C:96:ASN:OD1	4:C:501:NAG:H61	2.09	0.53
3:I:11:LYS:H	3:I:11:LYS:CE	2.21	0.53
3:I:77:PHE:HB2	3:I:325:ILE:HG21	1.91	0.53
3:C:186:ILE:O	3:C:189:TRP:HB3	2.08	0.53
3:I:285:LEU:CD2	3:I:404:ALA:HA	2.37	0.53
3:C:159:GLN:HE22	3:C:170:LEU:N	2.05	0.53
1:A:135:GLN:HB3	2:B:25:GLY:O	2.08	0.53
3:C:96:ASN:O	3:C:98:THR:N	2.42	0.53
2:B:151:GLN:OE1	3:C:399:ARG:NH1	2.32	0.53
3:I:304:LEU:CD2	3:I:420:ILE:HD11	2.39	0.53
2:H:55:ALA:HB3	2:H:58:CYS:SG	2.49	0.53
2:B:200:VAL:HG12	2:B:209:VAL:HA	1.90	0.53
2:B:209:VAL:CG2	2:B:231:VAL:HG21	2.38	0.53
3:I:47:ARG:O	3:I:50:GLU:HB3	2.08	0.53
3:I:260:TYR:CE2	3:I:400:VAL:HG11	2.44	0.53
3:C:414:GLU:O	3:C:418:ASN:HA	2.09	0.53
2:H:143:ARG:NH1	2:H:192:GLN:HB2	2.24	0.53
3:I:255:GLU:HG2	3:I:315:MET:CE	2.39	0.53
2:B:55:ALA:HB3	2:B:58:CYS:SG	2.48	0.53
1:A:131:PRO:HG2	1:A:134:LYS:CG	2.39	0.52
3:I:229:PHE:CZ	3:I:254:GLN:HG2	2.44	0.52
3:C:304:LEU:CD2	3:C:420:ILE:HD11	2.39	0.52
3:I:376:ASN:ND2	3:I:378:GLU:HG3	2.23	0.52
3:C:64:GLN:O	3:C:67:ALA:HB3	2.08	0.52
2:B:103:ILE:HG12	2:B:104:ALA:H	1.73	0.52
2:H:215:TRP:CE2	2:H:227:ILE:HG21	2.45	0.52
2:B:47:LEU:O	2:B:48:SER:HB3	2.08	0.52
3:I:231:PRO:HA	3:I:377:GLU:OE2	2.09	0.52
3:C:255:GLU:HG2	3:C:315:MET:CE	2.39	0.52
2:B:247:LEU:H	2:B:248:PRO:HD2	1.74	0.52
3:I:170:LEU:O	3:I:172:PRO:HD3	2.10	0.52
2:H:78:GLY:O	2:H:80:GLU:HG3	2.10	0.52
1:A:138:GLU:H	2:B:116:MET:HE3	1.74	0.52
2:B:215:TRP:CE2	2:B:227:ILE:HG21	2.45	0.52
3:C:229:PHE:CZ	3:C:254:GLN:HG2	2.44	0.52
2:B:57:HIS:CE1	2:B:195:ALA:HB1	2.45	0.52
2:H:231:VAL:C	2:H:233:ALA:H	2.13	0.52
3:C:77:PHE:HB2	3:C:325:ILE:HG21	1.91	0.52
1:A:138:GLU:H	2:B:116:MET:CE	2.23	0.52
2:B:143:ARG:NH1	2:B:192:GLN:HB2	2.24	0.52
3:C:51:LEU:HD11	3:C:119:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:180:MET:O	2:H:181:PHE:HB3	2.09	0.52
3:C:325:ILE:O	3:C:372:PHE:HA	2.11	0.52
3:I:267:THR:HA	3:I:286:PRO:HA	1.92	0.52
3:I:414:GLU:O	3:I:418:ASN:HA	2.09	0.52
3:C:376:ASN:ND2	3:C:378:GLU:HG3	2.24	0.52
6:C:601:NAG:O7	6:C:601:NAG:O3	2.18	0.51
2:H:57:HIS:CE1	2:H:195:ALA:HB1	2.45	0.51
2:H:199:HIS:HB3	2:H:211:GLY:O	2.10	0.51
1:L:131:PRO:HG2	1:L:134:LYS:CG	2.39	0.51
3:C:170:LEU:O	3:C:172:PRO:HD3	2.10	0.51
2:B:51:TYR:CE1	2:B:107:ARG:HG3	2.44	0.51
2:H:46:ILE:HA	2:H:52:ILE:HD13	1.91	0.51
3:I:51:LEU:HD11	3:I:119:ILE:HG13	1.92	0.51
3:C:415:VAL:HG12	3:C:416:PRO:HD3	1.91	0.51
3:I:316:LEU:HB3	3:I:400:VAL:HB	1.92	0.51
2:H:47:LEU:O	2:H:48:SER:HB3	2.10	0.51
3:I:317:VAL:HB	3:I:401:THR:HG23	1.92	0.51
2:H:209:VAL:CG2	2:H:231:VAL:HG21	2.38	0.51
3:C:99:LEU:O	3:C:100:GLN:C	2.49	0.51
3:I:148:GLY:N	3:I:170:LEU:HD21	2.26	0.51
2:H:188:GLU:O	2:H:189:ASP:HB2	2.11	0.51
2:B:188:GLU:O	2:B:189:ASP:HB2	2.11	0.51
2:B:180:MET:O	2:B:181:PHE:HB3	2.11	0.51
3:I:316:LEU:HA	3:I:400:VAL:O	2.11	0.51
3:C:317:VAL:HB	3:C:401:THR:HG23	1.92	0.51
2:H:241:SER:C	2:H:243:LYS:H	2.14	0.51
3:C:267:THR:HA	3:C:286:PRO:HA	1.92	0.51
3:I:415:VAL:HG12	3:I:416:PRO:HD3	1.91	0.51
3:C:15:ILE:HD13	3:C:15:ILE:O	2.11	0.51
2:B:231:VAL:C	2:B:233:ALA:H	2.13	0.50
3:C:305:GLN:HE21	3:C:309:ASP:CB	2.24	0.50
2:B:222:ARG:HB2	2:B:224:LYS:HG3	1.92	0.50
2:H:222:ARG:HB2	2:H:224:LYS:HG3	1.93	0.50
3:C:207:ILE:HG23	3:C:211:THR:CB	2.41	0.50
3:I:81:LEU:C	3:I:81:LEU:HD23	2.32	0.50
3:C:396:ASN:OD1	3:C:398:ASN:N	2.40	0.50
2:H:47:LEU:HG	2:H:53:LEU:HB2	1.93	0.50
3:C:148:GLY:N	3:C:170:LEU:HD21	2.26	0.50
2:B:181:PHE:HE2	2:B:211:GLY:HA3	1.75	0.50
2:B:199:HIS:HB3	2:B:211:GLY:O	2.11	0.50
3:I:346:PRO:HG3	3:I:363:TYR:CG	2.47	0.50
2:B:47:LEU:HG	2:B:53:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:284:ILE:HB	3:I:409:LEU:HB2	1.93	0.50
2:H:181:PHE:HE2	2:H:211:GLY:HA3	1.75	0.50
2:H:238:ILE:O	2:H:241:SER:N	2.44	0.50
2:B:248:PRO:O	2:B:249:LYS:CB	2.59	0.50
3:C:316:LEU:HA	3:C:400:VAL:O	2.11	0.50
3:I:183:ARG:C	3:I:185:ALA:H	2.15	0.50
2:H:151:GLN:OE1	3:I:399:ARG:NH1	2.31	0.50
3:I:207:ILE:HG23	3:I:211:THR:CB	2.41	0.50
3:I:336:GLN:HA	3:I:340:LEU:O	2.11	0.50
1:A:130:TYR:N	1:A:130:TYR:CD2	2.79	0.50
3:I:99:LEU:O	3:I:100:GLN:C	2.49	0.50
3:I:305:GLN:HE21	3:I:309:ASP:CB	2.24	0.50
3:I:70:LYS:HD2	3:I:76:ILE:HD12	1.94	0.50
2:H:191:CYS:O	2:H:194:ASP:HB2	2.12	0.50
3:C:183:ARG:C	3:C:185:ALA:H	2.15	0.50
3:C:346:PRO:HG3	3:C:363:TYR:CG	2.47	0.50
2:B:131(A):LEU:N	2:B:131(A):LEU:HD22	2.27	0.50
2:B:191:CYS:O	2:B:194:ASP:HB2	2.12	0.50
3:C:45:ASN:HB3	3:C:48:VAL:HG23	1.94	0.50
2:B:135:THR:HG22	2:B:161:PRO:HA	1.94	0.50
2:H:61(A):ALA:HA	3:I:397:PRO:CB	2.42	0.50
3:C:284:ILE:HB	3:C:409:LEU:HB2	1.93	0.50
3:I:12:PRO:HG3	3:I:121:PHE:CG	2.46	0.49
3:I:206:ALA:HB1	3:I:368:PHE:CZ	2.47	0.49
3:C:102:LEU:HD23	3:C:340:LEU:CD1	2.42	0.49
3:I:183:ARG:O	3:I:185:ALA:N	2.45	0.49
2:B:141:PHE:CE1	2:B:155:LEU:HB2	2.46	0.49
2:H:141:PHE:CE1	2:H:155:LEU:HB2	2.47	0.49
2:H:232:THR:CA	2:H:235:LEU:HD21	2.42	0.49
3:C:49:TRP:CA	3:C:417:LEU:HD11	2.42	0.49
2:H:131(A):LEU:N	2:H:131(A):LEU:HD22	2.26	0.49
2:B:163:VAL:HB	2:B:182:CYS:HB3	1.93	0.49
3:C:144:ASN:ND2	9:C:905:HOH:O	2.41	0.49
3:C:336:GLN:HA	3:C:340:LEU:O	2.12	0.49
3:I:325:ILE:O	3:I:372:PHE:HA	2.10	0.49
1:L:130:TYR:CD2	1:L:130:TYR:N	2.78	0.49
3:C:113:GLU:O	3:C:114:LYS:C	2.50	0.49
3:I:113:GLU:O	3:I:114:LYS:C	2.50	0.49
1:L:132:CYS:HA	2:H:120:PRO:HG2	1.94	0.49
3:I:238:LEU:HA	3:I:247:CYS:O	2.11	0.49
2:B:232:THR:CA	2:B:235:LEU:HD21	2.43	0.49
2:B:238:ILE:O	2:B:241:SER:N	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:241:SER:C	2:B:243:LYS:H	2.16	0.49
3:C:183:ARG:O	3:C:185:ALA:N	2.46	0.49
3:C:238:LEU:HA	3:C:247:CYS:O	2.12	0.49
3:C:81:LEU:HD23	3:C:81:LEU:C	2.32	0.49
3:I:108:PHE:O	3:I:111:ILE:HG12	2.13	0.49
3:C:408:PHE:CZ	3:C:426:VAL:HG21	2.48	0.49
3:C:324:ARG:O	3:C:325:ILE:HG13	2.13	0.49
8:C:902:NTO:O27	8:C:902:NTO:H1K	2.13	0.49
2:H:103:ILE:HG12	2:H:104:ALA:H	1.74	0.49
3:I:102:LEU:HD23	3:I:340:LEU:CD1	2.42	0.49
3:C:316:LEU:HB3	3:C:400:VAL:HB	1.93	0.49
3:I:79:SER:HB2	3:I:219:ILE:HD12	1.95	0.49
3:I:396:ASN:O	3:I:398:ASN:N	2.46	0.49
3:C:206:ALA:HB1	3:C:368:PHE:CZ	2.48	0.49
2:B:56:ALA:HB2	2:B:103:ILE:N	2.24	0.49
3:C:198:ILE:CD1	3:C:220:TYR:HB2	2.43	0.49
2:B:20:GLN:O	2:B:156:LYS:HA	2.13	0.49
1:L:135:GLN:HB3	2:H:25:GLY:O	2.13	0.49
3:C:108:PHE:O	3:C:111:ILE:HG12	2.13	0.48
3:I:7:ILE:CD1	3:I:7:ILE:H	2.26	0.48
1:A:115:TYR:HE1	1:A:131:PRO:HB2	1.74	0.48
3:C:42:GLU:O	3:C:43:ALA:C	2.51	0.48
1:L:115:TYR:HE1	1:L:131:PRO:HB2	1.74	0.48
3:I:171:GLN:HG3	3:I:173:LEU:HD21	1.95	0.48
3:I:61:THR:O	3:I:64:GLN:HB2	2.13	0.48
2:B:96:LYS:HG2	2:B:99:TYR:CE1	2.49	0.48
2:H:135:THR:HG22	2:H:161:PRO:HA	1.94	0.48
3:I:396:ASN:OD1	3:I:398:ASN:N	2.40	0.48
2:H:163:VAL:HB	2:H:182:CYS:HB3	1.93	0.48
3:I:327:ASP:HB3	3:I:329:PHE:HE1	1.79	0.48
2:H:158:LEU:HD11	2:H:188:GLU:HB3	1.94	0.48
3:C:46:ARG:CD	3:C:46:ARG:C	2.82	0.48
3:C:7:ILE:HD13	3:C:7:ILE:N	2.28	0.48
3:C:24:ARG:CZ	3:C:113:GLU:OE1	2.62	0.48
3:I:45:ASN:HB3	3:I:48:VAL:HG23	1.94	0.48
3:I:49:TRP:CA	3:I:417:LEU:HD11	2.42	0.48
2:B:178:GLN:H	2:B:178:GLN:NE2	2.11	0.48
2:H:215:TRP:C	3:I:393:ARG:HD3	2.34	0.48
3:C:100:GLN:O	3:C:103:MET:HB2	2.14	0.48
1:A:130:TYR:CE1	2:B:115:ARG:CA	2.88	0.48
3:I:190:VAL:HG21	3:I:201:VAL:HG11	1.95	0.48
3:I:198:ILE:CD1	3:I:220:TYR:HB2	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:408:PHE:CZ	3:I:426:VAL:HG21	2.48	0.48
3:C:327:ASP:HB3	3:C:329:PHE:HE1	1.79	0.48
2:B:177:THR:C	2:B:179:ASN:H	2.16	0.48
2:H:231:VAL:C	2:H:233:ALA:N	2.67	0.48
3:C:340:LEU:CD2	3:C:343:LEU:HD23	2.32	0.48
3:I:258:PHE:CE1	3:I:272:LEU:HD22	2.49	0.48
2:B:158:LEU:HD11	2:B:188:GLU:HB3	1.94	0.48
3:I:202:ILE:HG12	3:I:368:PHE:CD2	2.49	0.48
3:I:86:ALA:C	3:I:88:ALA:H	2.17	0.48
2:H:201:THR:CB	2:H:210:THR:HG21	2.43	0.48
3:C:61:THR:O	3:C:64:GLN:HB2	2.13	0.48
5:I:602:NAG:C7	5:I:602:NAG:O3	2.62	0.48
3:C:79:SER:HB3	3:C:82:SER:HB2	1.96	0.48
2:B:151:GLN:CD	3:C:399:ARG:HH12	2.14	0.48
3:C:71:ASN:O	3:C:73:ASN:N	2.47	0.48
3:I:42:GLU:O	3:I:43:ALA:C	2.51	0.48
3:I:92:LEU:HD13	3:I:120:HIS:CD2	2.49	0.47
3:I:91:LYS:HG2	3:I:99:LEU:CD1	2.44	0.47
3:C:79:SER:HB2	3:C:219:ILE:HD12	1.96	0.47
3:I:415:VAL:CG1	3:I:416:PRO:N	2.77	0.47
2:H:71:ARG:HG2	2:H:71:ARG:O	2.14	0.47
2:B:238:ILE:HG22	2:B:239:ASP:N	2.30	0.47
3:I:79:SER:HB3	3:I:82:SER:HB2	1.96	0.47
3:C:190:VAL:HG21	3:C:201:VAL:HG11	1.96	0.47
3:I:50:GLU:OE1	3:I:111:ILE:HA	2.13	0.47
3:I:157:THR:O	3:I:158:TYR:C	2.53	0.47
3:C:308:LEU:O	3:C:310:GLU:N	2.47	0.47
3:I:218:THR:HG22	3:I:370:LYS:CB	2.42	0.47
2:B:201:THR:CB	2:B:210:THR:HG21	2.44	0.47
3:C:238:LEU:HD23	3:C:247:CYS:O	2.15	0.47
2:H:178:GLN:H	2:H:178:GLN:NE2	2.12	0.47
2:B:195:ALA:HA	2:B:213:VAL:O	2.13	0.47
2:H:195:ALA:HA	2:H:213:VAL:O	2.14	0.47
3:C:91:LYS:HG2	3:C:99:LEU:CD1	2.44	0.47
2:B:61(A):ALA:HA	3:C:397:PRO:CB	2.43	0.47
3:I:193:LYS:C	3:I:195:GLU:H	2.17	0.47
2:B:231:VAL:C	2:B:233:ALA:N	2.68	0.47
2:B:234:PHE:C	2:B:236:LYS:N	2.67	0.47
2:B:231:VAL:HG12	2:B:235:LEU:CD1	2.45	0.47
3:C:92:LEU:HD13	3:C:120:HIS:CD2	2.49	0.47
3:C:157:THR:O	3:C:158:TYR:C	2.53	0.47
3:I:113:GLU:HB2	8:I:901:NTO:O5J	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:901:NTO:O27	8:I:901:NTO:H1K	2.13	0.47
2:H:51:TYR:HE1	2:H:107:ARG:HB2	1.79	0.47
2:H:20:GLN:O	2:H:156:LYS:HA	2.13	0.47
3:I:46:ARG:C	3:I:46:ARG:CD	2.82	0.47
3:I:385:SER:O	3:I:387:ALA:N	2.47	0.47
3:I:198:ILE:HG23	3:I:370:LYS:HG2	1.96	0.47
3:C:50:GLU:OE1	3:C:111:ILE:HA	2.14	0.47
2:B:133:GLN:HB2	2:B:133:GLN:HE21	1.60	0.47
2:H:96:LYS:HG2	2:H:99:TYR:CE1	2.49	0.47
3:C:86:ALA:C	3:C:88:ALA:H	2.17	0.47
3:C:11:LYS:H	3:C:11:LYS:HE2	1.78	0.47
3:I:238:LEU:HD23	3:I:247:CYS:O	2.15	0.47
2:H:232:THR:HA	2:H:235:LEU:HD21	1.96	0.47
3:I:79:SER:CB	3:I:219:ILE:HD12	2.45	0.47
3:C:329:PHE:CD1	3:C:329:PHE:N	2.82	0.47
3:C:396:ASN:O	3:C:398:ASN:N	2.47	0.47
2:B:29:TRP:HE3	2:B:120:PRO:O	1.98	0.47
2:H:116:MET:O	2:H:118:VAL:HG23	2.15	0.47
2:H:231:VAL:HG12	2:H:235:LEU:CD1	2.45	0.46
3:I:308:LEU:O	3:I:310:GLU:N	2.48	0.46
3:C:190:VAL:HG11	3:C:198:ILE:HG22	1.97	0.46
3:I:225:TRP:HA	3:I:225:TRP:CE3	2.50	0.46
3:C:225:TRP:HA	3:C:225:TRP:CE3	2.50	0.46
3:I:100:GLN:O	3:I:103:MET:HB2	2.14	0.46
3:I:324:ARG:O	3:I:325:ILE:HG13	2.14	0.46
3:C:159:GLN:CD	3:C:170:LEU:H	2.18	0.46
2:B:71:ARG:HG2	2:B:71:ARG:O	2.14	0.46
2:B:214:SER:OG	2:B:215:TRP:HD1	1.98	0.46
2:H:238:ILE:HG22	2:H:239:ASP:N	2.31	0.46
3:C:258:PHE:CE1	3:C:272:LEU:HD22	2.49	0.46
3:C:121:PHE:O	3:C:124:ALA:HB3	2.15	0.46
3:I:71:ASN:O	3:I:73:ASN:N	2.48	0.46
2:H:182:CYS:HA	2:H:226:GLY:O	2.15	0.46
3:C:130:LEU:HD11	3:C:419:THR:HG21	1.96	0.46
3:C:150:LYS:O	3:C:151:SER:C	2.54	0.46
3:I:20:MET:O	3:I:21:CYS:O	2.34	0.46
2:H:234:PHE:C	2:H:236:LYS:N	2.67	0.46
3:C:115:THR:C	3:C:117:ASP:N	2.68	0.46
3:I:121:PHE:O	3:I:124:ALA:HB3	2.15	0.46
3:I:159:GLN:CD	3:I:170:LEU:H	2.18	0.46
3:C:15:ILE:HD13	3:C:15:ILE:N	2.30	0.46
3:I:71:ASN:C	3:I:73:ASN:N	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:193:LYS:C	3:C:195:GLU:H	2.17	0.46
2:B:137:ILE:HG22	2:B:137:ILE:O	2.15	0.46
3:C:157:THR:HG21	6:C:601:NAG:H62	1.98	0.46
3:I:329:PHE:N	3:I:329:PHE:CD1	2.84	0.46
3:C:79:SER:CB	3:C:219:ILE:HD12	2.46	0.46
2:B:78:GLY:O	2:B:79:GLY:C	2.53	0.46
3:I:346:PRO:HG3	3:I:363:TYR:CD1	2.51	0.46
3:C:113:GLU:HB2	8:C:902:NTO:O5J	2.15	0.46
3:C:71:ASN:C	3:C:73:ASN:N	2.68	0.46
2:B:182:CYS:HA	2:B:226:GLY:O	2.16	0.46
3:C:334:GLN:O	3:C:335:LEU:C	2.54	0.46
2:H:211:GLY:CA	2:H:231:VAL:HG23	2.45	0.46
3:C:346:PRO:HG3	3:C:363:TYR:CD1	2.51	0.46
1:A:132:CYS:HA	2:B:120:PRO:HG2	1.98	0.46
1:A:115:TYR:HE2	9:A:27:HOH:O	1.99	0.46
3:C:82:SER:OG	3:C:219:ILE:HD11	2.16	0.46
2:B:99:TYR:CG	3:C:390:ILE:HG21	2.51	0.46
3:C:122:PHE:O	3:C:123:PHE:C	2.55	0.46
3:I:115:THR:C	3:I:117:ASP:N	2.67	0.46
2:H:177:THR:C	2:H:179:ASN:H	2.18	0.46
3:I:150:LYS:O	3:I:151:SER:C	2.55	0.46
3:C:278:ASP:O	3:C:279:ILE:HD13	2.16	0.46
3:I:130:LEU:HD11	3:I:419:THR:HG21	1.96	0.46
2:B:211:GLY:CA	2:B:231:VAL:HG23	2.45	0.46
2:B:180:MET:CE	2:B:215:TRP:HE1	2.29	0.46
2:B:232:THR:HA	2:B:235:LEU:HD21	1.97	0.46
3:C:102:LEU:HD23	3:C:340:LEU:HD11	1.98	0.46
3:C:198:ILE:HG23	3:C:370:LYS:HG2	1.97	0.46
2:H:161:PRO:HD3	2:H:185:TYR:CE1	2.51	0.46
2:H:29:TRP:HE3	2:H:120:PRO:O	1.97	0.46
3:C:71:ASN:C	3:C:73:ASN:H	2.19	0.46
2:B:183:ALA:HB3	2:B:228:TYR:HE1	1.76	0.46
1:A:134:LYS:CE	2:B:206:THR:HG23	2.42	0.46
3:I:349:SER:O	3:I:350:ALA:CB	2.64	0.46
2:H:52:ILE:HB	2:H:106:LEU:HB2	1.98	0.46
2:B:51:TYR:HE1	2:B:107:ARG:HB2	1.81	0.45
6:C:602:NAG:C7	6:C:602:NAG:O3	2.63	0.45
2:H:180:MET:CE	2:H:215:TRP:HE1	2.29	0.45
3:C:81:LEU:HD11	3:C:126:LEU:CD2	2.47	0.45
3:C:202:ILE:HG12	3:C:368:PHE:CD2	2.50	0.45
3:I:15:ILE:HD13	3:I:15:ILE:N	2.31	0.45
3:I:11:LYS:HE2	3:I:11:LYS:H	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:255:GLU:HG2	3:I:315:MET:HE1	1.97	0.45
3:I:157:THR:HG21	5:I:601:NAG:H62	1.98	0.45
3:C:220:TYR:OH	3:C:222:LYS:HE2	2.16	0.45
2:H:124:GLU:O	2:H:125:ARG:C	2.54	0.45
2:B:50:PHE:CE1	2:B:111:PRO:HB3	2.51	0.45
3:I:292:LEU:HD11	3:I:409:LEU:HG	1.98	0.45
3:C:146:LEU:HD11	3:C:215:LEU:CD1	2.47	0.45
2:H:145:HIS:O	2:H:147:GLU:C	2.54	0.45
2:B:215:TRP:HA	3:C:393:ARG:HD3	1.97	0.45
3:I:190:VAL:HG11	3:I:198:ILE:HG22	1.97	0.45
3:C:222:LYS:CD	3:C:374:GLU:HG2	2.46	0.45
3:I:334:GLN:O	3:I:335:LEU:C	2.53	0.45
2:B:145:HIS:O	2:B:147:GLU:C	2.54	0.45
3:I:222:LYS:CD	3:I:374:GLU:HG2	2.46	0.45
3:I:430:CYS:O	3:I:431:VAL:CB	2.65	0.45
3:C:293:ALA:O	3:C:296:GLU:N	2.49	0.45
3:C:44:THR:HG21	3:C:417:LEU:HD13	1.99	0.45
2:B:64:PHE:HD1	2:B:64:PHE:N	2.14	0.45
3:C:65:HIS:NE2	3:C:338:MET:HG2	2.31	0.45
3:I:102:LEU:HD23	3:I:340:LEU:HD11	1.99	0.45
3:I:293:ALA:O	3:I:296:GLU:N	2.50	0.45
3:I:71:ASN:C	3:I:73:ASN:H	2.20	0.45
3:I:15:ILE:O	3:I:15:ILE:HD13	2.15	0.45
3:C:6:ASP:O	3:C:8:CYS:N	2.50	0.45
3:I:81:LEU:HD11	3:I:126:LEU:CD2	2.46	0.45
2:H:175:ILE:HG12	2:H:176:ILE:H	1.82	0.45
3:C:270:LEU:HD23	3:C:283:LEU:HD12	1.98	0.45
3:I:430:CYS:O	3:I:431:VAL:HG23	2.17	0.45
3:C:430:CYS:O	3:C:431:VAL:CB	2.64	0.45
3:C:430:CYS:O	3:C:431:VAL:HG23	2.16	0.45
2:H:158:LEU:HD23	2:H:158:LEU:O	2.17	0.45
2:B:160:VAL:HA	2:B:161:PRO:HD3	1.81	0.45
2:B:161:PRO:HD3	2:B:185:TYR:CE1	2.51	0.45
3:I:220:TYR:OH	3:I:222:LYS:HE2	2.17	0.45
3:C:183:ARG:NH2	3:C:204:SER:CA	2.77	0.45
3:C:395:LEU:O	3:C:397:PRO:HD3	2.16	0.45
2:B:124:GLU:O	2:B:125:ARG:C	2.55	0.45
2:H:64:PHE:N	2:H:64:PHE:HD1	2.14	0.45
1:A:125:ILE:O	1:A:126:PRO:O	2.35	0.45
2:B:202:ARG:NH2	2:B:204:LYS:O	2.46	0.45
3:C:225:TRP:HA	3:C:225:TRP:HE3	1.82	0.45
3:I:256:GLY:C	3:I:315:MET:HE3	2.38	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:292:LEU:HD11	3:C:409:LEU:HG	1.98	0.45
3:I:65:HIS:NE2	3:I:338:MET:HG2	2.32	0.45
2:B:215:TRP:C	3:C:393:ARG:HD3	2.37	0.45
2:H:214:SER:OG	2:H:215:TRP:HD1	1.97	0.45
3:I:395:LEU:O	3:I:397:PRO:HD3	2.17	0.45
2:H:50:PHE:CE1	2:H:111:PRO:HB3	2.52	0.45
2:B:116:MET:O	2:B:118:VAL:HG23	2.16	0.45
3:C:255:GLU:HG2	3:C:315:MET:HE2	1.99	0.45
1:L:125:ILE:O	1:L:126:PRO:O	2.35	0.45
3:I:192:ASN:O	3:I:192:ASN:OD1	2.35	0.45
2:H:137:ILE:O	2:H:137:ILE:HG22	2.17	0.45
2:B:220:CYS:O	2:B:221:ALA:HB3	2.16	0.45
2:B:52:ILE:HB	2:B:106:LEU:HB2	1.98	0.44
3:I:291:SER:O	3:I:293:ALA:N	2.50	0.44
2:B:175:ILE:HG12	2:B:176:ILE:H	1.82	0.44
1:A:110:SER:O	1:A:111:CYS:SG	2.75	0.44
2:B:63:ARG:HG2	2:B:63:ARG:HH21	1.82	0.44
3:C:80:PRO:HG2	3:C:81:LEU:H	1.82	0.44
3:C:300:THR:OG1	3:C:302:GLU:HB2	2.16	0.44
2:B:247:LEU:N	2:B:248:PRO:HD2	2.32	0.44
3:I:212:VAL:HG23	3:I:213:LEU:N	2.33	0.44
3:C:145:ARG:NE	3:C:171:GLN:HB2	2.32	0.44
3:I:12:PRO:C	3:I:14:ASP:N	2.70	0.44
3:C:12:PRO:C	3:C:14:ASP:N	2.69	0.44
2:B:230:LYS:HG2	2:B:232:THR:HG23	2.00	0.44
3:I:204:SER:O	3:I:205:GLU:CB	2.64	0.44
3:C:143:ALA:HB2	3:C:194:THR:CG2	2.48	0.44
3:I:396:ASN:O	3:I:397:PRO:C	2.55	0.44
1:L:130:TYR:HD1	2:H:114:PHE:HB3	1.81	0.44
3:C:106:PHE:HB3	3:C:108:PHE:CZ	2.52	0.44
3:I:143:ALA:HB2	3:I:194:THR:CG2	2.47	0.44
3:I:145:ARG:NE	3:I:171:GLN:HB2	2.32	0.44
3:I:146:LEU:HD11	3:I:215:LEU:CD1	2.47	0.44
2:H:195:ALA:HB2	3:I:393:ARG:C	2.38	0.44
3:I:270:LEU:HD23	3:I:283:LEU:HD12	1.99	0.44
1:L:130:TYR:HD2	1:L:130:TYR:N	2.15	0.44
3:I:225:TRP:HA	3:I:225:TRP:HE3	1.83	0.44
3:I:122:PHE:O	3:I:125:LYS:N	2.51	0.44
3:C:291:SER:O	3:C:293:ALA:N	2.50	0.44
2:B:116:MET:O	2:B:117:ASN:HB2	2.17	0.44
3:C:376:ASN:HD21	3:C:378:GLU:HG3	1.83	0.44
3:I:278:ASP:O	3:I:279:ILE:HD13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:192:ASN:O	3:C:192:ASN:OD1	2.36	0.44
3:C:283:LEU:HD11	3:C:320:MET:CE	2.48	0.44
3:I:44:THR:HG21	3:I:417:LEU:HD13	1.99	0.44
3:C:12:PRO:HG3	3:C:121:PHE:CG	2.52	0.44
2:H:220:CYS:O	2:H:221:ALA:HB3	2.18	0.44
3:I:147:PHE:O	3:I:213:LEU:HD12	2.18	0.43
3:I:183:ARG:NH2	3:I:204:SER:CA	2.77	0.43
3:I:402:PHE:CE1	3:I:404:ALA:HB2	2.53	0.43
2:H:18:GLY:CA	2:H:188:GLU:OE2	2.66	0.43
2:B:127:TRP:CZ3	2:B:131(A):LEU:HD21	2.53	0.43
3:C:86:ALA:C	3:C:88:ALA:N	2.72	0.43
3:C:191:SER:C	3:C:193:LYS:H	2.21	0.43
1:A:130:TYR:HD1	2:B:114:PHE:HB3	1.83	0.43
3:I:82:SER:OG	3:I:219:ILE:HD11	2.17	0.43
3:C:187:ASN:O	3:C:188:LYS:C	2.57	0.43
3:C:212:VAL:HG23	3:C:213:LEU:N	2.33	0.43
3:C:131:TYR:CZ	3:C:135:ASN:ND2	2.87	0.43
1:A:138:GLU:CB	2:B:116:MET:HE1	2.48	0.43
3:I:7:ILE:CD1	3:I:7:ILE:N	2.80	0.43
3:I:191:SER:C	3:I:193:LYS:H	2.21	0.43
3:I:46:ARG:O	3:I:46:ARG:HD3	2.18	0.43
1:L:110:SER:O	1:L:111:CYS:SG	2.76	0.43
1:L:86:ARG:O	1:L:87:LYS:CB	2.66	0.43
2:B:239:ASP:C	2:B:239:ASP:OD2	2.57	0.43
3:C:77:PHE:CE1	3:C:373:LEU:HD22	2.53	0.43
3:I:355:VAL:CG2	3:I:356:ALA:H	2.21	0.43
3:C:349:SER:OG	3:C:350:ALA:N	2.51	0.43
3:C:127:ASN:O	3:C:131:TYR:N	2.51	0.43
3:I:80:PRO:HG2	3:I:81:LEU:H	1.83	0.43
3:I:187:ASN:O	3:I:188:LYS:C	2.57	0.43
1:L:95:ASP:O	1:L:122:LYS:HB3	2.18	0.43
2:B:195:ALA:HB2	3:C:393:ARG:C	2.38	0.43
3:I:283:LEU:HD11	3:I:320:MET:CE	2.49	0.43
3:C:48:VAL:HG21	8:C:902:NTO:O1A	2.18	0.43
3:I:106:PHE:HB3	3:I:108:PHE:CZ	2.53	0.43
3:I:122:PHE:O	3:I:123:PHE:C	2.54	0.43
3:I:131:TYR:CZ	3:I:135:ASN:ND2	2.86	0.43
3:C:396:ASN:O	3:C:397:PRO:C	2.55	0.43
2:B:158:LEU:HD23	2:B:158:LEU:O	2.19	0.43
2:H:127:TRP:CZ3	2:H:131(A):LEU:HD21	2.54	0.43
3:C:12:PRO:O	3:C:13:ARG:C	2.56	0.43
2:H:183:ALA:HB3	2:H:228:TYR:HE1	1.77	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:183:ARG:C	3:C:185:ALA:N	2.72	0.43
3:C:203:PRO:HG2	3:C:206:ALA:HB2	2.00	0.43
2:H:239:ASP:OD2	2:H:239:ASP:C	2.56	0.43
3:I:200:ASP:O	3:I:201:VAL:C	2.56	0.43
3:C:147:PHE:CE2	3:C:186:ILE:HG23	2.54	0.43
3:I:203:PRO:HG2	3:I:206:ALA:HB2	2.00	0.43
2:H:116:MET:O	2:H:117:ASN:HB2	2.18	0.43
3:I:7:ILE:H	3:I:7:ILE:HD13	1.81	0.43
2:H:63:ARG:HH21	2:H:63:ARG:HG2	1.82	0.43
3:I:271:GLU:HA	3:I:282:VAL:HA	2.01	0.43
3:C:204:SER:O	3:C:205:GLU:CB	2.63	0.43
2:B:122:CYS:HB2	2:B:208:PHE:HD1	1.81	0.43
3:C:121:PHE:CD2	3:C:121:PHE:C	2.91	0.43
2:H:77:GLU:OE1	2:H:80:GLU:OE1	2.36	0.43
3:I:300:THR:OG1	3:I:302:GLU:HB2	2.18	0.43
1:L:86:ARG:HG3	1:L:86:ARG:O	2.18	0.43
3:C:350:ALA:C	3:C:352:PRO:CD	2.87	0.43
3:C:183:ARG:O	3:C:186:ILE:N	2.47	0.43
3:I:376:ASN:HD21	3:I:378:GLU:HG3	1.83	0.43
3:I:260:TYR:HB2	3:I:316:LEU:HD21	2.00	0.43
3:C:349:SER:O	3:C:350:ALA:CB	2.64	0.43
3:I:183:ARG:C	3:I:185:ALA:N	2.71	0.43
3:I:75:ASN:OD1	3:I:427:ALA:N	2.50	0.43
1:A:130:TYR:N	1:A:130:TYR:HD2	2.16	0.43
3:I:350:ALA:C	3:I:352:PRO:CD	2.87	0.43
3:I:121:PHE:C	3:I:121:PHE:CD2	2.91	0.43
2:B:18:GLY:CA	2:B:188:GLU:OE2	2.67	0.43
2:B:16:ILE:CG2	2:B:17:VAL:N	2.81	0.43
2:H:74:GLU:C	2:H:75:GLN:HG3	2.38	0.43
1:A:95:ASP:O	1:A:122:LYS:HB3	2.18	0.43
3:C:260:TYR:HB2	3:C:316:LEU:HD21	2.00	0.42
3:I:430:CYS:O	3:I:431:VAL:HB	2.19	0.42
1:L:138:GLU:H	2:H:116:MET:CE	2.32	0.42
3:C:46:ARG:O	3:C:46:ARG:HD3	2.18	0.42
2:B:247:LEU:O	2:B:248:PRO:O	2.37	0.42
3:I:77:PHE:CE1	3:I:373:LEU:HD22	2.54	0.42
3:C:200:ASP:O	3:C:201:VAL:C	2.56	0.42
3:I:172:PRO:C	3:I:173:LEU:HD22	2.40	0.42
3:I:86:ALA:C	3:I:88:ALA:N	2.72	0.42
2:H:63:ARG:NH2	2:H:63:ARG:HG2	2.34	0.42
3:I:349:SER:OG	3:I:350:ALA:N	2.52	0.42
2:H:41:PHE:O	2:H:42:CYS:SG	2.77	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:127:ASN:O	3:I:131:TYR:N	2.53	0.42
3:I:47:ARG:CZ	3:I:114:LYS:HD3	2.49	0.42
3:C:47:ARG:CZ	3:C:114:LYS:HD3	2.50	0.42
3:C:81:LEU:HD11	3:C:126:LEU:HD21	2.00	0.42
3:I:22:ILE:HD13	3:I:24:ARG:CZ	2.50	0.42
2:H:160:VAL:HA	2:H:161:PRO:HD3	1.82	0.42
3:I:12:PRO:O	3:I:13:ARG:C	2.58	0.42
2:H:150:ARG:HA	3:I:253:TYR:CE1	2.55	0.42
3:C:92:LEU:HD23	3:C:158:TYR:CE1	2.54	0.42
3:I:326:GLU:HB3	3:I:372:PHE:CE2	2.51	0.42
3:C:147:PHE:O	3:C:213:LEU:HD12	2.19	0.42
3:C:430:CYS:O	3:C:431:VAL:HB	2.19	0.42
3:I:48:VAL:HG21	8:I:901:NTO:O1A	2.19	0.42
2:B:41:PHE:HB2	3:C:395:LEU:HB2	2.02	0.42
3:C:354:ILE:O	3:C:354:ILE:HG22	2.19	0.42
3:I:92:LEU:HD23	3:I:158:TYR:CE1	2.54	0.42
2:H:234:PHE:O	2:H:238:ILE:HG13	2.20	0.42
3:C:223:GLY:HA3	3:C:274:PHE:CE1	2.55	0.42
3:I:147:PHE:CE2	3:I:186:ILE:HG23	2.54	0.42
3:I:362:LEU:HD12	3:I:363:TYR:N	2.35	0.42
3:C:118:GLN:O	3:C:121:PHE:N	2.46	0.42
2:B:63:ARG:HG2	2:B:63:ARG:NH2	2.34	0.42
2:B:165:ARG:O	2:B:168:CYS:HB3	2.20	0.42
3:C:402:PHE:CE1	3:C:404:ALA:HB2	2.53	0.42
3:I:263:VAL:HG23	3:I:266:GLY:H	1.84	0.42
2:H:71:ARG:NH1	9:H:405:HOH:O	2.51	0.42
3:C:196:GLY:O	3:C:197:ARG:C	2.58	0.42
2:H:230:LYS:HG2	2:H:232:THR:HG23	2.01	0.42
3:I:147:PHE:O	3:I:213:LEU:HA	2.20	0.42
3:I:50:GLU:C	3:I:52:SER:N	2.73	0.42
3:I:155:ASN:OD1	3:I:156:GLU:N	2.53	0.42
3:I:285:LEU:HD11	3:I:406:ARG:CZ	2.49	0.42
2:H:165:ARG:O	2:H:168:CYS:HB3	2.20	0.42
3:I:101:GLN:HB3	3:I:340:LEU:HD12	2.02	0.42
3:I:354:ILE:O	3:I:354:ILE:HG22	2.19	0.42
3:C:96:ASN:O	3:C:97:ASP:C	2.58	0.42
2:H:16:ILE:CG2	2:H:17:VAL:N	2.82	0.42
3:C:230:SER:HA	3:C:231:PRO:HD3	1.87	0.42
3:C:122:PHE:O	3:C:125:LYS:N	2.52	0.41
3:C:101:GLN:O	3:C:103:MET:N	2.53	0.41
3:I:223:GLY:HA3	3:I:274:PHE:CE1	2.55	0.41
3:C:62:PHE:CD2	3:C:62:PHE:C	2.93	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:308:LEU:O	3:C:309:ASP:C	2.59	0.41
3:C:224:LEU:HD12	3:C:224:LEU:HA	1.90	0.41
3:C:285:LEU:HD11	3:C:406:ARG:CZ	2.50	0.41
3:I:81:LEU:HD11	3:I:126:LEU:HD21	2.00	0.41
2:H:29:TRP:CE3	2:H:120:PRO:O	2.73	0.41
1:L:97:ASP:CB	1:L:123:ALA:HA	2.49	0.41
3:I:196:GLY:O	3:I:197:ARG:C	2.58	0.41
3:I:346:PRO:HG3	3:I:363:TYR:CD2	2.56	0.41
3:C:332:LYS:CG	3:C:333:GLU:N	2.81	0.41
2:B:50:PHE:CZ	2:B:111:PRO:HB3	2.55	0.41
2:H:86:GLU:OE1	2:H:107:ARG:NH2	2.53	0.41
3:C:149:ASP:HA	3:C:173:LEU:O	2.21	0.41
2:B:234:PHE:O	2:B:238:ILE:HG13	2.21	0.41
3:I:101:GLN:O	3:I:103:MET:N	2.53	0.41
3:C:271:GLU:HA	3:C:282:VAL:HA	2.01	0.41
3:I:143:ALA:HB2	3:I:194:THR:HG22	2.03	0.41
2:B:159:GLU:O	2:B:160:VAL:HG13	2.20	0.41
2:H:28:PRO:HG2	2:H:29:TRP:CZ3	2.56	0.41
3:I:15:ILE:O	3:I:16:PRO:C	2.58	0.41
2:H:21:GLU:CD	2:H:154:ARG:HD3	2.41	0.41
3:C:360:ASP:O	3:C:361:ASP:CB	2.69	0.41
3:I:40:ILE:HA	3:I:41:PRO:HD3	1.81	0.41
2:B:51:TYR:HB2	2:B:242:MET:HE3	2.03	0.41
3:I:354:ILE:O	3:I:355:VAL:HG13	2.20	0.41
3:C:350:ALA:C	3:C:352:PRO:HD3	2.41	0.41
3:I:224:LEU:HD12	3:I:224:LEU:HA	1.88	0.41
3:C:286:PRO:O	3:C:406:ARG:NH2	2.54	0.41
3:I:80:PRO:HG2	3:I:81:LEU:N	2.36	0.41
2:B:124(A):PRO:HD3	2:B:208:PHE:HB3	2.03	0.41
2:H:61(A):ALA:HA	3:I:397:PRO:HB2	2.02	0.41
2:B:29:TRP:CE3	2:B:120:PRO:O	2.74	0.41
3:C:147:PHE:O	3:C:213:LEU:HA	2.20	0.41
2:B:41:PHE:O	2:B:42:CYS:SG	2.78	0.41
2:H:159:GLU:O	2:H:160:VAL:HG13	2.20	0.41
1:A:97:ASP:CB	1:A:123:ALA:HA	2.49	0.41
2:H:52:ILE:HD13	2:H:52:ILE:HA	1.85	0.41
1:A:117:LEU:HD11	1:A:121:GLY:O	2.21	0.41
2:B:46:ILE:HG12	2:B:52:ILE:HD11	2.03	0.41
2:H:56:ALA:HB2	2:H:103:ILE:O	2.20	0.41
3:C:82:SER:O	3:C:83:ILE:C	2.58	0.41
3:C:239:PHE:CE2	3:C:429:PRO:HG3	2.56	0.41
2:H:34:ILE:HG22	2:H:40:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:40:GLY:O	2:H:41:PHE:HB3	2.20	0.41
3:C:80:PRO:HG2	3:C:81:LEU:N	2.36	0.41
3:C:123:PHE:O	3:C:127:ASN:ND2	2.54	0.41
3:I:117:ASP:C	3:I:119:ILE:H	2.25	0.41
3:C:263:VAL:HG23	3:C:266:GLY:H	1.84	0.41
3:I:161:ILE:O	3:I:163:GLU:N	2.53	0.41
2:B:23:LYS:O	2:B:24:ASP:C	2.59	0.41
3:C:161:ILE:O	3:C:163:GLU:N	2.54	0.41
2:B:59:LEU:O	2:B:60:TYR:C	2.59	0.41
3:I:62:PHE:C	3:I:62:PHE:CD2	2.94	0.41
3:C:152:LEU:HD13	3:C:362:LEU:HD12	2.02	0.41
3:C:186:ILE:O	3:C:189:TRP:N	2.54	0.41
3:C:346:PRO:HG3	3:C:363:TYR:CD2	2.56	0.41
3:I:402:PHE:HE1	3:I:404:ALA:HB2	1.86	0.41
3:I:123:PHE:O	3:I:127:ASN:ND2	2.53	0.41
1:L:132:CYS:CA	2:H:120:PRO:HG2	2.51	0.41
2:H:50:PHE:CZ	2:H:111:PRO:HB3	2.55	0.41
2:H:78:GLY:C	2:H:80:GLU:N	2.72	0.41
2:H:76:GLU:HA	2:H:80:GLU:OE1	2.21	0.41
2:B:21:GLU:CD	2:B:154:ARG:HD3	2.42	0.41
1:A:115:TYR:OH	1:A:134:LYS:HE2	2.21	0.40
2:B:96:LYS:HA	2:B:99:TYR:CE1	2.56	0.40
3:I:183:ARG:O	3:I:186:ILE:N	2.47	0.40
3:I:186:ILE:O	3:I:189:TRP:N	2.54	0.40
3:C:332:LYS:O	3:C:333:GLU:C	2.59	0.40
3:C:50:GLU:C	3:C:52:SER:N	2.74	0.40
3:C:118:GLN:O	3:C:121:PHE:HB3	2.21	0.40
3:C:316:LEU:O	3:C:316:LEU:HD12	2.21	0.40
3:C:326:GLU:HB3	3:C:372:PHE:CE2	2.51	0.40
3:I:350:ALA:C	3:I:352:PRO:HD3	2.41	0.40
1:L:138:GLU:CB	2:H:116:MET:HE1	2.52	0.40
3:C:101:GLN:HB3	3:C:340:LEU:HD12	2.02	0.40
3:C:23:TYR:C	3:C:23:TYR:CD1	2.94	0.40
3:I:260:TYR:N	3:I:312:GLU:O	2.50	0.40
3:C:187:ASN:ND2	3:C:200:ASP:HA	2.36	0.40
3:I:149:ASP:HA	3:I:173:LEU:O	2.21	0.40
1:L:114:GLY:O	1:L:127:THR:HB	2.22	0.40
3:C:256:GLY:C	3:C:315:MET:HE3	2.41	0.40
1:L:99:PHE:HB2	1:L:110:SER:OG	2.21	0.40
3:I:332:LYS:O	3:I:333:GLU:C	2.60	0.40
1:A:89:CYS:SG	1:A:101:HIS:O	2.79	0.40
3:I:308:LEU:O	3:I:311:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:96:LYS:HA	2:H:99:TYR:CE1	2.57	0.40
2:B:177:THR:HB	2:B:180:MET:HG3	2.04	0.40
3:C:260:TYR:N	3:C:312:GLU:O	2.49	0.40
3:I:95:CYS:O	3:I:96:ASN:O	2.40	0.40
1:L:115:TYR:OH	1:L:134:LYS:HE2	2.21	0.40
3:I:286:PRO:O	3:I:406:ARG:NH2	2.54	0.40
3:C:402:PHE:HE1	3:C:404:ALA:HB2	1.87	0.40
2:B:35:ASN:O	2:B:38:ASN:N	2.50	0.40
3:I:118:GLN:O	3:I:121:PHE:HB3	2.22	0.40
3:C:4:PRO:O	3:C:5:VAL:CB	2.70	0.40
1:L:86:ARG:O	1:L:90:SER:CB	2.70	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	50/58 (86%)	36 (72%)	9 (18%)	5 (10%)	1	8
1	L	52/58 (90%)	37 (71%)	10 (19%)	5 (10%)	1	9
2	B	237/241 (98%)	174 (73%)	46 (19%)	17 (7%)	2	16
2	H	232/241 (96%)	174 (75%)	46 (20%)	12 (5%)	3	27
3	C	414/443 (94%)	290 (70%)	79 (19%)	45 (11%)	1	6
3	I	413/443 (93%)	294 (71%)	77 (19%)	42 (10%)	1	7
All	All	1398/1484 (94%)	1005 (72%)	267 (19%)	126 (9%)	1	10

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	87	LYS
1	L	102	GLU
1	L	126	PRO
2	H	125	ARG

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Mol	Chain	Res	Type
2	H	144	THR
3	I	21	CYS
3	I	42	GLU
3	I	96	ASN
3	I	97	ASP
3	I	113	GLU
3	I	116	SER
3	I	177	GLU
3	I	228	LYS
3	I	245	GLU
3	I	350	ALA
3	I	359	ARG
3	I	386	THR
3	I	430	CYS
1	A	102	GLU
1	A	126	PRO
2	B	79	GLY
2	B	125	ARG
2	B	144	THR
2	B	247	LEU
2	B	248	PRO
3	C	7	ILE
3	C	42	GLU
3	C	96	ASN
3	C	97	ASP
3	C	113	GLU
3	C	116	SER
3	C	177	GLU
3	C	228	LYS
3	C	245	GLU
3	C	350	ALA
3	C	355	VAL
3	C	361	ASP
3	C	385	SER
3	C	430	CYS
2	H	41	PHE
2	H	60	TYR
2	H	232	THR
2	H	242	MET
3	I	38	GLN
3	I	43	ALA
3	I	151	SER

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Mol	Chain	Res	Type
3	I	162	SER
3	I	179	ALA
3	I	197	ARG
3	I	241	LYS
3	I	309	ASP
3	I	355	VAL
3	I	358	GLY
3	I	383	ALA
2	B	41	PHE
2	B	60	TYR
2	B	78	GLY
2	B	232	THR
2	B	238	ILE
2	B	244	THR
3	C	5	VAL
3	C	21	CYS
3	C	38	GLN
3	C	43	ALA
3	C	151	SER
3	C	162	SER
3	C	197	ARG
3	C	241	LYS
3	C	309	ASP
3	C	356	ALA
3	C	386	THR
1	L	129	PRO
2	H	142	GLY
2	H	234	PHE
2	H	238	ILE
3	I	114	LYS
3	I	150	LYS
3	I	184	ALA
3	I	211	THR
3	I	357	GLU
3	I	407	PRO
3	I	429	PRO
1	A	88	LEU
1	A	129	PRO
2	B	142	GLY
2	B	234	PHE
2	B	242	MET
3	C	114	LYS

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Mol	Chain	Res	Type
3	C	150	LYS
3	C	179	ALA
3	C	184	ALA
3	C	211	THR
3	C	381	GLU
3	C	407	PRO
3	C	429	PRO
1	L	95	ASP
3	I	183	ARG
3	I	292	LEU
3	I	378	GLU
1	A	95	ASP
3	C	132	ARG
3	C	183	ARG
3	C	292	LEU
3	C	378	GLU
3	C	384	ALA
2	H	63	ARG
3	I	132	ARG
2	B	63	ARG
3	C	19	PRO
3	C	360	ASP
3	I	19	PRO
3	I	72	ASP
2	B	111	PRO
2	B	143	ARG
3	C	72	ASP
3	C	205	GLU
2	H	111	PRO
3	C	119	ILE
3	I	119	ILE
3	I	416	PRO
3	C	416	PRO
3	I	12	PRO
3	C	12	PRO
2	H	124(A)	PRO
3	I	161	ILE
3	I	421	ILE



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	33/50 (66%)	32 (97%)	1 (3%)	53	88
1	L	34/50 (68%)	32 (94%)	2 (6%)	28	73
2	B	189/203 (93%)	168 (89%)	21 (11%)	9	37
2	H	188/203 (93%)	169 (90%)	19 (10%)	11	42
3	C	331/389 (85%)	298 (90%)	33 (10%)	11	43
3	I	332/389 (85%)	298 (90%)	34 (10%)	11	42
All	All	1107/1284 (86%)	997 (90%)	110 (10%)	11	44

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	86	ARG
1	L	97	ASP
2	H	49	GLU
2	H	63	ARG
2	H	64	PHE
2	H	70	ASP
2	H	95	THR
2	H	115	ARG
2	H	118	VAL
2	H	133	GLN
2	H	144	THR
2	H	158	LEU
2	H	177	THR
2	H	178	GLN
2	H	181	PHE
2	H	185(B)	THR
2	H	205	ASP
2	H	206	THR
2	H	209	VAL
2	H	232	THR
2	H	235	LEU
3	I	7	ILE
3	I	11	LYS

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Mol	Chain	Res	Type
3	I	15	ILE
3	I	46	ARG
3	I	82	SER
3	I	110	THR
3	I	115	THR
3	I	119	ILE
3	I	123	PHE
3	I	144	ASN
3	I	149	ASP
3	I	217	ASN
3	I	222	LYS
3	I	237	GLU
3	I	245	GLU
3	I	247	CYS
3	I	260	TYR
3	I	282	VAL
3	I	287	LYS
3	I	300	THR
3	I	315	MET
3	I	316	LEU
3	I	317	VAL
3	I	327	ASP
3	I	329	PHE
3	I	332	LYS
3	I	342	ASP
3	I	361	ASP
3	I	366	ASP
3	I	393	ARG
3	I	407	PRO
3	I	414	GLU
3	I	415	VAL
3	I	430	CYS
1	A	97	ASP
2	B	49	GLU
2	B	63	ARG
2	B	64	PHE
2	B	70	ASP
2	B	80	GLU
2	B	95	THR
2	B	115	ARG
2	B	118	VAL
2	B	133	GLN

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Mol	Chain	Res	Type
2	B	144	THR
2	B	158	LEU
2	B	177	THR
2	B	178	GLN
2	B	181	PHE
2	B	185(B)	THR
2	B	205	ASP
2	B	206	THR
2	B	209	VAL
2	B	232	THR
2	B	235	LEU
2	B	248	PRO
3	C	7	ILE
3	C	11	LYS
3	C	15	ILE
3	C	46	ARG
3	C	82	SER
3	C	110	THR
3	C	115	THR
3	C	119	ILE
3	C	123	PHE
3	C	144	ASN
3	C	149	ASP
3	C	217	ASN
3	C	222	LYS
3	C	237	GLU
3	C	245	GLU
3	C	247	CYS
3	C	260	TYR
3	C	282	VAL
3	C	287	LYS
3	C	300	THR
3	C	315	MET
3	C	316	LEU
3	C	317	VAL
3	C	327	ASP
3	C	329	PHE
3	C	332	LYS
3	C	342	ASP
3	C	366	ASP
3	C	393	ARG
3	C	407	PRO

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Mol	Chain	Res	Type
3	C	414	GLU
3	C	415	VAL
3	C	430	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	133	GLN
2	H	178	GLN
3	I	18	ASN
3	I	144	ASN
3	I	305	GLN
3	I	319	HIS
3	I	336	GLN
2	B	133	GLN
2	B	178	GLN
3	C	18	ASN
3	C	73	ASN
3	C	144	ASN
3	C	305	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 ⓘ

8 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	C	601	3,6	12,14,15	0.49	0	15,19,21	0.69	0
6	NAG	C	602	6	12,14,15	0.46	0	15,19,21	0.69	0
5	NAG	I	601	3,5	12,14,15	0.48	0	15,19,21	0.70	0
5	NAG	I	602	5	12,14,15	0.49	0	15,19,21	0.69	0
5	BMA	I	603	5	10,11,12	0.50	0	11,15,17	0.40	0
5	MAN	I	604	5	10,11,12	0.46	0	11,15,17	0.35	0
5	MAN	I	605	5	10,11,12	0.47	0	11,15,17	0.20	0
5	MAN	I	606	5	9,10,12	1.12	1 (11%)	8,13,17	0.18	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
6	NAG	C	601	3,6	-	0/6/23/26	0/1/1/1
6	NAG	C	602	6	-	1/6/23/26	0/1/1/1
5	NAG	I	601	3,5	-	0/6/23/26	0/1/1/1
5	NAG	I	602	5	-	1/6/23/26	0/1/1/1
5	BMA	I	603	5	-	0/2/19/22	0/1/1/1
5	MAN	I	604	5	-	0/2/19/22	0/1/1/1
5	MAN	I	605	5	-	0/2/19/22	0/1/1/1
5	MAN	I	606	5	-	0/2/16/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	606	MAN	C1-C2	3.22	1.53	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	602	NAG	O7-C7-N2-C2
6	C	602	NAG	O7-C7-N2-C2

There are no ring outliers.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	C	501	3	12,14,15	0.68	0	15,19,21	1.33	2 (13%)
4	NAG	C	701	3	12,14,15	0.50	0	15,19,21	0.62	0
8	NTO	C	902	-	95,95,95	2.79	15 (15%)	147,150,150	1.54	28 (19%)
4	NAG	I	501	3	12,14,15	0.67	0	15,19,21	1.35	2 (13%)
4	NAG	I	701	3	12,14,15	0.51	0	15,19,21	0.62	0
8	NTO	I	901	-	95,95,95	2.78	15 (15%)	147,150,150	1.54	28 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	501	3	-	0/6/23/26	0/1/1/1
4	NAG	C	701	3	-	0/6/23/26	0/1/1/1
8	NTO	C	902	-	-	0/69/169/169	0/5/5/5
4	NAG	I	501	3	-	0/6/23/26	0/1/1/1
4	NAG	I	701	3	-	0/6/23/26	0/1/1/1
8	NTO	I	901	-	-	0/69/169/169	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	902	NTO	O3A-S3B	-10.68	1.43	1.60
8	I	901	NTO	O3A-S3B	-10.64	1.43	1.60
8	C	902	NTO	O4A-S4B	-10.60	1.43	1.60
8	I	901	NTO	O4A-S4B	-10.58	1.43	1.60
8	I	901	NTO	O1H-S1G	8.08	1.50	1.42
8	C	902	NTO	O1I-S1G	8.07	1.50	1.42
8	C	902	NTO	O5J-S5H	8.04	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	901	NTO	O5I-S5H	8.03	1.50	1.42
8	I	901	NTO	O3J-S3H	8.02	1.50	1.42
8	C	902	NTO	O1H-S1G	8.02	1.50	1.42
8	I	901	NTO	O5J-S5H	8.01	1.50	1.42
8	C	902	NTO	O3J-S3H	8.01	1.50	1.42
8	C	902	NTO	O3K-S3H	7.99	1.50	1.42
8	C	902	NTO	O5I-S5H	7.99	1.50	1.42
8	I	901	NTO	O1I-S1G	7.97	1.50	1.42
8	I	901	NTO	O3K-S3H	7.91	1.50	1.42
8	C	902	NTO	O54-S55	-4.12	1.43	1.57
8	C	902	NTO	O16-S17	-4.12	1.43	1.57
8	I	901	NTO	O54-S55	-4.09	1.43	1.57
8	I	901	NTO	O16-S17	-4.06	1.43	1.57
8	I	901	NTO	O34-S35	-4.02	1.43	1.57
8	C	902	NTO	O34-S35	-4.01	1.43	1.57
8	C	902	NTO	S3H-N3G	3.23	1.63	1.60
8	I	901	NTO	S3H-N3G	3.11	1.63	1.60
8	C	902	NTO	S5H-N5G	3.07	1.63	1.60
8	I	901	NTO	S5H-N5G	2.98	1.63	1.60
8	C	902	NTO	S1G-N1F	2.95	1.63	1.60
8	I	901	NTO	S1G-N1F	2.84	1.63	1.60
8	C	902	NTO	O5M-C5L	2.28	1.44	1.40
8	I	901	NTO	O5M-C5L	2.21	1.43	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	901	NTO	C39-O3A-S3B	-5.14	109.99	118.37
8	C	902	NTO	C39-O3A-S3B	-5.11	110.03	118.37
8	I	901	NTO	C1E-N1F-S1G	-4.63	107.73	120.83
8	C	902	NTO	C1E-N1F-S1G	-4.59	107.86	120.83
8	I	901	NTO	C5F-N5G-S5H	-3.71	110.33	120.83
8	C	902	NTO	O1J-S1G-O1I	-3.65	108.68	115.28
8	C	902	NTO	C5F-N5G-S5H	-3.65	110.50	120.83
8	C	902	NTO	O3K-S3H-O3J	-3.64	108.47	119.84
8	I	901	NTO	O3K-S3H-O3J	-3.60	108.61	119.84
8	I	901	NTO	O1J-S1G-O1I	-3.53	108.90	115.28
4	I	501	NAG	O5-C5-C4	3.50	115.10	110.65
4	C	501	NAG	O5-C5-C4	3.48	115.07	110.65
8	C	902	NTO	C49-O4A-S4B	-3.46	112.73	118.37
8	I	901	NTO	C49-O4A-S4B	-3.43	112.77	118.37
8	I	901	NTO	O5J-S5H-O5I	-3.37	109.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	902	NTO	O1I-S1G-O1H	-3.35	109.39	119.84
8	C	902	NTO	C33-O34-S35	3.33	121.04	116.76
8	I	901	NTO	C1K-O1L-C20	-3.33	109.50	117.99
8	C	902	NTO	O5J-S5H-O5I	-3.32	109.49	119.84
8	C	902	NTO	C1K-O1L-C20	-3.31	109.55	117.99
8	I	901	NTO	O1I-S1G-O1H	-3.30	109.56	119.84
8	C	902	NTO	C3F-N3G-S3H	-3.28	111.55	120.83
8	I	901	NTO	C5N-O5M-C5L	-3.28	108.34	113.33
8	I	901	NTO	C33-O34-S35	3.27	120.97	116.76
8	I	901	NTO	C3F-N3G-S3H	-3.25	111.65	120.83
8	I	901	NTO	O3I-S3H-O3K	-3.19	109.52	115.28
8	I	901	NTO	O1J-S1G-O1H	-3.18	109.53	115.28
8	C	902	NTO	O5K-S5H-O5J	-3.15	109.59	115.28
8	C	902	NTO	O3I-S3H-O3J	-3.15	109.59	115.28
8	C	902	NTO	C5N-O5M-C5L	-3.14	108.56	113.33
8	I	901	NTO	O3I-S3H-O3J	-3.13	109.63	115.28
8	C	902	NTO	O1J-S1G-O1H	-3.11	109.66	115.28
8	C	902	NTO	O5K-S5H-O5I	-3.08	109.71	115.28
8	I	901	NTO	O5K-S5H-O5I	-3.07	109.73	115.28
8	I	901	NTO	O5K-S5H-O5J	-3.07	109.74	115.28
8	C	902	NTO	O3I-S3H-O3K	-3.07	109.74	115.28
8	C	902	NTO	C4F-O4G-C50	-2.87	110.66	117.99
8	I	901	NTO	C4F-O4G-C50	-2.85	110.71	117.99
4	C	501	NAG	C4-C3-C2	-2.81	104.45	111.32
4	I	501	NAG	C4-C3-C2	-2.78	104.51	111.32
8	C	902	NTO	C20-C21-C23	-2.74	107.78	111.89
8	I	901	NTO	C15-C13-C12	-2.72	105.69	111.87
8	I	901	NTO	C20-C21-C23	-2.69	107.86	111.89
8	C	902	NTO	C15-C13-C12	-2.68	105.78	111.87
8	I	901	NTO	C40-C41-C43	-2.50	108.14	111.89
8	I	901	NTO	O34-C33-C31	2.41	112.39	107.81
8	C	902	NTO	O34-C33-C31	2.32	112.22	107.81
8	C	902	NTO	O5M-C5L-C5F	2.31	111.20	107.94
8	C	902	NTO	C40-C41-C43	-2.29	108.46	111.89
8	I	901	NTO	O5M-C5L-C5F	2.20	111.05	107.94
8	I	901	NTO	C33-C31-C30	-2.16	108.07	113.30
8	C	902	NTO	C2C-O2D-C30	-2.16	112.49	117.99
8	I	901	NTO	C15-O16-S17	2.11	119.47	116.76
8	C	902	NTO	C33-C31-C30	-2.11	108.19	113.30
8	I	901	NTO	C2C-O2D-C30	-2.11	112.62	117.99
8	C	902	NTO	O32-C31-C33	2.08	110.80	106.61
8	C	902	NTO	O4A-C49-C4F	2.08	110.46	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	902	NTO	C59-C50-C51	-2.03	106.30	110.85
8	I	901	NTO	C59-C50-C51	-2.02	106.33	110.85
8	I	901	NTO	O16-C15-C13	2.01	111.63	107.81

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9	
1	A	52/58 (89%)	0.31	0	100	100	29, 65, 82, 83	1 (1%)
1	L	54/58 (93%)	0.02	0	100	100	29, 65, 81, 83	0
2	B	239/241 (99%)	-0.26	0	100	100	1, 19, 45, 80	3 (1%)
2	H	234/241 (97%)	-0.29	0	100	100	1, 19, 38, 53	3 (1%)
3	C	418/443 (94%)	-0.08	3 (0%)	84	42	1, 41, 87, 99	6 (1%)
3	I	417/443 (94%)	-0.07	2 (0%)	88	51	1, 39, 85, 103	3 (0%)
All	All	1414/1484 (95%)	-0.12	5 (0%)	91	57	1, 31, 83, 103	16 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	387	ALA	2.7
3	C	387	ALA	2.5
3	I	359	ARG	2.4
3	C	358	GLY	2.2
3	C	386	THR	2.1

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	I	606	10/12	0.44	-	148,149,150,150	0
5	BMA	I	603	11/12	0.43	-	129,134,135,139	0
5	NAG	I	602	14/15	0.34	-	107,110,117,121	0
5	MAN	I	605	11/12	0.48	-	143,145,147,147	0
6	NAG	C	602	14/15	0.33	-	106,110,114,115	0
5	MAN	I	604	11/12	0.34	-	135,136,137,137	0
6	NAG	C	601	14/15	0.22	-	85,87,93,100	0
5	NAG	I	601	14/15	0.21	-	84,88,94,101	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	701	14/15	0.50	-	92,94,97,97	0
7	CA	B	401	1/1	0.07	-	12,12,12,12	0
8	NTO	I	901	91/91	0.17	-	27,44,59,65	0
4	NAG	I	701	14/15	0.53	-	92,94,97,97	0
8	NTO	C	902	91/91	0.17	-	28,45,59,66	0
7	CA	H	401	1/1	0.11	-	19,19,19,19	0
4	NAG	C	501	14/15	0.30	-	102,109,110,110	0
4	NAG	I	501	14/15	0.30	-	103,108,110,110	0

## 6.5 Other polymers

There are no such residues in this entry.