



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID : 2B4X  
Title : Crystal Structure of Antithrombin-III  
Authors : Adams, T.E.; Huntington, J.A.; Johnson, D.J.D.; Bock, S.C.  
Deposited on : 2005-09-27  
Resolution : 2.80 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

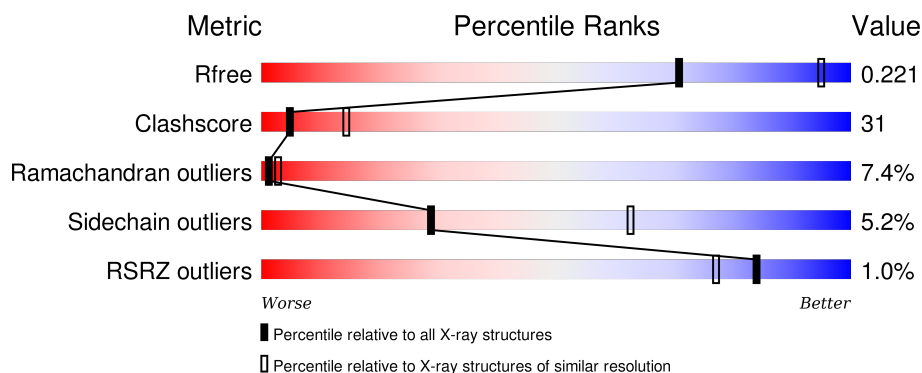
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	I	427	<div> <div></div> <div> <div></div> <div>46%</div> <div>44%</div> <div>5%</div> <div>.</div> </div> </div>
2	L	427	<div> <div></div> <div> <div></div> <div>47%</div> <div>42%</div> <div>7%</div> <div>.</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	I	861	-	-	X	-
4	NAG	I	841	X	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6560 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	413	3203	2044	528	615	16	0	0	0

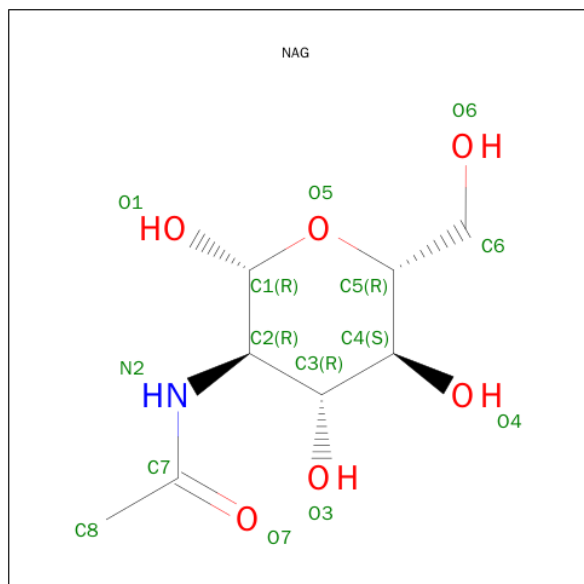
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	135	ALA	ASN	ENGINEERED	UNP P01008
I	220	LEU	TYR	ENGINEERED	UNP P01008

- Molecule 2 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	410	3078	1969	497	595	17	0	0	0

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



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			27	16	2	9		

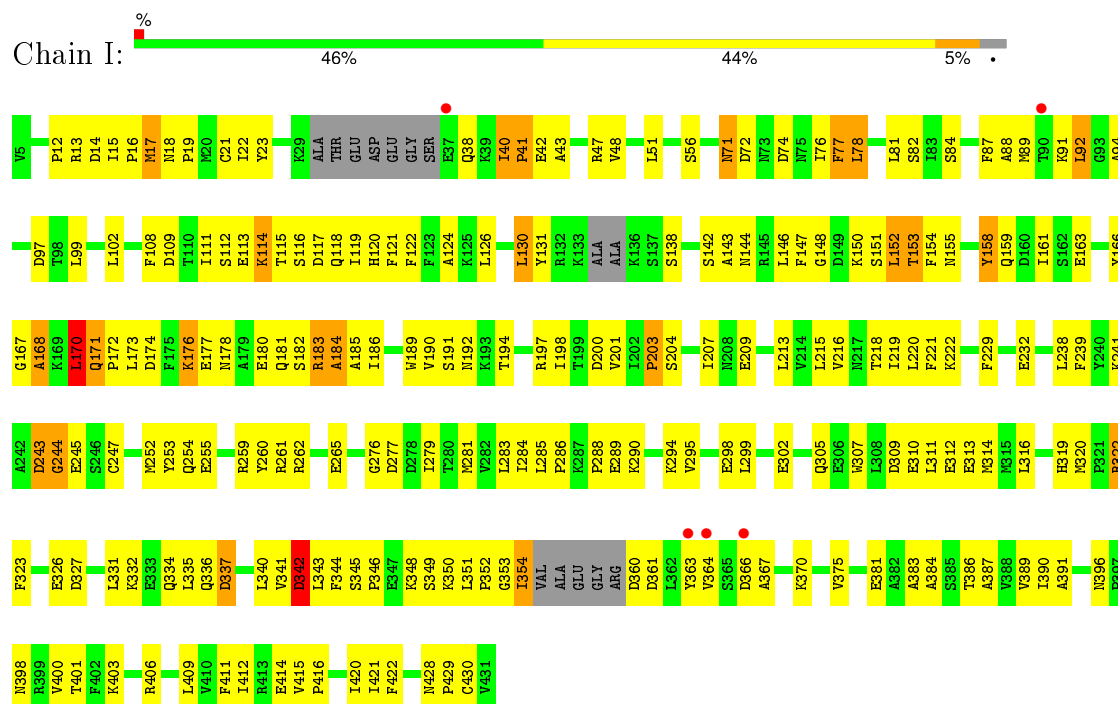
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	84	Total	O	0	0
			84	84		
5	L	56	Total	O	0	0
			56	56		

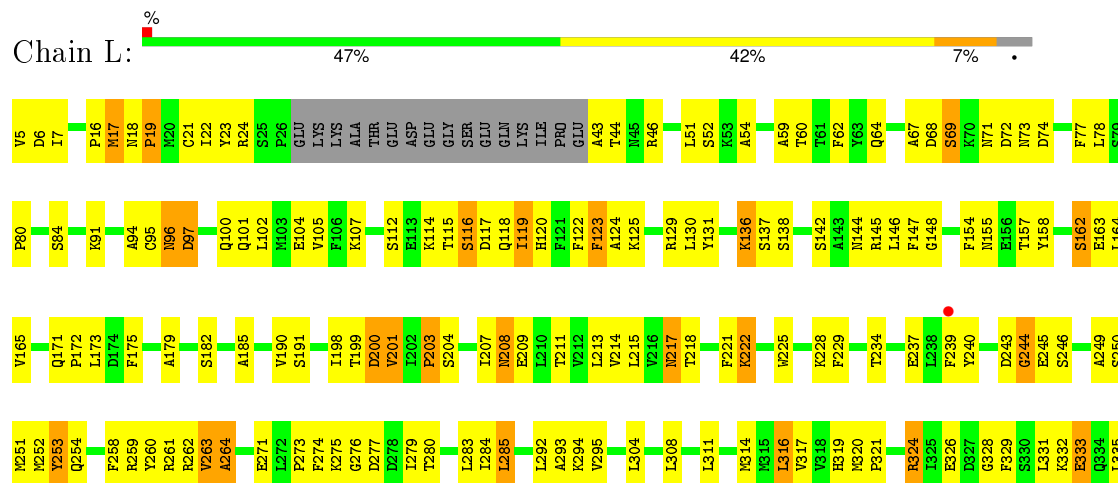
### 3 Residue-property plots

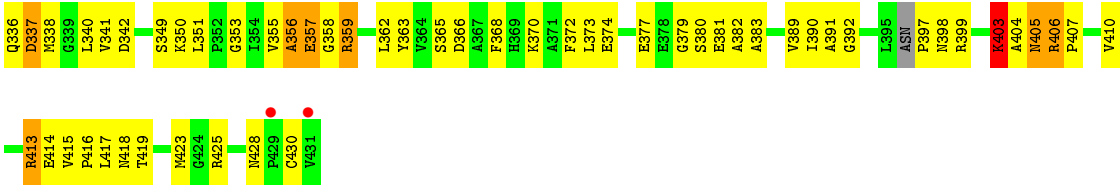
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Antithrombin-III



#### • Molecule 2: Antithrombin-III





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.47Å 98.67Å 89.24Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 54.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.80) 99.9 (54.94-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.228 , 0.283 0.231 , 0.221	Depositor DCC
$R_{free}$ test set	1436 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 28330 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	I	0.40	0/3265	0.67	0/4423
2	L	0.40	0/3141	0.66	0/4277
All	All	0.40	0/6406	0.66	0/8700

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	841	NAG	C1

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	I	3203	0	3086	199	0
2	L	3078	0	2857	196	0
3	I	42	0	39	9	0
3	L	42	0	39	5	0
4	I	28	0	25	1	0
4	L	27	0	25	0	0
5	I	84	0	0	7	0
5	L	56	0	0	3	0
All	All	6560	0	6071	393	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 31.

All (393) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:LYS:HA	1:I:172:PRO:HB2	1.42	0.99
2:L:404:ALA:HB2	2:L:428:ASN:ND2	1.78	0.98
2:L:7:ILE:H	2:L:7:ILE:HD12	1.30	0.96
2:L:404:ALA:HB2	2:L:428:ASN:HD22	1.32	0.94
2:L:94:ALA:HA	2:L:351:LEU:HD23	1.52	0.91
1:I:190:VAL:HB	1:I:201:VAL:HG21	1.51	0.91
2:L:292:LEU:HD23	2:L:407:PRO:HG2	1.54	0.89
1:I:143:ALA:HB3	1:I:218:THR:HG23	1.51	0.89
2:L:124:ALA:HB2	2:L:165:VAL:HG13	1.58	0.84
2:L:211:THR:HA	2:L:391:ALA:O	1.78	0.83
2:L:365:SER:HB3	2:L:392:GLY:H	1.46	0.81
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.64	0.79
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.64	0.79
2:L:215:LEU:HD12	2:L:215:LEU:H	1.48	0.79
2:L:285:LEU:HD23	2:L:285:LEU:N	1.99	0.78
1:I:232:GLU:OE1	2:L:262:ARG:HD2	1.84	0.78
2:L:73:ASN:HB3	2:L:404:ALA:O	1.84	0.77
2:L:239:PHE:HE1	2:L:404:ALA:HB1	1.50	0.77
2:L:71:ASN:HB2	5:L:652:HOH:O	1.82	0.77
1:I:192:ASN:HD21	3:I:861:NAG:H2	1.49	0.77
1:I:183:ARG:HB2	1:I:207:ILE:HD12	1.66	0.76
2:L:145:ARG:HG2	2:L:147:PHE:CE1	2.22	0.74
1:I:176:LYS:HA	1:I:209:GLU:HG3	1.69	0.74
2:L:215:LEU:HD12	2:L:215:LEU:N	2.04	0.73
2:L:62:PHE:HA	2:L:338:MET:HE1	1.70	0.73
2:L:213:LEU:HB3	2:L:390:ILE:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:244:GLY:HA2	5:L:537:HOH:O	1.90	0.71
2:L:91:LYS:NZ	2:L:120:HIS:NE2	2.37	0.71
1:I:261:ARG:HA	1:I:261:ARG:NH1	2.05	0.71
1:I:192:ASN:HD21	3:I:861:NAG:C2	2.03	0.71
1:I:161:ILE:C	1:I:163:GLU:H	1.92	0.70
1:I:154:PHE:HA	1:I:354:ILE:HG23	1.74	0.70
1:I:213:LEU:HD23	1:I:364:VAL:HG22	1.74	0.70
2:L:252:MET:HE2	2:L:320:MET:HG2	1.73	0.69
1:I:354:ILE:HD12	1:I:354:ILE:N	2.08	0.69
2:L:190:VAL:HG21	2:L:201:VAL:HG21	1.73	0.69
1:I:192:ASN:HD21	3:I:861:NAG:C1	2.06	0.68
2:L:59:ALA:HB1	2:L:423:MET:CE	2.23	0.68
2:L:91:LYS:HE2	2:L:120:HIS:NE2	2.07	0.68
1:I:183:ARG:HE	1:I:204:SER:HA	1.59	0.68
1:I:336:GLN:HA	1:I:340:LEU:O	1.93	0.68
1:I:262:ARG:HG3	1:I:262:ARG:HH11	1.59	0.67
2:L:405:ASN:CG	2:L:406:ARG:H	1.97	0.66
1:I:332:LYS:O	1:I:336:GLN:HG3	1.95	0.66
2:L:7:ILE:HG12	2:L:164:LEU:O	1.96	0.66
2:L:77:PHE:CZ	2:L:373:LEU:HB2	2.30	0.66
1:I:91:LYS:NZ	1:I:120:HIS:NE2	2.38	0.66
3:L:841:NAG:O4	3:L:842:NAG:C1	2.44	0.66
1:I:146:LEU:HD13	1:I:215:LEU:HD13	1.78	0.66
2:L:77:PHE:CE2	2:L:373:LEU:HB2	2.32	0.65
2:L:324:ARG:HG3	2:L:324:ARG:O	1.96	0.65
1:I:259:ARG:NH2	1:I:311:LEU:HB2	2.11	0.65
2:L:292:LEU:CD2	2:L:407:PRO:HG2	2.26	0.65
2:L:355:VAL:HG23	2:L:362:LEU:HD11	1.77	0.65
1:I:143:ALA:HB3	1:I:218:THR:CG2	2.23	0.64
2:L:91:LYS:CE	2:L:120:HIS:NE2	2.60	0.64
2:L:59:ALA:HB1	2:L:423:MET:HE3	1.78	0.64
2:L:341:VAL:HG23	2:L:342:ASP:H	1.61	0.64
2:L:413:ARG:NH2	2:L:415:VAL:HG13	2.12	0.64
1:I:71:ASN:HD22	1:I:72:ASP:H	1.45	0.64
2:L:182:SER:O	2:L:185:ALA:HB3	1.97	0.64
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.79	0.64
2:L:237:GLU:HB2	5:L:656:HOH:O	1.97	0.64
1:I:294:LYS:O	1:I:298:GLU:HG3	1.96	0.64
2:L:365:SER:CB	2:L:392:GLY:H	2.12	0.63
2:L:239:PHE:CE1	2:L:404:ALA:HB1	2.32	0.63
2:L:261:ARG:HG3	2:L:263:VAL:CG1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:SER:O	1:I:184:ALA:N	2.25	0.63
1:I:174:ASP:HB3	1:I:178:ASN:HB2	1.79	0.63
1:I:312:GLU:HB2	5:I:588:HOH:O	1.99	0.63
2:L:71:ASN:ND2	2:L:73:ASN:HB2	2.14	0.62
1:I:183:ARG:HG2	1:I:183:ARG:O	2.00	0.62
2:L:341:VAL:HG23	2:L:342:ASP:N	2.14	0.62
1:I:78:LEU:HD23	1:I:78:LEU:N	2.15	0.62
1:I:190:VAL:HG21	1:I:201:VAL:HG11	1.80	0.62
1:I:343:LEU:HD11	1:I:364:VAL:HG23	1.83	0.61
1:I:144:ASN:HB2	5:I:519:HOH:O	1.99	0.61
2:L:125:LYS:O	2:L:129:ARG:HG2	2.00	0.61
2:L:331:LEU:O	2:L:335:LEU:HB2	1.99	0.61
2:L:229:PHE:HB2	2:L:377:GLU:HA	1.82	0.61
2:L:175:PHE:O	2:L:209:GLU:HA	2.01	0.61
1:I:331:LEU:HB2	1:I:367:ALA:HB3	1.82	0.61
2:L:191:SER:OG	2:L:199:THR:HG22	2.01	0.61
1:I:326:GLU:HG2	1:I:370:LYS:HE3	1.82	0.60
1:I:190:VAL:CB	1:I:201:VAL:HG21	2.27	0.60
2:L:222:LYS:HG2	2:L:381:GLU:HG3	1.82	0.60
1:I:51:LEU:HA	1:I:111:ILE:HD11	1.83	0.60
1:I:170:LEU:O	1:I:171:GLN:HB3	2.02	0.60
2:L:261:ARG:O	2:L:263:VAL:HG13	2.02	0.60
1:I:194:THR:O	1:I:197:ARG:HG2	2.02	0.60
2:L:91:LYS:HZ3	2:L:120:HIS:CD2	2.19	0.59
2:L:274:PHE:HD2	2:L:279:ILE:O	1.84	0.59
1:I:283:LEU:HD11	1:I:320:MET:HE1	1.84	0.59
2:L:119:ILE:HG22	2:L:120:HIS:N	2.16	0.59
1:I:18:ASN:O	1:I:21:CYS:HB2	2.03	0.59
5:I:609:HOH:O	2:L:249:ALA:HB2	2.02	0.59
2:L:102:LEU:HD23	2:L:340:LEU:HD11	1.84	0.59
1:I:159:GLN:CB	1:I:170:LEU:HD21	2.32	0.59
1:I:111:ILE:O	1:I:114:LYS:HB2	2.03	0.58
1:I:182:SER:O	1:I:185:ALA:N	2.36	0.58
1:I:108:PHE:HB3	1:I:119:ILE:HG12	1.85	0.58
1:I:183:ARG:HG2	1:I:183:ARG:HH11	1.67	0.58
2:L:221:PHE:CE1	2:L:279:ILE:HG21	2.39	0.58
2:L:144:ASN:HD22	2:L:217:ASN:HA	1.68	0.58
2:L:252:MET:CE	2:L:320:MET:HG2	2.34	0.58
2:L:428:ASN:OD1	2:L:430:CYS:HB2	2.03	0.58
1:I:183:ARG:CB	1:I:207:ILE:HD12	2.34	0.58
1:I:391:ALA:O	2:L:321:PRO:HD3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:ILE:H	2:L:7:ILE:CD1	2.07	0.58
2:L:24:ARG:HA	2:L:114:LYS:O	2.04	0.58
2:L:54:ALA:HB1	2:L:107:LYS:O	2.03	0.58
1:I:289:GLU:CD	1:I:289:GLU:H	2.08	0.58
2:L:292:LEU:HD21	2:L:407:PRO:O	2.05	0.57
1:I:47:ARG:HB3	1:I:122:PHE:CD1	2.39	0.57
2:L:254:GLN:NE2	2:L:258:PHE:HZ	2.02	0.57
1:I:115:THR:H	1:I:118:GLN:NE2	2.03	0.57
1:I:286:PRO:HB3	1:I:295:VAL:HG21	1.86	0.57
2:L:207:ILE:HG23	2:L:211:THR:HG21	1.85	0.56
2:L:208:ASN:C	2:L:208:ASN:HD22	2.08	0.56
1:I:115:THR:H	1:I:118:GLN:HE21	1.51	0.56
1:I:161:ILE:C	1:I:163:GLU:N	2.59	0.56
1:I:331:LEU:HB3	1:I:335:LEU:HD11	1.87	0.56
2:L:52:SER:HB2	2:L:419:THR:HG22	1.87	0.56
1:I:260:TYR:CD2	1:I:261:ARG:N	2.73	0.56
2:L:261:ARG:HG3	2:L:263:VAL:HG13	1.87	0.56
2:L:131:TYR:CE1	2:L:142:SER:HB2	2.39	0.56
1:I:396:ASN:OD1	1:I:398:ASN:N	2.36	0.56
1:I:71:ASN:HD22	1:I:72:ASP:N	2.03	0.56
1:I:387:ALA:O	2:L:316:LEU:HB2	2.06	0.56
1:I:284:ILE:HD13	1:I:307:TRP:HZ3	1.70	0.56
1:I:183:ARG:HG2	1:I:183:ARG:NH1	2.21	0.56
2:L:116:SER:O	2:L:118:GLN:N	2.40	0.55
1:I:285:LEU:HD11	1:I:406:ARG:HG3	1.87	0.55
2:L:7:ILE:HD12	2:L:7:ILE:N	2.11	0.55
1:I:51:LEU:HD22	1:I:122:PHE:CB	2.36	0.55
2:L:222:LYS:CG	2:L:381:GLU:HG3	2.37	0.55
2:L:96:ASN:ND2	3:L:801:NAG:C1	2.70	0.55
2:L:366:ASP:OD2	2:L:368:PHE:CZ	2.60	0.55
1:I:192:ASN:ND2	3:I:861:NAG:H2	2.18	0.55
2:L:332:LYS:O	2:L:336:GLN:HG3	2.07	0.55
1:I:191:SER:HA	1:I:198:ILE:O	2.07	0.54
1:I:342:ASP:O	1:I:349:SER:HA	2.06	0.54
2:L:148:GLY:HA3	2:L:154:PHE:CE2	2.42	0.54
2:L:198:ILE:HG23	2:L:370:LYS:HG2	1.88	0.54
1:I:177:GLU:C	1:I:178:ASN:HD22	2.11	0.54
1:I:17:MET:HG2	1:I:117:ASP:HB3	1.88	0.54
1:I:76:ILE:O	1:I:77:PHE:HB2	2.08	0.54
1:I:412:ILE:O	1:I:421:ILE:HB	2.08	0.54
1:I:221:PHE:CE1	1:I:279:ILE:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:ARG:HG3	1:I:262:ARG:NH1	2.23	0.54
2:L:234:THR:HG23	2:L:251:MET:O	2.07	0.54
2:L:115:THR:HG23	2:L:118:GLN:CB	2.38	0.54
2:L:328:GLY:O	2:L:329:PHE:HB3	2.09	0.53
2:L:372:PHE:O	2:L:382:ALA:HA	2.08	0.53
2:L:405:ASN:ND2	2:L:406:ARG:N	2.55	0.53
1:I:389:VAL:HA	5:I:655:HOH:O	2.07	0.53
2:L:199:THR:O	2:L:200:ASP:HB3	2.08	0.53
1:I:238:LEU:HA	1:I:247:CYS:O	2.08	0.53
1:I:331:LEU:HB3	1:I:335:LEU:CD1	2.39	0.53
2:L:403:LYS:HD3	2:L:404:ALA:N	2.24	0.53
2:L:18:ASN:O	2:L:19:PRO:O	2.26	0.53
1:I:183:ARG:HB2	1:I:207:ILE:CD1	2.37	0.53
1:I:183:ARG:CA	1:I:207:ILE:HD12	2.39	0.53
2:L:221:PHE:CG	2:L:222:LYS:N	2.77	0.53
2:L:105:VAL:HG21	2:L:340:LEU:HB2	1.91	0.52
1:I:345:SER:HB3	1:I:348:LYS:HB2	1.91	0.52
1:I:232:GLU:CD	2:L:262:ARG:HD2	2.30	0.52
1:I:260:TYR:CG	1:I:261:ARG:N	2.78	0.52
2:L:283:LEU:HD11	2:L:320:MET:CE	2.39	0.52
1:I:182:SER:C	1:I:184:ALA:H	2.12	0.52
2:L:71:ASN:C	2:L:73:ASN:H	2.13	0.52
2:L:71:ASN:HD21	2:L:73:ASN:HB2	1.74	0.52
2:L:22:ILE:N	2:L:22:ILE:HD12	2.24	0.52
2:L:130:LEU:HD23	2:L:417:LEU:HD13	1.92	0.52
2:L:283:LEU:O	2:L:284:ILE:HG13	2.08	0.52
1:I:213:LEU:HB3	1:I:364:VAL:HA	1.92	0.52
2:L:259:ARG:HD3	2:L:271:GLU:OE1	2.09	0.52
1:I:261:ARG:HD3	1:I:262:ARG:N	2.25	0.51
1:I:302:GLU:CD	1:I:302:GLU:H	2.13	0.51
2:L:91:LYS:HE2	2:L:120:HIS:CE1	2.45	0.51
1:I:89:MET:HA	1:I:166:TYR:CD2	2.45	0.51
1:I:170:LEU:HD23	1:I:170:LEU:H	1.76	0.51
2:L:67:ALA:O	2:L:69:SER:N	2.40	0.51
1:I:155:ASN:HB3	1:I:353:GLY:O	2.11	0.51
2:L:404:ALA:CB	2:L:428:ASN:HB2	2.41	0.51
2:L:179:ALA:HB1	2:L:207:ILE:O	2.11	0.51
2:L:74:ASP:O	2:L:425:ARG:HD2	2.10	0.51
1:I:153:THR:HG22	1:I:354:ILE:C	2.32	0.50
1:I:154:PHE:HA	1:I:354:ILE:CG2	2.40	0.50
1:I:15:ILE:N	1:I:16:PRO:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:213:LEU:HG	2:L:214:VAL:N	2.25	0.50
3:I:862:NAG:H3	3:I:862:NAG:O7	2.09	0.50
2:L:349:SER:OG	2:L:363:TYR:HA	2.11	0.50
1:I:19:PRO:C	1:I:21:CYS:H	2.13	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.11	0.50
2:L:60:THR:O	2:L:64:GLN:HG3	2.12	0.50
2:L:304:LEU:O	2:L:308:LEU:HG	2.12	0.50
1:I:71:ASN:ND2	1:I:72:ASP:N	2.58	0.50
2:L:78:LEU:N	2:L:78:LEU:HD23	2.27	0.50
1:I:241:LYS:HD3	1:I:428:ASN:HD22	1.77	0.50
2:L:405:ASN:ND2	2:L:406:ARG:H	2.10	0.49
1:I:84:SER:O	1:I:88:ALA:HB2	2.12	0.49
2:L:292:LEU:O	2:L:295:VAL:N	2.41	0.49
1:I:313:GLU:O	1:I:314:MET:HG3	2.12	0.49
2:L:410:VAL:O	2:L:423:MET:HA	2.13	0.49
2:L:155:ASN:ND2	3:L:841:NAG:C7	2.76	0.49
1:I:182:SER:C	1:I:184:ALA:N	2.66	0.49
2:L:366:ASP:OD2	2:L:368:PHE:CE1	2.66	0.49
2:L:23:TYR:HB3	2:L:116:SER:OG	2.12	0.49
2:L:21:CYS:C	2:L:22:ILE:HD12	2.33	0.49
2:L:285:LEU:CD2	2:L:285:LEU:N	2.70	0.49
1:I:284:ILE:HD13	1:I:307:TRP:CZ3	2.47	0.49
2:L:374:GLU:O	2:L:380:SER:HA	2.13	0.49
1:I:91:LYS:HE3	1:I:120:HIS:CE1	2.47	0.49
2:L:23:TYR:CE1	2:L:100:GLN:HG3	2.47	0.49
2:L:355:VAL:O	2:L:355:VAL:HG12	2.12	0.49
2:L:100:GLN:O	2:L:104:GLU:HG3	2.13	0.49
1:I:92:LEU:HB3	1:I:158:TYR:CE1	2.48	0.49
2:L:5:VAL:HG12	2:L:6:ASP:N	2.28	0.49
2:L:284:ILE:C	2:L:285:LEU:HD23	2.33	0.48
2:L:51:LEU:CD2	2:L:123:PHE:HA	2.43	0.48
1:I:186:ILE:O	1:I:189:TRP:N	2.46	0.48
1:I:71:ASN:ND2	1:I:72:ASP:H	2.11	0.48
1:I:170:LEU:N	1:I:170:LEU:HD23	2.28	0.48
2:L:414:GLU:OE1	2:L:416:PRO:HG2	2.14	0.48
1:I:147:PHE:CE2	1:I:186:ILE:HG12	2.49	0.48
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.79	0.48
1:I:19:PRO:C	1:I:21:CYS:N	2.64	0.48
1:I:261:ARG:HD3	1:I:262:ARG:H	1.78	0.48
1:I:400:VAL:HG12	1:I:401:THR:N	2.28	0.48
1:I:89:MET:HA	1:I:166:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:ASN:HB3	1:I:181:GLN:HG3	1.96	0.48
1:I:76:ILE:HG22	1:I:77:PHE:N	2.29	0.48
2:L:326:GLU:HG2	2:L:372:PHE:HD2	1.79	0.47
1:I:346:PRO:HG3	1:I:363:TYR:CE2	2.49	0.47
2:L:158:TYR:HB2	2:L:353:GLY:O	2.13	0.47
1:I:396:ASN:HB2	2:L:240:TYR:CZ	2.49	0.47
1:I:260:TYR:CZ	1:I:400:VAL:HG11	2.50	0.47
2:L:214:VAL:HG22	2:L:389:VAL:HG22	1.97	0.47
2:L:215:LEU:CD1	2:L:215:LEU:H	2.23	0.47
2:L:96:ASN:O	2:L:97:ASP:HB2	2.14	0.47
1:I:261:ARG:NH1	5:I:658:HOH:O	2.46	0.47
2:L:355:VAL:O	2:L:357:GLU:N	2.48	0.47
2:L:355:VAL:CG2	2:L:362:LEU:HD11	2.45	0.47
2:L:308:LEU:HD13	2:L:413:ARG:NH2	2.30	0.47
1:I:87:PHE:CE1	1:I:335:LEU:HD13	2.49	0.47
1:I:22:ILE:HG22	1:I:23:TYR:N	2.30	0.47
2:L:119:ILE:O	2:L:122:PHE:N	2.48	0.47
1:I:261:ARG:CZ	1:I:261:ARG:HA	2.44	0.47
2:L:217:ASN:ND2	2:L:218:THR:N	2.63	0.47
1:I:390:ILE:HA	2:L:319:HIS:HB2	1.96	0.47
3:I:801:NAG:O7	3:I:801:NAG:H3	2.14	0.47
2:L:276:GLY:O	2:L:277:ASP:HB2	2.14	0.47
1:I:281:MET:HA	1:I:411:PHE:O	2.14	0.47
1:I:71:ASN:HB3	1:I:74:ASP:OD2	2.15	0.47
2:L:146:LEU:HD11	2:L:162:SER:HB3	1.97	0.47
1:I:51:LEU:HD22	1:I:122:PHE:HB3	1.97	0.47
1:I:121:PHE:O	1:I:124:ALA:HB3	2.15	0.47
2:L:404:ALA:HB2	2:L:428:ASN:CG	2.33	0.46
1:I:91:LYS:CB	1:I:102:LEU:HD13	2.42	0.46
1:I:326:GLU:CG	1:I:370:LYS:HE3	2.44	0.46
1:I:40:ILE:HG23	1:I:40:ILE:O	2.14	0.46
2:L:163:GLU:HG2	2:L:163:GLU:O	2.15	0.46
1:I:261:ARG:HH11	1:I:261:ARG:HA	1.80	0.46
2:L:215:LEU:CD1	2:L:215:LEU:N	2.76	0.46
2:L:131:TYR:CZ	2:L:142:SER:HB2	2.50	0.46
1:I:346:PRO:HA	1:I:363:TYR:CD1	2.50	0.46
1:I:155:ASN:O	1:I:158:TYR:HB3	2.16	0.46
2:L:405:ASN:O	2:L:406:ARG:C	2.54	0.46
2:L:398:ASN:CG	2:L:399:ARG:H	2.19	0.46
1:I:351:LEU:C	1:I:353:GLY:H	2.18	0.46
1:I:87:PHE:HD2	1:I:87:PHE:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:229:PHE:CE2	1:I:254:GLN:HG2	2.51	0.46
1:I:265:GLU:CD	1:I:290:LYS:HZ2	2.18	0.46
1:I:151:SER:O	1:I:152:LEU:O	2.34	0.46
3:I:861:NAG:H5	3:I:862:NAG:C1	2.46	0.46
2:L:95:CYS:O	2:L:350:LYS:HB2	2.16	0.46
1:I:51:LEU:HD22	1:I:122:PHE:HB2	1.97	0.46
2:L:71:ASN:O	2:L:73:ASN:N	2.49	0.45
1:I:190:VAL:HB	1:I:201:VAL:CG2	2.35	0.45
2:L:101:GLN:O	2:L:105:VAL:HG23	2.15	0.45
1:I:351:LEU:O	1:I:353:GLY:N	2.49	0.45
2:L:221:PHE:CE1	2:L:279:ILE:HD13	2.52	0.45
2:L:333:GLU:O	2:L:337:ASP:OD1	2.34	0.45
1:I:319:HIS:CB	1:I:403:LYS:HG3	2.46	0.45
2:L:326:GLU:HG2	2:L:372:PHE:CD2	2.52	0.45
2:L:16:PRO:O	2:L:17:MET:C	2.55	0.45
2:L:172:PRO:O	2:L:173:LEU:HG	2.16	0.45
1:I:327:ASP:O	1:I:370:LYS:HD2	2.16	0.45
2:L:43:ALA:HB3	2:L:46:ARG:CB	2.47	0.45
1:I:56:SER:OG	1:I:420:ILE:HD12	2.17	0.45
1:I:89:MET:HE2	1:I:166:TYR:HB3	1.99	0.45
1:I:253:TYR:OH	1:I:255:GLU:OE2	2.34	0.45
5:I:609:HOH:O	2:L:239:PHE:HB2	2.17	0.45
1:I:331:LEU:C	1:I:335:LEU:HD12	2.38	0.45
1:I:219:ILE:HG22	1:I:220:LEU:N	2.32	0.45
2:L:145:ARG:HG2	2:L:147:PHE:CZ	2.51	0.44
2:L:200:ASP:O	2:L:201:VAL:C	2.56	0.44
1:I:276:GLY:O	1:I:277:ASP:HB2	2.17	0.44
2:L:404:ALA:HB2	2:L:428:ASN:CB	2.47	0.44
2:L:418:ASN:O	2:L:418:ASN:OD1	2.35	0.44
2:L:294:LYS:O	2:L:294:LYS:HG2	2.18	0.44
2:L:71:ASN:N	2:L:74:ASP:OD2	2.46	0.44
2:L:199:THR:O	2:L:200:ASP:CB	2.64	0.44
1:I:78:LEU:H	1:I:78:LEU:HD23	1.80	0.44
2:L:258:PHE:O	2:L:314:MET:N	2.49	0.44
2:L:263:VAL:O	2:L:264:ALA:C	2.57	0.44
2:L:258:PHE:HB2	2:L:316:LEU:HD21	2.00	0.44
1:I:180:GLU:C	1:I:182:SER:H	2.22	0.43
1:I:346:PRO:HG3	1:I:363:TYR:CZ	2.53	0.43
2:L:404:ALA:HB2	2:L:428:ASN:HB2	1.99	0.43
2:L:91:LYS:HZ3	2:L:120:HIS:CE1	2.34	0.43
1:I:332:LYS:HG3	1:I:344:PHE:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:285:LEU:HD12	1:I:286:PRO:HD2	2.00	0.43
1:I:219:ILE:HB	1:I:422:PHE:CZ	2.53	0.43
2:L:245:GLU:HG2	2:L:246:SER:N	2.34	0.43
1:I:360:ASP:OD2	1:I:361:ASP:N	2.52	0.43
2:L:358:GLY:O	2:L:359:ARG:C	2.57	0.43
1:I:239:PHE:CD2	1:I:429:PRO:HG3	2.53	0.43
1:I:198:ILE:HG23	1:I:370:LYS:HG2	2.01	0.43
1:I:151:SER:HB3	1:I:152:LEU:H	1.54	0.43
1:I:192:ASN:ND2	3:I:861:NAG:C1	2.80	0.43
2:L:157:THR:OG1	3:L:841:NAG:H5	2.19	0.43
2:L:258:PHE:HB2	2:L:316:LEU:CD2	2.48	0.43
2:L:157:THR:CB	3:L:841:NAG:H5	2.49	0.43
1:I:288:PRO:HB2	1:I:289:GLU:OE2	2.18	0.43
2:L:171:GLN:HA	2:L:172:PRO:HD3	1.81	0.43
1:I:192:ASN:ND2	3:I:861:NAG:C2	2.77	0.43
1:I:153:THR:O	1:I:354:ILE:HG22	2.18	0.43
1:I:241:LYS:CD	1:I:428:ASN:HD22	2.32	0.43
1:I:89:MET:O	1:I:92:LEU:HB2	2.19	0.42
1:I:284:ILE:HB	1:I:409:LEU:HB2	2.01	0.42
1:I:14:ASP:C	1:I:16:PRO:HD3	2.40	0.42
1:I:154:PHE:O	1:I:155:ASN:C	2.57	0.42
1:I:22:ILE:CG2	1:I:23:TYR:N	2.81	0.42
2:L:356:ALA:C	2:L:358:GLY:N	2.73	0.42
1:I:167:GLY:O	1:I:168:ALA:HB2	2.19	0.42
1:I:94:ALA:HB3	1:I:99:LEU:HD13	2.01	0.42
1:I:341:VAL:O	1:I:343:LEU:N	2.52	0.42
2:L:80:PRO:HG3	2:L:423:MET:HE2	2.02	0.42
1:I:421:ILE:HG22	1:I:422:PHE:CD2	2.54	0.42
2:L:259:ARG:NH2	2:L:311:LEU:HB2	2.33	0.42
2:L:365:SER:OG	2:L:389:VAL:HG12	2.20	0.42
1:I:155:ASN:HA	4:I:841:NAG:C8	2.50	0.42
1:I:113:GLU:O	1:I:114:LYS:C	2.57	0.42
1:I:414:GLU:HB2	1:I:421:ILE:HD11	2.01	0.42
2:L:356:ALA:O	2:L:358:GLY:N	2.53	0.42
2:L:136:LYS:O	2:L:137:SER:HB2	2.20	0.42
1:I:189:TRP:O	1:I:192:ASN:HB3	2.20	0.42
2:L:245:GLU:HG2	2:L:246:SER:H	1.85	0.42
2:L:356:ALA:C	2:L:358:GLY:H	2.22	0.42
2:L:138:SER:HB3	2:L:279:ILE:HD12	2.02	0.42
2:L:225:TRP:CD1	2:L:379:GLY:HA2	2.55	0.42
1:I:334:GLN:O	1:I:335:LEU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:LEU:C	1:I:299:LEU:HD13	2.41	0.42
1:I:337:ASP:OD2	1:I:337:ASP:O	2.37	0.42
1:I:81:LEU:HD21	1:I:130:LEU:CD1	2.50	0.42
1:I:183:ARG:NE	1:I:203:PRO:O	2.52	0.41
1:I:354:ILE:CD1	1:I:354:ILE:N	2.77	0.41
1:I:341:VAL:C	1:I:343:LEU:H	2.24	0.41
2:L:217:ASN:C	2:L:217:ASN:ND2	2.74	0.41
1:I:222:LYS:HB2	1:I:381:GLU:HG2	2.01	0.41
1:I:343:LEU:CD1	1:I:364:VAL:HG23	2.49	0.41
2:L:273:PRO:HA	2:L:280:THR:HG22	2.02	0.41
1:I:243:ASP:OD1	1:I:244:GLY:N	2.42	0.41
2:L:341:VAL:CG2	2:L:342:ASP:N	2.83	0.41
1:I:138:SER:OG	1:I:138:SER:O	2.37	0.41
1:I:305:GLN:HG2	5:I:586:HOH:O	2.21	0.41
2:L:372:PHE:CD1	2:L:372:PHE:C	2.93	0.41
1:I:48:VAL:HG13	1:I:126:LEU:HD13	2.03	0.41
1:I:131:TYR:CZ	1:I:142:SER:HB2	2.56	0.41
2:L:102:LEU:CD2	2:L:340:LEU:HD11	2.51	0.41
2:L:91:LYS:HE2	2:L:91:LYS:HB3	1.80	0.41
1:I:114:LYS:HD2	1:I:114:LYS:N	2.34	0.41
1:I:241:LYS:HD3	1:I:428:ASN:ND2	2.35	0.41
2:L:221:PHE:HE1	2:L:279:ILE:HD13	1.86	0.41
1:I:81:LEU:HD21	1:I:130:LEU:HD11	2.02	0.41
1:I:323:PHE:CZ	1:I:375:VAL:HG21	2.56	0.41
1:I:252:MET:HG3	1:I:322:ARG:HG2	2.01	0.41
1:I:361:ASP:O	1:I:361:ASP:OD1	2.39	0.40
2:L:105:VAL:HG13	2:L:338:MET:HB3	2.02	0.40
1:I:200:ASP:OD1	1:I:370:LYS:HE2	2.21	0.40
1:I:40:ILE:HA	1:I:41:PRO:HD2	2.01	0.40
1:I:150:LYS:N	1:I:173:LEU:O	2.54	0.40
2:L:260:TYR:O	2:L:261:ARG:HB2	2.21	0.40
2:L:253:TYR:CD1	2:L:253:TYR:C	2.94	0.40
2:L:253:TYR:CE2	2:L:317:VAL:CG1	3.05	0.40
2:L:283:LEU:HD11	2:L:320:MET:HE3	2.02	0.40
2:L:373:LEU:HD12	2:L:374:GLU:H	1.86	0.40
1:I:119:ILE:HG22	1:I:120:HIS:N	2.35	0.40
2:L:251:MET:CE	2:L:319:HIS:HB3	2.52	0.40
2:L:372:PHE:N	2:L:383:ALA:O	2.54	0.40
2:L:203:PRO:HB2	2:L:204:SER:H	1.69	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	I	405/427 (95%)	309 (76%)	65 (16%)	31 (8%)	1	2
2	L	404/427 (95%)	328 (81%)	47 (12%)	29 (7%)	1	3
All	All	809/854 (95%)	637 (79%)	112 (14%)	60 (7%)	1	3

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	42	GLU
1	I	152	LEU
1	I	170	LEU
1	I	176	LYS
1	I	430	CYS
2	L	19	PRO
2	L	96	ASN
2	L	112	SER
2	L	116	SER
2	L	117	ASP
2	L	136	LYS
2	L	200	ASP
2	L	203	PRO
2	L	228	LYS
2	L	250	SER
2	L	264	ALA
2	L	356	ALA
2	L	403	LYS
1	I	184	ALA
1	I	245	GLU
1	I	350	LYS
1	I	383	ALA
1	I	384	ALA
2	L	44	THR
2	L	69	SER

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Mol	Chain	Res	Type
2	L	72	ASP
2	L	243	ASP
1	I	77	PHE
1	I	168	ALA
1	I	183	ARG
1	I	243	ASP
1	I	244	GLY
1	I	337	ASP
1	I	342	ASP
2	L	17	MET
2	L	68	ASP
2	L	293	ALA
2	L	359	ARG
1	I	38	GLN
1	I	82	SER
1	I	158	TYR
1	I	203	PRO
1	I	352	PRO
1	I	386	THR
2	L	244	GLY
2	L	357	GLU
1	I	12	PRO
1	I	43	ALA
1	I	116	SER
1	I	130	LEU
1	I	171	GLN
2	L	222	LYS
2	L	406	ARG
1	I	40	ILE
1	I	112	SER
2	L	275	LYS
2	L	333	GLU
1	I	41	PRO
2	L	263	VAL
2	L	119	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	I	341/378 (90%)	323 (95%)	18 (5%)	28	61
2	L	312/379 (82%)	296 (95%)	16 (5%)	29	63
All	All	653/757 (86%)	619 (95%)	34 (5%)	29	62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	13	ARG
1	I	17	MET
1	I	71	ASN
1	I	78	LEU
1	I	92	LEU
1	I	97	ASP
1	I	109	ASP
1	I	114	LYS
1	I	153	THR
1	I	170	LEU
1	I	216	VAL
1	I	309	ASP
1	I	310	GLU
1	I	316	LEU
1	I	322	ARG
1	I	342	ASP
1	I	354	ILE
1	I	366	ASP
2	L	84	SER
2	L	97	ASP
2	L	123	PHE
2	L	162	SER
2	L	201	VAL
2	L	208	ASN
2	L	217	ASN
2	L	253	TYR
2	L	285	LEU
2	L	316	LEU
2	L	324	ARG
2	L	337	ASP
2	L	397	PRO
2	L	403	LYS
2	L	405	ASN
2	L	413	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	55	ASN
1	I	71	ASN
1	I	118	GLN
1	I	178	ASN
1	I	192	ASN
1	I	334	GLN
1	I	428	ASN
2	L	55	ASN
2	L	65	HIS
2	L	71	ASN
2	L	96	ASN
2	L	144	ASN
2	L	208	ASN
2	L	217	ASN
2	L	254	GLN
2	L	336	GLN
2	L	405	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

4 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
4	NAG	I	841	1,4	14,14,15	0.77	0	15,19,21	0.99	1 (6%)
4	NAG	I	842	4	14,14,15	0.58	0	15,19,21	0.80	1 (6%)
4	NAG	L	861	2,4	14,14,15	0.75	0	15,19,21	0.97	1 (6%)
4	NAG	L	862	4	13,13,15	0.85	0	11,17,21	0.31	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
4	NAG	I	841	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	I	842	4	-	0/6/23/26	0/1/1/1
4	NAG	L	861	2,4	-	0/6/23/26	0/1/1/1
4	NAG	L	862	4	-	0/5/22/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	841	NAG	C2-N2-C7	-2.75	119.51	123.04
4	L	861	NAG	C2-N2-C7	-2.39	119.97	123.04
4	I	842	NAG	C2-N2-C7	-2.36	120.01	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	841	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	841	NAG	1	0

## 5.6 Ligand geometry ⓘ

6 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	$\# Z  > 2$
3	NAG	I	801	1	14,14,15	0.72	1 (7%)	15,19,21	0.64	0
3	NAG	I	861	-	14,14,15	0.60	0	15,19,21	0.82	1 (6%)
3	NAG	I	862	-	14,14,15	0.55	0	15,19,21	0.60	0
3	NAG	L	801	-	14,14,15	0.57	0	15,19,21	0.61	0
3	NAG	L	841	2	14,14,15	0.66	0	15,19,21	1.01	2 (13%)
3	NAG	L	842	-	14,14,15	0.46	0	15,19,21	0.63	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
3	NAG	I	801	1	-	0/6/23/26	0/1/1/1
3	NAG	I	861	-	-	0/6/23/26	0/1/1/1
3	NAG	I	862	-	-	0/6/23/26	0/1/1/1
3	NAG	L	801	-	-	0/6/23/26	0/1/1/1
3	NAG	L	841	2	-	0/6/23/26	0/1/1/1
3	NAG	L	842	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	801	NAG	C1-C2	2.05	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	861	NAG	C2-N2-C7	-2.34	120.04	123.04
3	L	841	NAG	C4-C3-C2	2.10	114.49	111.23
3	L	841	NAG	C3-C4-C5	2.24	114.11	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	801	NAG	1	0
3	I	861	NAG	7	0
3	I	862	NAG	2	0
3	L	801	NAG	1	0
3	L	841	NAG	4	0
3	L	842	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	I	413/427 (96%)	-0.06	5 (1%) 81 73	36, 79, 115, 151	0
2	L	410/427 (96%)	-0.13	3 (0%) 89 84	42, 77, 121, 141	0
All	All	823/854 (96%)	-0.10	8 (0%) 84 77	36, 78, 120, 151	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	366	ASP	3.1
1	I	90	THR	3.1
1	I	363	TYR	2.9
1	I	37	GLU	2.6
2	L	429	PRO	2.3
2	L	431	VAL	2.3
2	L	239	PHE	2.2
1	I	364	VAL	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	I	841	14/15	0.82	0.46	5.62	106,112,116,118	0
4	NAG	L	862	13/15	0.88	0.17	-	127,128,129,129	0
4	NAG	L	861	14/15	0.80	0.24	-	115,119,122,124	0
4	NAG	I	842	14/15	0.80	0.35	-	120,122,122,122	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	L	841	14/15	0.89	0.17	-0.48	86,93,96,97	0
3	NAG	L	842	14/15	0.83	0.39	-	148,150,151,152	0
3	NAG	L	801	14/15	0.70	0.28	-	126,128,129,129	0
3	NAG	I	861	14/15	0.58	0.25	-	139,143,145,147	0
3	NAG	I	862	14/15	0.67	0.23	-	160,162,163,163	0
3	NAG	I	801	14/15	0.83	0.30	-	125,128,130,130	0

## 6.5 Other polymers

There are no such residues in this entry.