Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:29 AM GMT

PDB ID	:	3EVJ
Title	:	Intermediate structure of antithrombin bound to the natural pentasaccharide
Authors	:	Huntington, J.A.; Belzar, K.J.
Deposited on	:	2008-10-13
Resolution	:	3.00 Å(reported)

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

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

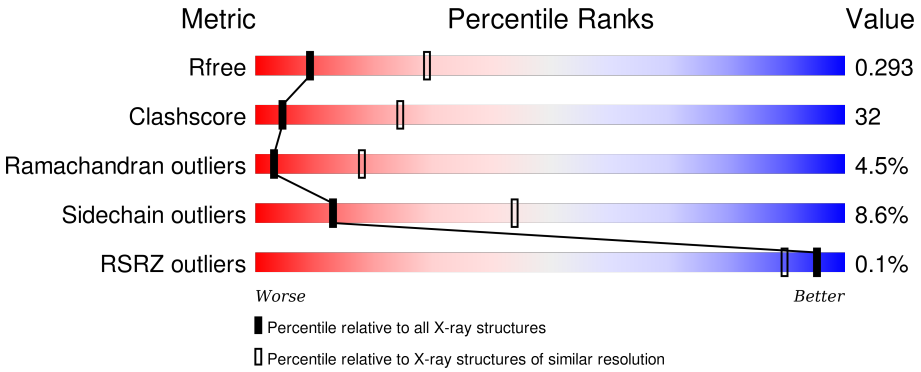
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	I	432	44% 43% 7% 6%
1	L	432	48% 43% 5% •

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	MAN	I	843	X	-	-	-
6	MAN	L	863	X	-	-	-

2 Entry composition

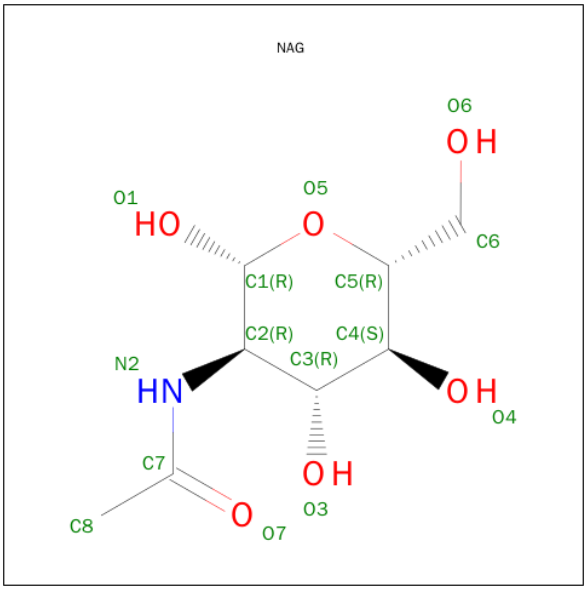
There are 7 unique types of molecules in this entry. The entry contains 6574 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	I	404	Total	C	N	O	S	0	0	0
			3016	1922	498	579	17			
1	L	417	Total	C	N	O	S	0	0	0
			3148	2009	517	605	17			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	6	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

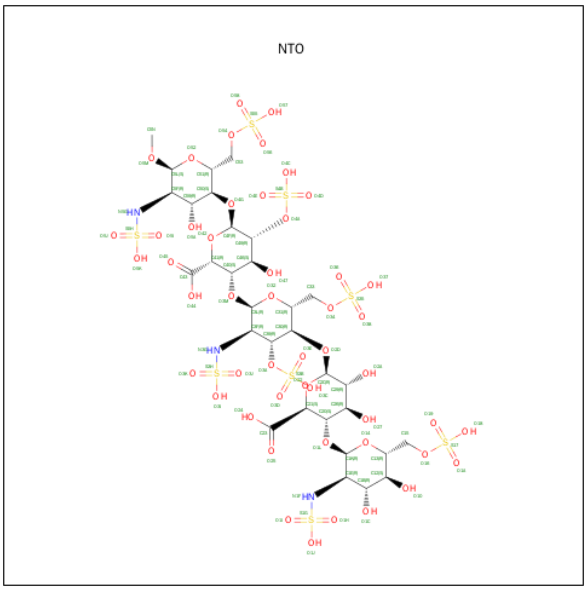
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	3	Total	C	N	O	0	0
			38	21	2	15		

- 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
			28	16	2	10		

- Molecule 5 is TRISULFOAMINO HEPARIN PENTASACCHARIDE (three-letter code: NTO) (formula: $C_{31}H_{53}N_3O_{49}S_8$).



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

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

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

- Molecule 7 is water.

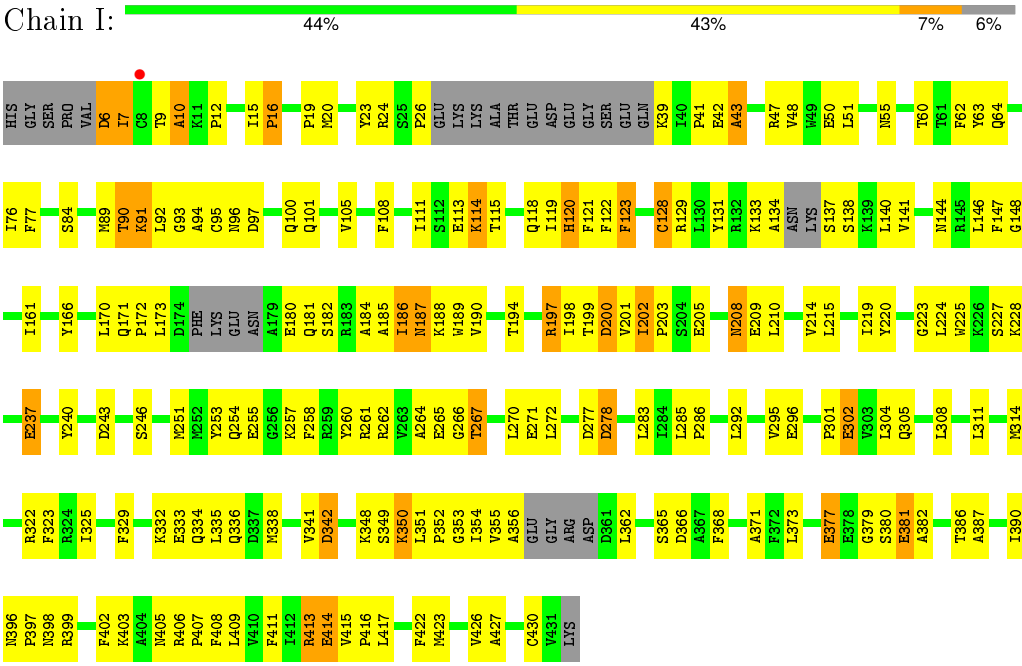
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	24	Total O 24 24	0	0
7	L	21	Total O 21 21	0	0

3 Residue-property plots (i)

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

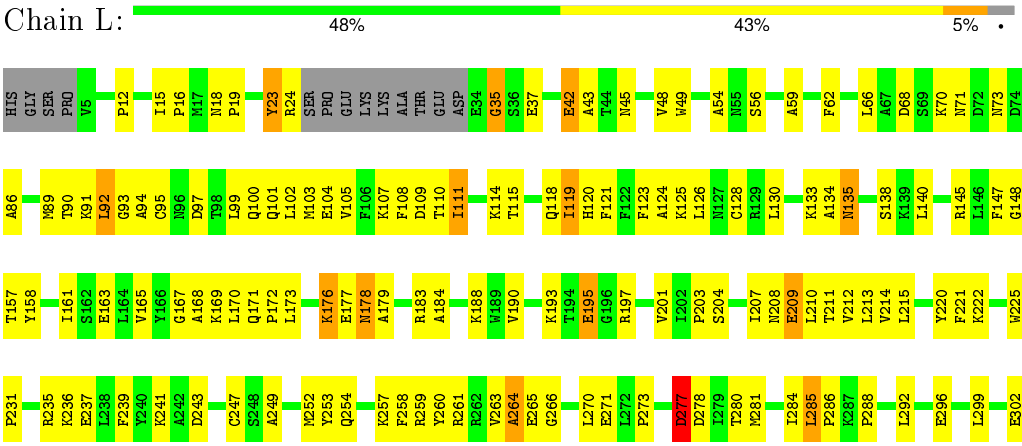
- Molecule 1: Antithrombin-III

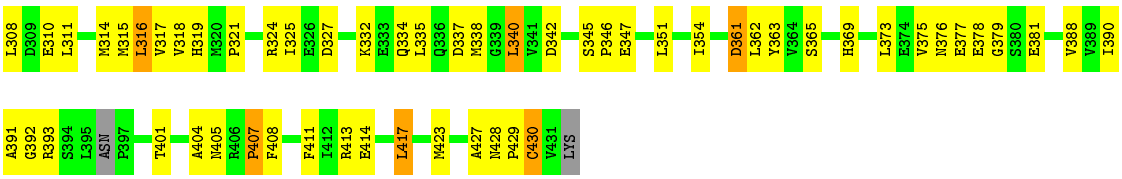
Chain I:



- Molecule 1: Antithrombin-III

Chain L:




L308
D309
E310
L311
M314
M315
L316
V317
V318
H319
M320
P321
R324
I325
E326
D327
K332
E333
Q334
L335
Q336
D337
M338
G339
L340
V341
D342
S345
P346
E347
L351
I354
D361
L362
Y363
V364
S365
H369
L373
E374
V375
N376
E377
E378
G379
S380
E381
V388
V389
I390
A391
G392
R393
S394
L395
ASN
P397
T401
A404
N405
R406
P407
F408
F411
I412
R413
E414
L417
M423
A427
N428
P429
C430
V431
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.85Å 87.06Å 92.38Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	63.24 – 3.00 63.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (63.24-3.00) 99.1 (63.24-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.289 0.235 , 0.293	Depositor DCC
R_{free} test set	1016 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	70.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	3 of 20055 reflections (0.015%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6574	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	I	0.43	0/3076	0.67	0/4187
1	L	0.46	0/3211	0.74	2/4365 (0.0%)
All	All	0.44	0/6287	0.70	2/8552 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
3	I	1	0
6	L	1	0
All	All	2	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	35	GLY	N-CA-C	6.30	128.86	113.10
1	L	95	CYS	N-CA-C	5.19	125.02	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	843	MAN	C1
6	L	863	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	63	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3016	0	2762	223	0
1	L	3148	0	2933	170	0
2	I	14	0	13	0	0
2	L	14	0	13	0	0
3	I	38	0	30	8	0
4	I	28	0	25	2	0
4	L	28	0	25	2	0
5	I	91	0	51	3	0
5	L	91	0	51	5	0
6	L	61	0	52	4	0
7	I	24	0	0	2	0
7	L	21	0	0	0	0
All	All	6574	0	5955	401	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 32.

All (401) 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:332:LYS:O	1:I:336:GLN:HG3	1.71	0.89
1:L:258:PHE:HB2	1:L:316:LEU:HD21	1.55	0.88
1:L:178:ASN:N	1:L:178:ASN:HD22	1.68	0.88
6:L:861:NAG:H62	6:L:862:NAG:HN2	1.39	0.88
1:L:102:LEU:HD23	1:L:340:LEU:HD21	1.56	0.87
1:L:171:GLN:HE21	1:L:173:LEU:HD21	1.39	0.85
1:L:365:SER:HB3	1:L:392:GLY:H	1.41	0.85
1:I:390:ILE:HG12	1:L:319:HIS:HB2	1.61	0.80
1:I:316:LEU:HD23	1:I:316:LEU:H	1.45	0.80
1:I:93:GLY:HA2	1:I:353:GLY:HA3	1.64	0.80
1:I:186:ILE:O	1:I:189:TRP:N	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:LEU:HD23	1:L:407:PRO:HG2	1.65	0.79
1:I:258:PHE:HB2	1:I:316:LEU:HD21	1.63	0.79
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.65	0.78
1:L:292:LEU:CD2	1:L:407:PRO:HG2	2.14	0.78
1:L:286:PRO:HG3	1:L:292:LEU:HD13	1.67	0.77
6:L:861:NAG:C6	6:L:862:NAG:HN2	1.99	0.75
1:I:90:THR:C	1:I:92:LEU:H	1.90	0.74
1:I:395:LEU:HB2	1:I:399:ARG:HH12	1.53	0.74
1:L:172:PRO:O	1:L:173:LEU:HD23	1.88	0.74
1:I:148:GLY:HA3	1:I:170:LEU:HD21	1.70	0.74
1:I:47:ARG:HH21	1:I:114:LYS:HZ3	1.37	0.73
1:I:302:GLU:CD	1:I:302:GLU:H	1.90	0.73
1:L:428:ASN:OD1	1:L:430:CYS:HB2	1.88	0.73
4:L:841:NAG:H62	4:L:842:NAG:O5	1.89	0.72
1:I:93:GLY:CA	1:I:353:GLY:HA3	2.19	0.72
5:L:869:NTO:O27	5:L:869:NTO:H1K	1.89	0.72
3:I:842:NAG:N2	3:I:842:NAG:C3	2.53	0.72
1:I:354:ILE:HD12	1:I:354:ILE:N	2.04	0.72
1:I:286:PRO:HB3	1:I:295:VAL:HG21	1.72	0.72
1:L:158:TYR:CE2	1:L:354:ILE:HG23	2.26	0.71
1:L:190:VAL:HG11	1:L:201:VAL:HG21	1.70	0.71
1:L:114:LYS:NZ	5:L:869:NTO:O3C	2.24	0.71
1:I:386:THR:HG22	1:I:387:ALA:N	2.05	0.71
1:I:187:ASN:ND2	1:I:200:ASP:HA	2.05	0.70
1:I:147:PHE:CE1	1:I:186:ILE:HG12	2.27	0.69
1:L:111:ILE:HD12	1:L:115:THR:HG22	1.73	0.69
1:L:91:LYS:HE2	1:L:103:MET:HE3	1.72	0.69
1:L:119:ILE:HD12	1:L:120:HIS:H	1.58	0.69
1:I:415:VAL:HG13	1:I:416:PRO:HA	1.74	0.69
1:L:299:LEU:HD11	1:L:304:LEU:HD21	1.75	0.69
1:I:380:SER:C	1:I:382:ALA:H	1.95	0.69
1:L:177:GLU:C	1:L:178:ASN:HD22	1.94	0.69
1:L:92:LEU:HD11	1:L:161:ILE:HG21	1.75	0.69
1:I:202:ILE:HG22	1:I:203:PRO:HD2	1.74	0.68
1:I:47:ARG:NH2	1:I:114:LYS:HZ3	1.90	0.68
1:I:229:PHE:HB2	1:I:377:GLU:HA	1.76	0.68
1:L:15:ILE:N	1:L:16:PRO:HD3	2.08	0.68
1:I:134:ALA:HB1	1:I:137:SER:N	2.08	0.68
1:L:178:ASN:N	1:L:178:ASN:ND2	2.40	0.68
1:I:148:GLY:CA	1:I:170:LEU:HD21	2.24	0.68
1:I:386:THR:HG22	1:I:387:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:GLY:N	1:I:170:LEU:HD21	2.09	0.67
1:L:93:GLY:O	1:L:351:LEU:HA	1.94	0.67
1:L:270:LEU:HD12	1:L:271:GLU:N	2.10	0.67
1:I:51:LEU:HD21	1:I:123:PHE:CD2	2.29	0.67
1:I:187:ASN:HD22	1:I:200:ASP:HA	1.59	0.67
1:L:119:ILE:HD12	1:L:120:HIS:N	2.09	0.67
1:I:395:LEU:HB2	1:I:399:ARG:NH1	2.10	0.66
5:I:863:NTO:H1K	5:I:863:NTO:O27	1.95	0.66
1:I:194:THR:HG21	1:I:198:ILE:HB	1.78	0.66
1:I:332:LYS:HG2	1:I:336:GLN:NE2	2.10	0.65
1:L:100:GLN:O	1:L:104:GLU:HG3	1.96	0.65
3:I:842:NAG:C1	3:I:842:NAG:N2	2.60	0.65
1:I:94:ALA:HA	1:I:351:LEU:HD23	1.79	0.65
1:I:60:THR:O	1:I:64:GLN:HG3	1.97	0.65
6:L:864:MAN:H62	6:L:864:MAN:O2	1.95	0.64
1:L:70:LYS:HE2	1:L:75:ASN:O	1.98	0.64
1:I:181:GLN:O	1:I:184:ALA:HB3	1.97	0.64
1:I:352:PRO:HA	1:I:355:VAL:HG22	1.80	0.64
1:L:119:ILE:O	1:L:123:PHE:HB2	1.98	0.64
1:L:229:PHE:HB2	1:L:377:GLU:HA	1.80	0.64
1:I:47:ARG:HH21	1:I:114:LYS:NZ	1.95	0.64
1:L:209:GLU:OE1	1:L:210:LEU:HG	1.98	0.64
1:L:195:GLU:HG3	1:L:220:TYR:CZ	2.32	0.64
1:L:270:LEU:HD12	1:L:271:GLU:H	1.60	0.64
1:L:179:ALA:HB1	1:L:207:ILE:O	1.97	0.63
1:I:186:ILE:CG2	1:I:202:ILE:HD11	2.29	0.63
1:I:285:LEU:HD12	1:I:286:PRO:HD2	1.81	0.63
1:I:214:VAL:HG13	1:I:366:ASP:O	2.00	0.62
1:I:71:ASN:HD21	1:I:73:ASN:HB2	1.64	0.62
1:L:171:GLN:NE2	1:L:173:LEU:HD21	2.13	0.62
1:I:23:TYR:O	1:I:24:ARG:NH1	2.31	0.62
1:I:12:PRO:HG3	1:I:121:PHE:CE2	2.35	0.62
1:I:302:GLU:CD	1:I:302:GLU:N	2.54	0.61
1:L:111:ILE:HD12	1:L:115:THR:CG2	2.30	0.61
1:L:124:ALA:HB2	1:L:165:VAL:HG13	1.82	0.61
1:I:180:GLU:C	1:I:182:SER:N	2.52	0.61
1:L:91:LYS:CD	1:L:103:MET:HE3	2.31	0.61
1:I:7:ILE:HD12	1:I:7:ILE:H	1.66	0.61
1:I:96:ASN:OD1	1:I:97:ASP:N	2.28	0.61
1:I:120:HIS:HD2	1:I:121:PHE:H	1.49	0.60
1:I:377:GLU:CD	1:I:377:GLU:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LEU:HD23	1:I:382:ALA:CB	2.32	0.60
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.84	0.60
1:I:396:ASN:HD21	1:I:398:ASN:HB3	1.65	0.60
1:I:101:GLN:O	1:I:105:VAL:HG23	2.02	0.60
1:I:101:GLN:OE1	1:I:342:ASP:HB2	2.01	0.59
1:I:47:ARG:NH2	1:I:114:LYS:NZ	2.48	0.59
1:L:226:LYS:HD2	1:L:277:ASP:OD1	2.02	0.59
1:L:110:THR:O	1:L:111:ILE:HG23	2.01	0.59
1:I:47:ARG:HD2	1:I:115:THR:OG1	2.03	0.59
1:I:225:TRP:NE1	1:I:379:GLY:HA2	2.17	0.59
1:I:119:ILE:HG23	1:I:120:HIS:N	2.18	0.59
1:I:77:PHE:CE2	1:I:373:LEU:HB2	2.38	0.58
1:L:335:LEU:HD23	1:L:338:MET:HE3	1.84	0.58
1:I:120:HIS:CD2	1:I:121:PHE:H	2.22	0.58
1:L:104:GLU:HG2	1:L:109:ASP:OD2	2.03	0.58
1:L:375:VAL:HG12	1:L:376:ASN:N	2.19	0.58
1:L:92:LEU:HD11	1:L:161:ILE:CG2	2.34	0.58
1:I:180:GLU:C	1:I:182:SER:H	2.04	0.58
6:L:861:NAG:H62	6:L:862:NAG:N2	2.13	0.57
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.04	0.57
1:L:273:PRO:HA	1:L:280:THR:HG22	1.85	0.57
1:L:184:ALA:O	1:L:188:LYS:HB2	2.04	0.57
1:I:147:PHE:CD1	1:I:186:ILE:HG12	2.39	0.57
1:I:380:SER:O	1:I:382:ALA:N	2.36	0.57
1:I:146:LEU:HG	1:I:215:LEU:HD13	1.86	0.57
1:L:365:SER:CB	1:L:392:GLY:H	2.16	0.57
1:I:386:THR:HG23	1:L:315:MET:O	2.05	0.57
1:L:263:VAL:CG1	1:L:264:ALA:N	2.68	0.56
1:I:140:LEU:HD11	1:I:219:ILE:HD11	1.86	0.56
1:L:285:LEU:HD12	1:L:408:PHE:HB2	1.87	0.56
3:I:842:NAG:C1	3:I:842:NAG:C3	2.83	0.56
1:L:91:LYS:CE	1:L:103:MET:HE3	2.34	0.56
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.40	0.56
1:I:90:THR:O	1:I:92:LEU:N	2.38	0.56
1:I:71:ASN:HB3	1:I:74:ASP:OD2	2.06	0.56
1:I:391:ALA:O	1:L:321:PRO:HD3	2.04	0.56
1:I:90:THR:C	1:I:92:LEU:N	2.59	0.56
1:I:197:ARG:HG3	1:I:220:TYR:CZ	2.41	0.56
1:I:390:ILE:HG12	1:L:319:HIS:CB	2.33	0.55
1:I:186:ILE:HD12	1:I:202:ILE:CD1	2.36	0.55
1:L:188:LYS:HD3	1:L:188:LYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:121:PHE:O	1:L:124:ALA:HB3	2.07	0.55
1:I:266:GLY:O	1:I:267:THR:C	2.45	0.55
1:L:286:PRO:CG	1:L:292:LEU:HD13	2.36	0.55
1:L:130:LEU:HD23	1:L:414:GLU:OE1	2.07	0.55
4:I:861:NAG:O7	4:I:861:NAG:H3	2.06	0.55
1:L:123:PHE:O	1:L:126:LEU:HB3	2.06	0.54
1:L:140:LEU:HD12	1:L:220:TYR:O	2.08	0.54
1:L:284:ILE:HD12	1:L:411:PHE:HE1	1.72	0.54
1:L:236:LYS:HA	1:L:249:ALA:O	2.08	0.54
1:I:20:MET:HE3	3:I:841:NAG:H2	1.87	0.54
1:I:148:GLY:O	1:I:172:PRO:HA	2.07	0.54
1:I:301:PRO:HB2	1:I:302:GLU:OE2	2.07	0.54
1:I:225:TRP:CD1	1:I:379:GLY:HA2	2.42	0.54
1:I:415:VAL:CG1	1:I:416:PRO:HA	2.38	0.54
1:I:366:ASP:HB3	1:I:368:PHE:CZ	2.43	0.54
1:I:270:LEU:HD12	1:I:271:GLU:N	2.22	0.54
1:L:404:ALA:HB3	1:L:427:ALA:HB1	1.90	0.54
1:L:208:ASN:HD22	1:L:393:ARG:HD3	1.73	0.54
1:I:146:LEU:HG	1:I:215:LEU:CD1	2.38	0.54
1:I:237:GLU:OE1	1:I:403:LYS:HE3	2.08	0.54
1:L:103:MET:HE1	1:L:108:PHE:CD2	2.43	0.53
1:L:15:ILE:N	1:L:16:PRO:CD	2.71	0.53
1:I:240:TYR:CD1	1:I:246:SER:HB3	2.43	0.53
1:I:48:VAL:HG21	5:I:863:NTO:O1A	2.08	0.53
1:I:278:ASP:O	1:I:414:GLU:HG2	2.08	0.53
1:I:197:ARG:HA	1:I:197:ARG:HE	1.72	0.53
1:L:91:LYS:HD3	1:L:103:MET:CE	2.38	0.53
1:I:197:ARG:HG3	1:I:220:TYR:OH	2.09	0.53
1:I:19:PRO:HB3	1:I:92:LEU:HD12	1.91	0.52
1:I:285:LEU:HD11	1:I:406:ARG:HG3	1.91	0.52
1:I:292:LEU:O	1:I:296:GLU:HG3	2.09	0.52
1:L:56:SER:O	1:L:59:ALA:HB3	2.09	0.52
1:I:396:ASN:ND2	1:I:398:ASN:HB3	2.24	0.52
1:L:404:ALA:O	1:L:405:ASN:HB2	2.10	0.52
1:I:335:LEU:O	1:I:338:MET:HB2	2.09	0.52
1:L:261:ARG:CB	1:L:311:LEU:HD23	2.40	0.52
1:L:176:LYS:O	1:L:209:GLU:HB3	2.10	0.52
1:L:259:ARG:NH2	1:L:311:LEU:O	2.41	0.52
1:L:149:ASP:HB3	1:L:152:LEU:HD12	1.92	0.52
1:I:62:PHE:CD2	1:I:338:MET:HE2	2.45	0.52
1:I:23:TYR:C	1:I:24:ARG:HH11	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:TYR:C	1:I:133:LYS:H	2.13	0.52
1:I:184:ALA:O	1:I:188:LYS:CB	2.58	0.51
1:I:224:LEU:HD23	1:I:382:ALA:HB1	1.93	0.51
1:L:77:PHE:CZ	1:L:373:LEU:HB2	2.45	0.51
1:L:125:LYS:O	1:L:128:CYS:HB2	2.10	0.51
1:I:119:ILE:HG23	1:I:120:HIS:H	1.74	0.51
1:L:302:GLU:CD	1:L:302:GLU:H	2.14	0.51
1:L:148:GLY:O	1:L:172:PRO:HA	2.10	0.51
1:I:386:THR:CG2	1:I:387:ALA:H	2.23	0.51
1:L:62:PHE:HD1	1:L:338:MET:CE	2.24	0.51
1:I:199:THR:O	1:I:200:ASP:C	2.49	0.51
1:I:272:LEU:HD12	1:I:283:LEU:HD11	1.92	0.50
1:I:71:ASN:ND2	1:I:73:ASN:HB2	2.26	0.50
1:L:211:THR:HA	1:L:391:ALA:O	2.11	0.50
1:L:91:LYS:HE2	1:L:119:ILE:HD11	1.93	0.50
1:L:24:ARG:HH12	1:L:109:ASP:HB2	1.77	0.50
1:L:213:LEU:HD22	1:L:354:ILE:HG21	1.93	0.50
1:I:386:THR:CG2	1:I:387:ALA:N	2.72	0.50
1:I:144:ASN:HB3	1:I:166:TYR:OH	2.12	0.50
1:L:225:TRP:NE1	1:L:376:ASN:O	2.41	0.50
1:I:243:ASP:OD1	1:I:243:ASP:N	2.43	0.50
1:I:335:LEU:HD23	1:I:338:MET:CE	2.42	0.50
1:I:325:ILE:HD11	1:I:426:VAL:HG22	1.94	0.50
1:I:186:ILE:HD12	1:I:202:ILE:HD11	1.94	0.49
1:I:187:ASN:OD1	1:I:202:ILE:HG13	2.12	0.49
1:I:270:LEU:HD23	1:I:402:PHE:CD1	2.47	0.49
1:L:48:VAL:HG21	5:L:869:NTO:O1A	2.12	0.49
1:I:219:ILE:HG12	1:I:220:TYR:N	2.27	0.49
1:I:155:ASN:OD1	1:I:356:ALA:HA	2.13	0.49
1:L:90:THR:OG1	1:L:215:LEU:HD22	2.11	0.49
1:L:401:THR:O	1:L:401:THR:HG22	2.12	0.49
1:L:145:ARG:HG2	1:L:147:PHE:CZ	2.48	0.49
1:L:261:ARG:HB3	1:L:311:LEU:HD23	1.94	0.49
1:I:197:ARG:HA	1:I:197:ARG:NE	2.28	0.49
1:L:125:LYS:HA	1:L:125:LYS:HE2	1.93	0.49
1:L:78:LEU:HB2	1:L:369:HIS:NE2	2.27	0.49
1:I:138:SER:CB	1:I:223:GLY:HA2	2.42	0.49
1:L:316:LEU:H	1:L:316:LEU:HD23	1.78	0.49
1:I:51:LEU:O	1:I:51:LEU:HD12	2.13	0.49
1:L:257:LYS:HA	1:L:314:MET:O	2.13	0.49
1:L:228:LYS:O	1:L:254:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:ILE:HD11	3:I:842:NAG:H82	1.95	0.48
1:L:62:PHE:HD1	1:L:338:MET:HE2	1.78	0.48
1:L:345:SER:O	1:L:347:GLU:N	2.46	0.48
1:L:163:GLU:OE2	1:L:169:LYS:HG2	2.13	0.48
1:L:263:VAL:HG12	1:L:264:ALA:N	2.27	0.48
1:I:403:LYS:HD3	1:I:405:ASN:ND2	2.28	0.48
1:L:163:GLU:HA	1:L:168:ALA:H	1.78	0.48
1:I:350:LYS:C	1:I:352:PRO:HD3	2.34	0.48
1:I:23:TYR:CE2	1:I:100:GLN:HG3	2.48	0.48
1:I:219:ILE:O	1:I:371:ALA:HA	2.13	0.48
4:I:861:NAG:C3	4:I:861:NAG:O7	2.62	0.48
1:I:39:LYS:O	1:I:41:PRO:HD3	2.13	0.48
1:I:120:HIS:CD2	1:I:121:PHE:N	2.81	0.48
1:I:20:MET:CE	3:I:841:NAG:H2	2.43	0.48
1:L:92:LEU:CD2	1:L:120:HIS:CE1	2.96	0.48
1:I:329:PHE:HB2	7:I:876:HOH:O	2.12	0.48
1:I:62:PHE:HD2	1:I:338:MET:CE	2.27	0.48
1:L:18:ASN:O	1:L:161:ILE:HD11	2.14	0.48
1:I:89:MET:SD	1:I:166:TYR:HB2	2.53	0.48
1:L:281:MET:HA	1:L:411:PHE:O	2.14	0.48
1:L:149:ASP:OD2	1:L:151:SER:N	2.43	0.48
1:L:91:LYS:CE	1:L:119:ILE:HD11	2.43	0.48
1:I:51:LEU:HD11	1:I:123:PHE:CE2	2.49	0.48
1:I:208:ASN:C	1:I:210:LEU:H	2.15	0.48
1:I:161:ILE:HD11	3:I:842:NAG:C8	2.44	0.47
1:I:411:PHE:CE2	1:I:423:MET:HE3	2.49	0.47
1:I:186:ILE:CB	1:I:202:ILE:HD11	2.45	0.47
1:I:316:LEU:CD2	1:I:316:LEU:H	2.20	0.47
1:L:324:ARG:O	1:L:325:ILE:HG22	2.14	0.47
1:I:283:LEU:HD23	1:I:408:PHE:CE2	2.49	0.47
1:I:316:LEU:HD23	1:I:316:LEU:N	2.20	0.47
1:L:208:ASN:HB3	1:L:393:ARG:CZ	2.43	0.47
1:L:221:PHE:CG	1:L:222:LYS:N	2.82	0.47
1:I:351:LEU:N	1:I:352:PRO:HD3	2.29	0.47
1:L:23:TYR:CG	1:L:24:ARG:N	2.80	0.47
1:I:180:GLU:O	1:I:180:GLU:CG	2.63	0.47
1:L:214:VAL:HA	1:L:388:VAL:O	2.14	0.47
1:I:190:VAL:HG21	1:I:201:VAL:HG21	1.97	0.47
1:L:253:TYR:CE1	1:L:317:VAL:HG13	2.49	0.47
1:I:155:ASN:N	1:I:354:ILE:O	2.37	0.47
1:L:304:LEU:O	1:L:308:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:TYR:HE2	1:I:100:GLN:HG3	1.80	0.47
1:I:352:PRO:HA	1:I:355:VAL:CG2	2.44	0.47
1:I:93:GLY:O	1:I:351:LEU:HA	2.15	0.47
1:L:225:TRP:CD1	1:L:379:GLY:HA2	2.50	0.47
1:I:319:HIS:CE1	1:I:403:LYS:HZ2	2.32	0.47
1:I:260:TYR:CG	1:I:261:ARG:N	2.82	0.46
1:L:120:HIS:HB3	1:L:165:VAL:HG11	1.97	0.46
1:L:230:SER:O	1:L:231:PRO:C	2.53	0.46
3:I:841:NAG:H5	3:I:842:NAG:O7	2.14	0.46
1:I:305:GLN:O	1:I:308:LEU:N	2.47	0.46
1:L:97:ASP:O	1:L:101:GLN:HG3	2.15	0.46
1:I:214:VAL:HG22	1:I:365:SER:OG	2.16	0.46
1:L:91:LYS:HD3	1:L:103:MET:HE2	1.97	0.46
1:I:120:HIS:N	1:I:120:HIS:CD2	2.83	0.46
1:I:7:ILE:HD13	1:I:128:CYS:SG	2.56	0.46
1:I:148:GLY:O	1:I:173:LEU:N	2.49	0.46
1:I:224:LEU:CD2	1:I:382:ALA:HB1	2.46	0.46
1:L:110:THR:O	1:L:111:ILE:CG2	2.63	0.46
1:L:91:LYS:CD	1:L:103:MET:CE	2.93	0.46
1:I:75:ASN:OD1	1:I:427:ALA:N	2.48	0.45
1:I:237:GLU:CD	1:I:251:MET:HG2	2.37	0.45
1:L:259:ARG:CZ	1:L:311:LEU:HB2	2.45	0.45
1:I:380:SER:C	1:I:382:ALA:N	2.64	0.45
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.97	0.45
1:I:158:TYR:CD2	1:I:354:ILE:HG23	2.51	0.45
1:L:91:LYS:HG3	1:L:99:LEU:CD1	2.47	0.45
1:L:259:ARG:NH1	1:L:311:LEU:HB2	2.31	0.45
1:I:228:LYS:O	1:I:254:GLN:NE2	2.50	0.45
1:I:257:LYS:HA	1:I:314:MET:O	2.17	0.45
1:I:157:THR:O	1:I:161:ILE:HG13	2.16	0.45
1:I:170:LEU:C	1:I:170:LEU:HD23	2.36	0.45
1:I:406:ARG:HB2	1:I:407:PRO:HD2	1.98	0.45
1:L:12:PRO:HB3	1:L:118:GLN:OE1	2.17	0.45
1:I:271:GLU:OE2	1:I:413:ARG:NH1	2.50	0.45
1:I:264:ALA:O	1:I:265:GLU:HB2	2.17	0.45
1:I:185:ALA:O	1:I:189:TRP:HB2	2.16	0.44
1:L:321:PRO:HG3	1:L:429:PRO:HB3	1.99	0.44
1:L:302:GLU:N	1:L:302:GLU:CD	2.71	0.44
1:L:417:LEU:N	1:L:417:LEU:CD2	2.80	0.44
1:I:9:THR:O	1:I:10:ALA:O	2.35	0.44
1:L:71:ASN:HD21	1:L:73:ASN:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:PHE:CE1	1:I:422:PHE:HB3	2.52	0.44
1:I:286:PRO:HB3	1:I:295:VAL:CG2	2.45	0.44
1:L:345:SER:C	1:L:347:GLU:H	2.19	0.44
1:I:209:GLU:O	1:I:209:GLU:HG2	2.17	0.44
1:L:292:LEU:HD22	1:L:407:PRO:O	2.17	0.44
1:L:114:LYS:HB2	5:L:869:NTO:H5F	1.99	0.44
1:L:375:VAL:CG1	1:L:376:ASN:N	2.80	0.44
1:I:261:ARG:HB3	1:I:311:LEU:HD23	2.00	0.44
1:I:322:ARG:O	1:I:323:PHE:HB3	2.18	0.44
1:I:108:PHE:O	1:I:111:ILE:HG12	2.16	0.44
1:L:23:TYR:O	1:L:24:ARG:CB	2.65	0.44
1:I:197:ARG:NH2	1:I:381:GLU:OE1	2.50	0.44
1:I:6:ASP:HA	7:I:886:HOH:O	2.17	0.44
1:I:89:MET:O	1:I:92:LEU:N	2.51	0.44
1:I:202:ILE:HG23	1:I:368:PHE:CD2	2.53	0.44
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.00	0.44
1:I:129:ARG:NH1	5:I:863:NTO:O18	2.51	0.44
1:L:163:GLU:OE2	1:L:169:LYS:CG	2.66	0.44
1:L:170:LEU:HD23	1:L:170:LEU:C	2.37	0.43
1:L:91:LYS:HD3	1:L:103:MET:HE3	2.00	0.43
1:I:411:PHE:HE2	1:I:423:MET:HE3	1.82	0.43
1:L:241:LYS:CE	1:L:247:CYS:SG	3.06	0.43
1:L:310:GLU:O	1:L:311:LEU:C	2.57	0.43
1:L:101:GLN:O	1:L:105:VAL:HG23	2.18	0.43
1:L:66:LEU:HD12	1:L:66:LEU:HA	1.90	0.43
1:L:197:ARG:NH2	1:L:381:GLU:OE1	2.51	0.43
1:L:212:VAL:HG12	1:L:213:LEU:N	2.32	0.43
1:I:329:PHE:CD2	1:I:329:PHE:N	2.86	0.43
1:I:231:PRO:HG3	1:I:377:GLU:HG2	2.00	0.43
1:I:42:GLU:O	1:I:43:ALA:C	2.56	0.43
1:L:134:ALA:O	1:L:135:ASN:C	2.57	0.43
1:I:390:ILE:HG12	1:L:319:HIS:ND1	2.34	0.43
1:I:89:MET:O	1:I:90:THR:C	2.58	0.43
1:I:186:ILE:O	1:I:188:LYS:N	2.52	0.42
1:I:197:ARG:HD3	1:I:381:GLU:OE1	2.18	0.42
1:L:345:SER:C	1:L:347:GLU:N	2.72	0.42
1:I:50:GLU:OE1	1:I:111:ILE:HB	2.19	0.42
1:I:315:MET:CE	1:I:395:LEU:HD21	2.49	0.42
1:I:76:ILE:HG22	1:I:77:PHE:N	2.34	0.42
1:L:42:GLU:HB3	1:L:43:ALA:H	1.51	0.42
1:I:351:LEU:HB3	1:I:354:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:ASN:ND2	1:I:55:ASN:O	2.53	0.42
1:I:253:TYR:CE1	1:I:317:VAL:HG13	2.53	0.42
1:I:354:ILE:CD1	1:I:354:ILE:N	2.76	0.42
1:I:171:GLN:NE2	1:I:172:PRO:HD2	2.34	0.42
1:L:260:TYR:CG	1:L:261:ARG:N	2.87	0.42
1:I:262:ARG:HD3	1:I:266:GLY:O	2.19	0.42
1:I:332:LYS:HE2	1:I:336:GLN:HE22	1.83	0.42
1:I:316:LEU:CD2	1:I:316:LEU:N	2.80	0.42
1:I:47:ARG:HG3	1:I:122:PHE:CE1	2.54	0.42
1:L:221:PHE:CD1	1:L:222:LYS:N	2.88	0.42
1:L:49:TRP:CD1	1:L:417:LEU:HB2	2.54	0.42
1:I:317:VAL:HG12	1:I:318:VAL:N	2.34	0.42
1:L:193:LYS:HD3	1:L:193:LYS:HA	1.85	0.42
1:L:308:LEU:HA	1:L:311:LEU:HG	2.01	0.42
1:I:353:GLY:C	1:I:354:ILE:HD12	2.38	0.42
1:I:395:LEU:CB	1:I:399:ARG:NH1	2.81	0.42
1:I:24:ARG:O	1:I:26:PRO:HD3	2.19	0.42
1:I:335:LEU:HD23	1:I:338:MET:HE1	2.00	0.42
1:I:231:PRO:C	1:I:233:ASN:H	2.23	0.42
1:I:323:PHE:HE2	1:I:373:LEU:HD23	1.85	0.42
1:L:163:GLU:O	1:L:167:GLY:HA2	2.20	0.42
1:I:92:LEU:HD23	1:I:158:TYR:CE1	2.55	0.41
1:I:341:VAL:HG13	1:I:342:ASP:N	2.34	0.41
1:I:230:SER:HA	1:I:231:PRO:HD3	1.95	0.41
1:L:273:PRO:CA	1:L:280:THR:HG22	2.49	0.41
1:L:423:MET:HE2	1:L:423:MET:HB2	1.91	0.41
1:L:252:MET:O	1:L:319:HIS:HA	2.21	0.41
1:L:346:PRO:HG3	1:L:363:TYR:CE2	2.55	0.41
1:I:332:LYS:CE	1:I:336:GLN:HE22	2.33	0.41
1:L:125:LYS:O	1:L:128:CYS:N	2.53	0.41
1:L:302:GLU:O	1:L:306:GLU:HB2	2.20	0.41
1:L:45:ASN:HB3	1:L:48:VAL:HG23	2.02	0.41
1:L:264:ALA:C	1:L:266:GLY:H	2.24	0.41
1:I:15:ILE:O	1:I:16:PRO:C	2.59	0.41
1:I:186:ILE:CD1	1:I:202:ILE:HD11	2.51	0.41
1:I:255:GLU:HG2	1:I:395:LEU:HD12	2.03	0.41
4:L:842:NAG:H3	4:L:842:NAG:O7	2.19	0.41
1:I:62:PHE:CD2	1:I:338:MET:CE	3.02	0.41
1:I:89:MET:O	1:I:91:LYS:N	2.54	0.41
1:L:292:LEU:O	1:L:296:GLU:HG3	2.21	0.41
5:L:869:NTO:H3L	5:L:869:NTO:O3K	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:PRO:HD3	1:L:121:PHE:CZ	2.56	0.41
1:L:278:ASP:OD1	1:L:278:ASP:N	2.47	0.41
1:L:253:TYR:HA	1:L:318:VAL:O	2.21	0.41
1:L:378:GLU:OE1	1:L:378:GLU:N	2.54	0.41
1:L:76:ILE:HA	1:L:327:ASP:OD2	2.21	0.41
1:I:332:LYS:HG2	1:I:336:GLN:HE21	1.86	0.40
1:I:148:GLY:H	1:I:170:LEU:HD21	1.82	0.40
1:L:86:ALA:O	1:L:89:MET:HB2	2.21	0.40
1:I:92:LEU:HD13	1:I:120:HIS:CE1	2.56	0.40
1:L:286:PRO:HD3	1:L:292:LEU:HD13	2.03	0.40
1:I:335:LEU:O	1:I:338:MET:N	2.50	0.40
1:I:336:GLN:C	1:I:338:MET:N	2.73	0.40
1:I:332:LYS:CG	1:I:336:GLN:NE2	2.83	0.40
1:I:75:ASN:OD1	1:I:426:VAL:HA	2.21	0.40
1:L:363:TYR:O	1:L:390:ILE:HG23	2.21	0.40
1:I:393:ARG:NH2	1:L:237:GLU:OE1	2.54	0.40
1:I:392:GLY:O	1:L:239:PHE:CE2	2.74	0.40
1:L:54:ALA:HB1	1:L:107:LYS:O	2.21	0.40
1:I:93:GLY:HA3	1:I:353:GLY:HA3	2.02	0.40
1:L:91:LYS:HD2	1:L:99:LEU:HD11	2.03	0.40
1:I:96:ASN:CG	1:I:97:ASP:H	2.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	394/432 (91%)	315 (80%)	63 (16%)	16 (4%)	3	20
1	L	411/432 (95%)	336 (82%)	55 (13%)	20 (5%)	3	16
All	All	805/864 (93%)	651 (81%)	118 (15%)	36 (4%)	3	18

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	10	ALA
1	I	186	ILE
1	I	348	LYS
1	I	430	CYS
1	L	42	GLU
1	L	264	ALA
1	I	43	ALA
1	I	237	GLU
1	I	349	SER
1	I	350	LYS
1	L	19	PRO
1	L	133	LYS
1	L	203	PRO
1	L	277	ASP
1	L	361	ASP
1	L	430	CYS
1	I	91	LYS
1	I	187	ASN
1	I	377	GLU
1	L	135	ASN
1	L	138	SER
1	L	150	LYS
1	L	332	LYS
1	I	90	THR
1	I	381	GLU
1	L	37	GLU
1	L	119	ILE
1	L	228	LYS
1	I	16	PRO
1	I	267	THR
1	L	195	GLU
1	I	208	ASN
1	L	35	GLY
1	L	68	ASP
1	L	111	ILE
1	L	288	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	299/383 (78%)	270 (90%)	29 (10%)	10 37
1	L	318/383 (83%)	294 (92%)	24 (8%)	17 51
All	All	617/766 (80%)	564 (91%)	53 (9%)	13 44

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	6	ASP
1	I	7	ILE
1	I	84	SER
1	I	95	CYS
1	I	113	GLU
1	I	114	LYS
1	I	118	GLN
1	I	120	HIS
1	I	123	PHE
1	I	128	CYS
1	I	141	VAL
1	I	157	THR
1	I	197	ARG
1	I	200	ASP
1	I	202	ILE
1	I	205	GLU
1	I	227	SER
1	I	277	ASP
1	I	278	ASP
1	I	302	GLU
1	I	304	LEU
1	I	316	LEU
1	I	333	GLU
1	I	334	GLN
1	I	342	ASP
1	I	362	LEU
1	I	413	ARG
1	I	414	GLU
1	I	417	LEU
1	L	23	TYR
1	L	92	LEU
1	L	157	THR
1	L	176	LYS

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Mol	Chain	Res	Type
1	L	178	ASN
1	L	183	ARG
1	L	204	SER
1	L	209	GLU
1	L	235	ARG
1	L	243	ASP
1	L	265	GLU
1	L	277	ASP
1	L	285	LEU
1	L	306	GLU
1	L	316	LEU
1	L	334	GLN
1	L	337	ASP
1	L	340	LEU
1	L	342	ASP
1	L	361	ASP
1	L	362	LEU
1	L	407	PRO
1	L	413	ARG
1	L	417	LEU

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

Mol	Chain	Res	Type
1	I	71	ASN
1	I	118	GLN
1	I	120	HIS
1	I	171	GLN
1	I	181	GLN
1	I	254	GLN
1	I	336	GLN
1	I	405	ASN
1	L	71	ASN
1	L	171	GLN
1	L	178	ASN
1	L	334	GLN
1	L	405	ASN

5.3.3 RNA

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)

12 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	I	841	1,3	14,14,15	0.64	0	15,19,21	1.08	1 (6%)
3	NAG	I	842	3	11,11,15	0.53	0	11,12,21	0.81	0
3	MAN	I	843	3	11,11,12	0.61	0	14,15,17	0.47	0
4	NAG	I	861	1,4	14,14,15	0.76	0	15,19,21	0.78	0
4	NAG	I	862	4	14,14,15	0.55	0	15,19,21	0.58	0
4	NAG	L	841	1,4	14,14,15	0.76	0	15,19,21	1.14	1 (6%)
4	NAG	L	842	4	14,14,15	0.70	1 (7%)	15,19,21	0.67	0
6	NAG	L	861	1,6	14,14,15	0.65	0	15,19,21	0.62	0
6	NAG	L	862	6	14,14,15	0.57	0	15,19,21	0.65	0
6	MAN	L	863	6	11,11,12	0.70	0	14,15,17	0.95	1 (7%)
6	MAN	L	864	6	11,11,12	0.70	0	14,15,17	1.30	1 (7%)
6	MAN	L	868	6	11,11,12	0.62	0	14,15,17	0.62	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	841	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	842	3	-	0/10/10/26	0/0/0/1
3	MAN	I	843	3	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	I	861	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	862	4	-	0/6/23/26	0/1/1/1
4	NAG	L	841	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	842	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	861	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	862	6	-	0/6/23/26	0/1/1/1
6	MAN	L	863	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	L	864	6	-	0/2/19/22	1/1/1/1
6	MAN	L	868	6	-	0/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	842	NAG	C1-C2	2.09	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	841	NAG	C2-N2-C7	-2.64	119.65	123.04
4	L	841	NAG	C3-C4-C5	2.61	114.74	110.20
6	L	863	MAN	C1-C2-C3	2.67	112.70	109.54
6	L	864	MAN	C1-O5-C5	4.33	117.75	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	863	MAN	C1
3	I	843	MAN	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	868	MAN	C1-C2-C3-C4-C5-O5
6	L	864	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	841	NAG	3	0
3	I	842	NAG	6	0
4	I	861	NAG	2	0
4	L	841	NAG	1	0
4	L	842	NAG	2	0
6	L	861	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	862	NAG	3	0
6	L	864	MAN	1	0

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	I	801	1	14,14,15	0.57	0	15,19,21	0.85	0
5	NTO	I	863	-	83,95,95	2.55	12 (14%)	109,150,150	1.10	8 (7%)
2	NAG	L	801	1	14,14,15	0.54	0	15,19,21	0.89	0
5	NTO	L	869	-	83,95,95	2.55	12 (14%)	109,150,150	1.13	8 (7%)

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
2	NAG	I	801	1	-	0/6/23/26	0/1/1/1
5	NTO	I	863	-	-	0/61/169/169	0/5/5/5
2	NAG	L	801	1	-	0/6/23/26	0/1/1/1
5	NTO	L	869	-	-	0/61/169/169	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	863	NTO	O54-S55	-4.32	1.43	1.57
5	L	869	NTO	O16-S17	-4.26	1.43	1.57
5	L	869	NTO	O54-S55	-4.26	1.43	1.57
5	I	863	NTO	O16-S17	-4.26	1.43	1.57
5	I	863	NTO	O34-S35	-4.25	1.43	1.57
5	L	869	NTO	O4A-S4B	-4.25	1.43	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	863	NTO	O4A-S4B	-4.23	1.43	1.57
5	L	869	NTO	O34-S35	-4.22	1.43	1.57
5	I	863	NTO	O3A-S3B	-4.22	1.43	1.57
5	L	869	NTO	O3A-S3B	-4.21	1.43	1.57
5	L	869	NTO	O5M-C5L	2.10	1.43	1.40
5	I	863	NTO	O5M-C5L	2.19	1.43	1.40
5	I	863	NTO	O3K-S3H	8.21	1.50	1.42
5	L	869	NTO	O5I-S5H	8.22	1.50	1.42
5	L	869	NTO	O5J-S5H	8.24	1.50	1.42
5	L	869	NTO	O1H-S1G	8.24	1.50	1.42
5	L	869	NTO	O3K-S3H	8.25	1.50	1.42
5	I	863	NTO	O5I-S5H	8.26	1.50	1.42
5	I	863	NTO	O1H-S1G	8.27	1.50	1.42
5	I	863	NTO	O3J-S3H	8.28	1.50	1.42
5	I	863	NTO	O1I-S1G	8.29	1.50	1.42
5	I	863	NTO	O5J-S5H	8.29	1.50	1.42
5	L	869	NTO	O3J-S3H	8.31	1.50	1.42
5	L	869	NTO	O1I-S1G	8.37	1.50	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	869	NTO	C49-O4A-S4B	-4.33	110.52	118.77
5	L	869	NTO	C39-O3A-S3B	-4.12	110.92	118.77
5	I	863	NTO	C49-O4A-S4B	-3.84	111.45	118.77
5	I	863	NTO	C39-O3A-S3B	-3.57	111.96	118.77
5	I	863	NTO	C4F-O4G-C50	-2.98	110.21	118.01
5	L	869	NTO	C3L-O3M-C40	-2.92	110.37	118.01
5	I	863	NTO	C1K-O1L-C20	-2.74	110.85	118.01
5	L	869	NTO	C5N-O5M-C5L	-2.68	108.91	113.29
5	I	863	NTO	C5N-O5M-C5L	-2.62	109.00	113.29
5	L	869	NTO	C1K-O1L-C20	-2.42	111.67	118.01
5	I	863	NTO	C2C-O2D-C30	-2.33	111.92	118.01
5	L	869	NTO	C4F-O4G-C50	-2.32	111.94	118.01
5	L	869	NTO	C2C-O2D-C30	-2.16	112.37	118.01
5	I	863	NTO	C3L-O3M-C40	-2.07	112.60	118.01
5	L	869	NTO	O5M-C5L-C5F	2.04	111.34	108.03
5	I	863	NTO	O16-C15-C13	2.53	112.77	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	863	NTO	3	0
5	L	869	NTO	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	I	404/432 (93%)	-0.37	1 (0%) 95 87	37, 65, 90, 100	0
1	L	417/432 (96%)	-0.39	0 100 100	33, 59, 90, 106	0
All	All	821/864 (95%)	-0.38	1 (0%) 95 90	33, 62, 90, 106	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	8	CYS	2.4

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	I	842	13/15	0.89	0.30	1.62	63,71,74,79	0
4	NAG	L	841	14/15	0.88	0.21	0.94	63,71,75,82	0
6	MAN	L	868	11/12	0.82	0.19	-0.23	76,81,83,84	0
3	NAG	I	841	14/15	0.91	0.19	-0.46	69,72,75,76	0
4	NAG	L	842	14/15	0.67	0.38	-	87,90,92,92	0
6	MAN	L	863	11/12	0.87	0.18	-	79,81,85,89	0
6	MAN	L	864	11/12	0.84	0.17	-	90,91,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	I	862	14/15	0.40	0.40	-	128,132,134,134	0
6	NAG	L	861	14/15	0.90	0.18	-	64,67,68,71	0
3	MAN	I	843	11/12	0.83	0.20	-	82,85,87,87	0
6	NAG	L	862	14/15	0.91	0.17	-	68,74,77,79	0
4	NAG	I	861	14/15	0.82	0.20	-	110,114,118,123	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NTO	I	863	91/91	0.88	0.22	0.24	76,97,110,116	0
5	NTO	L	869	91/91	0.85	0.22	0.08	86,100,111,113	0
2	NAG	L	801	14/15	0.88	0.22	-	80,81,83,83	0
2	NAG	I	801	14/15	0.71	0.21	-	105,107,108,109	6

6.5 Other polymers

There are no such residues in this entry.