



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2ANT  
Title : THE 2.6 Å STRUCTURE OF ANTITHROMBIN INDICATES A CONFORMATIONAL CHANGE AT THE HEPARIN BINDING SITE  
Authors : Skinner, R.; Abrahams, J.-P.; Whisstock, J.C.; Lesk, A.M.; Carrell, R.W.; Wardell, M.R.  
Deposited on : 1997-01-28  
Resolution : 2.60 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.

---

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

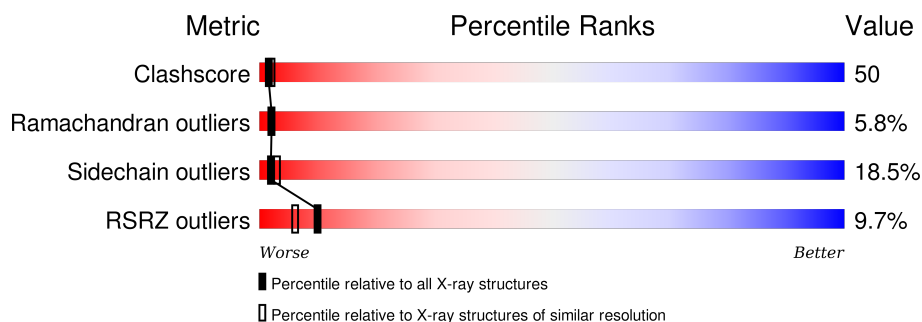
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

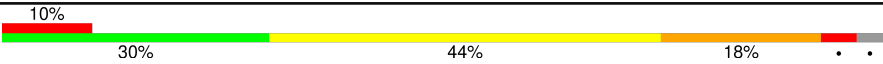
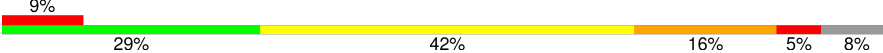
The reported resolution of this entry is 2.60 Å.

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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	432	
1	L	432	

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
2	NAA	L	500	X	-	-	-

## 2 Entry composition [i](#)

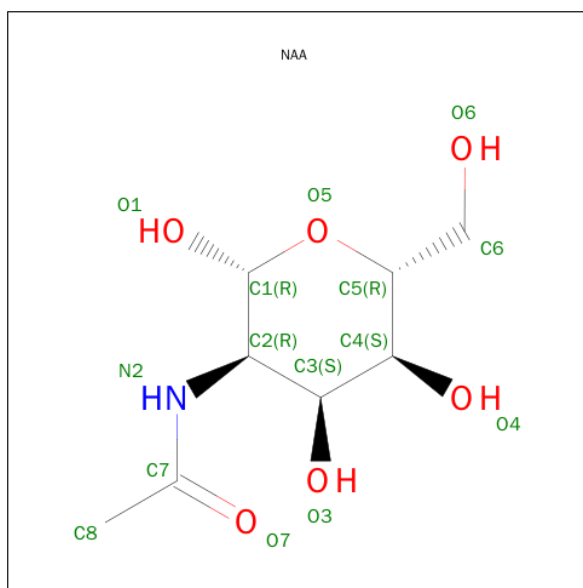
There are 3 unique types of molecules in this entry. The entry contains 6636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	398	Total	C	N	O	S	0	0	0
			3181	2029	534	600	18			
1	I	419	Total	C	N	O	S	0	0	0
			3348	2133	568	629	18			

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

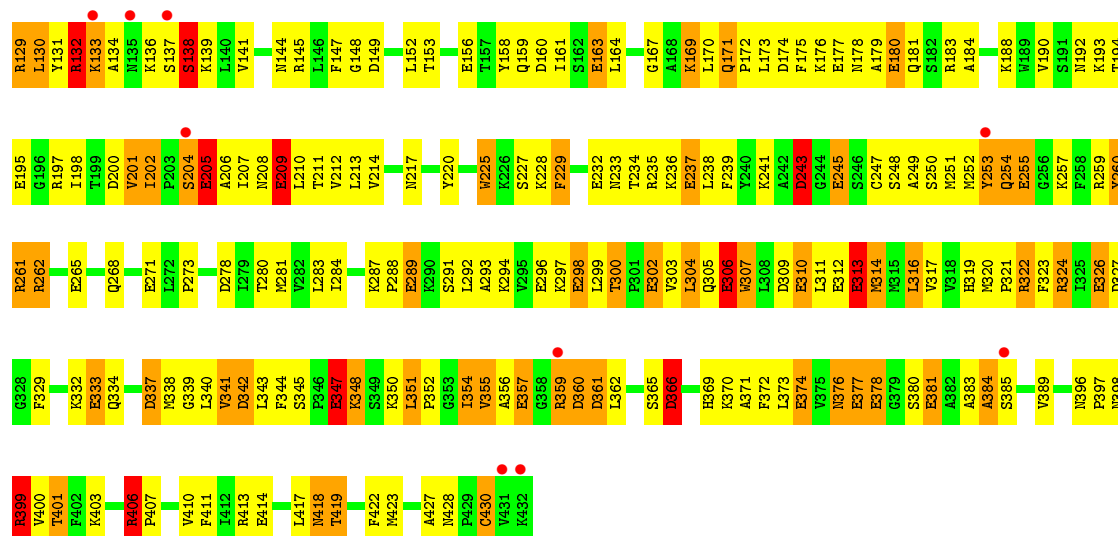


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	N	O	1	0
			14	8	1	5		
2	I	1	Total	C	N	O	1	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	42	Total 42	O 42	0	0
3	L	37	Total 37	O 37	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.41Å 98.31Å 90.41Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	26.90 – 2.60 19.92 – 2.62	Depositor EDS
% Data completeness (in resolution range)	74.0 (26.90-2.60) 78.3 (19.92-2.62)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.63Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, $R_{free}$	0.217 , 0.290 0.228 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 86.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25487 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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

### 5.1 Standard geometry

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

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	0.91	27/3415 (0.8%)	1.34	42/4608 (0.9%)
1	L	0.92	30/3240 (0.9%)	1.43	56/4367 (1.3%)
All	All	0.91	57/6655 (0.9%)	1.38	98/8975 (1.1%)

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	L	1	0

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	377	GLU	CD-OE2	6.52	1.32	1.25
1	L	104	GLU	CD-OE2	6.48	1.32	1.25
1	L	232	GLU	CD-OE2	6.23	1.32	1.25
1	I	312	GLU	CD-OE1	6.22	1.32	1.25
1	L	195	GLU	CD-OE2	6.19	1.32	1.25
1	L	156	GLU	CD-OE2	6.12	1.32	1.25
1	I	310	GLU	CD-OE2	6.11	1.32	1.25
1	L	271	GLU	CD-OE2	6.07	1.32	1.25
1	I	255	GLU	CD-OE2	6.06	1.32	1.25
1	I	245	GLU	CD-OE2	5.97	1.32	1.25
1	L	310	GLU	CD-OE2	5.87	1.32	1.25
1	L	180	GLU	CD-OE2	5.71	1.31	1.25
1	I	414	GLU	CD-OE2	5.69	1.31	1.25
1	I	180	GLU	CD-OE2	5.66	1.31	1.25
1	I	357	GLU	CD-OE2	5.64	1.31	1.25
1	L	296	GLU	CD-OE2	5.63	1.31	1.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	347	GLU	CD-OE2	5.62	1.31	1.25
1	I	163	GLU	CD-OE2	5.62	1.31	1.25
1	L	289	GLU	CD-OE2	5.62	1.31	1.25
1	I	302	GLU	CD-OE2	5.60	1.31	1.25
1	L	381	GLU	CD-OE2	5.59	1.31	1.25
1	L	313	GLU	CD-OE2	5.57	1.31	1.25
1	L	237	GLU	CD-OE2	5.57	1.31	1.25
1	L	378	GLU	CD-OE2	5.57	1.31	1.25
1	I	27	GLU	CD-OE2	5.54	1.31	1.25
1	L	209	GLU	CD-OE2	5.53	1.31	1.25
1	I	298	GLU	CD-OE2	5.52	1.31	1.25
1	L	163	GLU	CD-OE2	5.50	1.31	1.25
1	L	347	GLU	CD-OE2	5.50	1.31	1.25
1	I	306	GLU	CD-OE2	5.47	1.31	1.25
1	L	255	GLU	CD-OE2	5.47	1.31	1.25
1	I	104	GLU	CD-OE2	5.46	1.31	1.25
1	L	333	GLU	CD-OE2	5.46	1.31	1.25
1	I	326	GLU	CD-OE2	5.44	1.31	1.25
1	I	205	GLU	CD-OE2	5.44	1.31	1.25
1	I	237	GLU	CD-OE2	5.43	1.31	1.25
1	L	177	GLU	CD-OE1	5.40	1.31	1.25
1	L	357	GLU	CD-OE1	5.38	1.31	1.25
1	I	209	GLU	CD-OE2	5.37	1.31	1.25
1	L	205	GLU	CD-OE2	5.35	1.31	1.25
1	L	326	GLU	CD-OE1	5.31	1.31	1.25
1	I	177	GLU	CD-OE2	5.30	1.31	1.25
1	I	289	GLU	CD-OE2	5.29	1.31	1.25
1	L	113	GLU	CD-OE2	5.28	1.31	1.25
1	L	374	GLU	CD-OE1	5.24	1.31	1.25
1	I	313	GLU	CD-OE1	5.23	1.31	1.25
1	L	312	GLU	CD-OE2	5.22	1.31	1.25
1	I	232	GLU	CD-OE2	5.22	1.31	1.25
1	L	298	GLU	CD-OE2	5.22	1.31	1.25
1	I	50	GLU	CD-OE2	5.22	1.31	1.25
1	L	302	GLU	CD-OE1	5.22	1.31	1.25
1	I	195	GLU	CD-OE2	5.22	1.31	1.25
1	L	306	GLU	CD-OE2	5.20	1.31	1.25
1	L	50	GLU	CD-OE2	5.10	1.31	1.25
1	L	407	PRO	N-CD	5.10	1.54	1.47
1	I	333	GLU	CD-OE2	5.09	1.31	1.25
1	I	381	GLU	CD-OE2	5.01	1.31	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	406	ARG	C-N-CD	-27.57	59.94	120.60
1	I	406	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	L	18	ASN	C-N-CD	-10.48	97.55	120.60
1	I	3	SER	C-N-CD	-10.25	98.05	120.60
1	L	135	ASN	N-CA-C	9.99	137.97	111.00
1	L	407	PRO	CA-N-CD	-9.95	97.57	111.50
1	L	135	ASN	CA-C-N	-9.40	96.51	117.20
1	L	134	ALA	C-N-CA	8.61	143.24	121.70
1	I	261	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	L	407	PRO	N-CA-CB	8.03	112.93	103.30
1	L	408	PHE	N-CA-C	7.89	132.29	111.00
1	L	174	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	L	359	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	L	135	ASN	C-N-CA	7.67	140.86	121.70
1	I	366	ASP	CB-CG-OD1	7.41	124.97	118.30
1	I	278	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	L	109	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	I	261	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	L	243	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	L	200	ASP	CB-CG-OD1	7.05	124.64	118.30
1	I	342	ASP	CB-CG-OD1	7.04	124.64	118.30
1	L	337	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	I	174	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	L	97	ASP	CB-CG-OD1	6.80	124.42	118.30
1	L	277	ASP	CB-CG-OD2	6.76	124.39	118.30
1	I	74	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	L	112	SER	N-CA-CB	6.75	120.63	110.50
1	L	97	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	L	277	ASP	CB-CG-OD1	-6.65	112.32	118.30
1	I	200	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	I	74	ASP	CB-CG-OD1	6.59	124.23	118.30
1	I	366	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	I	278	ASP	CB-CG-OD1	6.55	124.20	118.30
1	L	407	PRO	C-N-CA	6.49	137.94	121.70
1	I	399	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	L	149	ASP	CB-CG-OD1	6.35	124.01	118.30
1	L	14	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	L	243	ASP	CB-CG-OD1	6.30	123.97	118.30
1	I	342	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	I	117	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	L	366	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	L	360	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	L	14	ASP	CB-CG-OD1	6.12	123.81	118.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	337	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	I	14	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	L	309	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	I	109	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	L	117	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	I	14	ASP	CB-CG-OD1	5.90	123.61	118.30
1	L	342	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	L	200	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	L	174	ASP	CB-CG-OD1	5.82	123.54	118.30
1	I	68	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	L	135	ASN	CA-C-O	5.78	132.24	120.10
1	I	337	ASP	CB-CG-OD1	5.78	123.50	118.30
1	L	337	ASP	CB-CG-OD1	5.72	123.45	118.30
1	I	174	ASP	CB-CG-OD1	5.72	123.45	118.30
1	I	6	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	L	68	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	I	309	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	I	361	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	L	361	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	L	261	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	L	309	ASP	CB-CG-OD1	5.56	123.30	118.30
1	L	149	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	L	109	ASP	CB-CG-OD1	5.53	123.28	118.30
1	L	406	ARG	C-N-CA	5.49	145.06	122.00
1	I	399	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	I	160	ASP	CB-CG-OD1	5.48	123.23	118.30
1	I	72	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	I	97	ASP	CA-CB-CG	-5.44	101.43	113.40
1	L	74	ASP	CB-CG-OD1	5.42	123.18	118.30
1	I	360	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	I	243	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	I	132	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	L	74	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	L	235	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	L	135	ASN	O-C-N	5.30	131.18	122.70
1	I	327	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	L	361	ASP	CB-CG-OD1	5.26	123.03	118.30
1	L	68	ASP	CB-CG-OD1	5.24	123.01	118.30
1	I	360	ASP	CB-CG-OD1	5.23	123.01	118.30
1	I	68	ASP	CB-CG-OD1	5.21	122.99	118.30
1	L	327	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	I	262	ARG	NE-CZ-NH2	-5.21	117.70	120.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	327	ASP	CB-CG-OD1	5.18	122.97	118.30
1	L	324	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	L	278	ASP	CB-CG-OD1	5.16	122.95	118.30
1	L	135	ASN	CB-CA-C	-5.16	100.08	110.40
1	I	97	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	I	117	ASP	CB-CG-OD1	5.12	122.91	118.30
1	L	197	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	I	361	ASP	CB-CG-OD1	5.10	122.89	118.30
1	L	360	ASP	CB-CG-OD1	5.09	122.88	118.30
1	L	72	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	I	109	ASP	CB-CG-OD1	5.07	122.86	118.30
1	I	112	SER	CB-CA-C	5.03	119.66	110.10
1	L	322	ARG	NE-CZ-NH1	5.01	122.81	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	112	SER	CA

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3348	0	3357	348	10
1	L	3181	0	3183	316	10
2	I	14	0	12	1	0
2	L	14	0	12	2	0
3	I	42	0	0	10	0
3	L	37	0	0	8	0
All	All	6636	0	6564	662	10

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 50.

All (662) 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:L:50:GLU:HB3	1:L:111:ILE:HG22	1.22	1.19
1:L:355:VAL:HG13	1:L:359:ARG:HD2	1.31	1.08
1:L:355:VAL:H	1:L:359:ARG:HD3	1.20	1.06
1:I:75:ASN:ND2	1:I:427:ALA:H	1.56	1.04
1:I:152:LEU:HA	1:I:356:ALA:HB1	1.40	1.03
1:I:359:ARG:NH1	1:I:360:ASP:H	1.57	1.03
1:I:1:HIS:CD2	1:I:124:ALA:HB1	1.99	0.97
1:I:75:ASN:HD21	1:I:428:ASN:H	1.06	0.95
1:I:11:LYS:HB3	1:I:12:PRO:HD3	1.47	0.94
1:L:355:VAL:HG13	1:L:359:ARG:CD	2.00	0.91
1:L:359:ARG:NE	1:L:362:LEU:HD13	1.87	0.90
1:I:75:ASN:HD22	1:I:427:ALA:H	1.20	0.90
1:I:5:VAL:HG21	1:I:133:LYS:NZ	1.86	0.89
1:L:283:LEU:HD13	1:L:408:PHE:HZ	1.35	0.89
1:L:179:ALA:HB1	1:L:207:ILE:HG22	1.56	0.88
1:I:314:MET:CE	1:I:400:VAL:HG13	2.04	0.87
1:I:62:PHE:HA	1:I:338:MET:HE1	1.55	0.87
1:I:7:ILE:HD12	1:I:9:THR:HB	1.56	0.87
1:L:7:ILE:HG12	1:L:16:PRO:HG2	1.57	0.87
1:L:62:PHE:HA	1:L:338:MET:HE2	1.56	0.86
1:L:355:VAL:N	1:L:359:ARG:HD3	1.91	0.86
1:L:86:ALA:HA	1:L:89:MET:HE3	1.56	0.85
1:L:18:ASN:HA	1:L:161:ILE:HD11	1.58	0.85
1:L:283:LEU:HD13	1:L:408:PHE:CZ	2.12	0.84
1:L:158:TYR:CE2	1:L:354:ILE:HG23	2.13	0.83
1:L:237:GLU:HG3	1:L:238:LEU:H	1.43	0.83
1:L:252:MET:HE1	1:L:377:GLU:N	1.94	0.83
1:L:252:MET:HE3	1:L:376:ASN:HA	1.61	0.83
1:I:75:ASN:HD21	1:I:428:ASN:N	1.76	0.83
1:I:359:ARG:HG3	1:I:360:ASP:N	1.94	0.81
1:L:78:LEU:HD22	1:L:80:PRO:HD3	1.61	0.81
1:L:293:ALA:HB1	1:L:297:LYS:NZ	1.95	0.81
1:I:16:PRO:HA	1:I:161:ILE:HD11	1.61	0.81
1:I:53:LYS:HZ3	1:I:57:ARG:HH22	1.28	0.81
1:I:71:ASN:HD21	1:I:73:ASN:HB2	1.44	0.80
1:L:44:THR:HG23	1:L:47:ARG:NH1	1.95	0.80
1:I:15:ILE:N	1:I:16:PRO:HD3	1.96	0.80
1:I:133:LYS:HG2	1:I:134:ALA:N	1.96	0.80
1:I:406:ARG:HH11	1:I:406:ARG:HG2	1.45	0.80
1:I:23:TYR:HB2	1:I:100:GLN:HE22	1.46	0.80
1:L:73:ASN:HB3	1:L:405:ASN:N	1.96	0.80
1:I:75:ASN:ND2	1:I:427:ALA:N	2.29	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:432:LYS:H	1:L:432:LYS:HD3	1.46	0.79
1:I:5:VAL:H	1:I:132:ARG:HB2	1.47	0.79
1:I:129:ARG:HG2	1:I:417:LEU:HD11	1.62	0.79
1:I:91:LYS:HE2	1:I:103:MET:SD	2.22	0.79
1:L:24:ARG:HB3	1:L:114:LYS:CE	2.14	0.78
1:L:62:PHE:HA	1:L:338:MET:CE	2.13	0.78
1:I:345:SER:OG	1:I:348:LYS:HB2	1.83	0.78
1:I:12:PRO:CG	1:I:15:ILE:HB	2.13	0.78
1:L:86:ALA:HA	1:L:89:MET:CE	2.13	0.78
1:I:83:ILE:HD13	1:I:217:ASN:HD21	1.48	0.78
1:L:50:GLU:HB3	1:L:111:ILE:CG2	2.10	0.78
1:I:153:THR:H	1:I:356:ALA:CB	1.97	0.78
1:I:53:LYS:HZ3	1:I:57:ARG:NH2	1.80	0.78
1:L:324:ARG:O	1:L:431:VAL:HG11	1.84	0.77
1:I:47:ARG:HD2	1:I:122:PHE:CE1	2.19	0.77
1:I:53:LYS:HZ3	1:I:57:ARG:HH12	1.32	0.77
1:L:101:GLN:O	1:L:105:VAL:HG23	1.85	0.77
1:I:284:ILE:HD12	1:I:411:PHE:HE1	1.50	0.77
1:I:183:ARG:HB2	1:I:207:ILE:HD12	1.67	0.76
1:I:53:LYS:HZ3	1:I:57:ARG:NH1	1.83	0.76
1:L:354:ILE:HB	1:L:359:ARG:CZ	2.15	0.76
1:I:5:VAL:HG22	1:I:132:ARG:HG2	1.68	0.75
1:I:281:MET:HE2	1:I:283:LEU:HD21	1.66	0.75
1:L:261:ARG:HD3	1:L:310:GLU:O	1.86	0.75
1:I:47:ARG:HD2	1:I:122:PHE:HE1	1.51	0.75
1:L:20:MET:HB3	3:L:504:HOH:O	1.87	0.75
1:I:53:LYS:NZ	1:I:57:ARG:HH22	1.84	0.74
1:I:294:LYS:O	1:I:298:GLU:HG3	1.87	0.74
1:L:262:ARG:HE	1:L:266:GLY:HA2	1.53	0.74
1:L:261:ARG:NH2	1:L:310:GLU:HG2	2.02	0.74
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.23	0.74
1:I:12:PRO:CB	1:I:15:ILE:HB	2.17	0.74
1:L:24:ARG:HB3	1:L:114:LYS:HE3	1.69	0.73
1:L:261:ARG:CZ	1:L:310:GLU:HG2	2.18	0.73
1:L:121:PHE:CZ	1:L:125:LYS:HE2	2.23	0.73
1:I:314:MET:HE3	1:I:400:VAL:HG13	1.70	0.73
1:L:53:LYS:O	1:L:57:ARG:HG3	1.89	0.73
1:L:234:THR:HG22	1:L:252:MET:HA	1.68	0.73
1:L:47:ARG:HG2	1:L:47:ARG:HH11	1.54	0.73
1:I:316:LEU:HG	1:I:400:VAL:HG22	1.71	0.72
1:L:237:GLU:HG3	1:L:238:LEU:N	2.04	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.70	0.72
1:L:359:ARG:HE	1:L:362:LEU:HD13	1.53	0.72
1:L:92:LEU:HD13	1:L:120:HIS:NE2	2.05	0.72
1:I:45:ASN:ND2	1:I:46:ARG:HG3	2.03	0.72
1:L:252:MET:CE	1:L:322:ARG:HB2	2.20	0.72
1:I:1:HIS:HB2	1:I:9:THR:CG2	2.19	0.72
1:I:60:THR:O	1:I:64:GLN:HG3	1.90	0.72
1:I:322:ARG:HD2	3:I:535:HOH:O	1.90	0.72
1:L:7:ILE:HG22	1:L:124:ALA:HB1	1.70	0.71
1:I:121:PHE:CE1	1:I:125:LYS:HE3	2.25	0.71
1:L:355:VAL:HG12	1:L:359:ARG:HH11	1.55	0.71
1:I:26:PRO:HG2	1:I:29:LYS:O	1.89	0.71
1:I:304:LEU:O	1:I:307:TRP:HB2	1.90	0.71
1:I:16:PRO:HG2	1:I:117:ASP:OD2	1.89	0.71
1:L:238:LEU:HD21	1:L:240:TYR:HE2	1.54	0.71
1:L:59:ALA:O	1:L:423:MET:HE1	1.90	0.71
1:I:5:VAL:HG21	1:I:133:LYS:HZ2	1.54	0.71
1:I:334:GLN:O	1:I:338:MET:HG3	1.90	0.71
1:I:236:LYS:HA	1:I:249:ALA:O	1.91	0.71
1:L:113:GLU:O	1:L:115:THR:HG22	1.91	0.71
1:L:351:LEU:O	1:L:359:ARG:HG2	1.92	0.70
1:L:7:ILE:HG22	1:L:124:ALA:CB	2.21	0.70
1:I:11:LYS:CB	1:I:12:PRO:HD3	2.15	0.70
1:I:71:ASN:ND2	1:I:73:ASN:HB2	2.06	0.70
1:L:154:PHE:HA	1:L:355:VAL:HA	1.74	0.70
1:I:184:ALA:O	1:I:188:LYS:HG2	1.92	0.70
1:I:359:ARG:HH11	1:I:360:ASP:H	1.35	0.70
1:I:159:GLN:HG2	1:I:170:LEU:HD12	1.72	0.69
1:L:238:LEU:HD11	1:L:240:TYR:CE2	2.27	0.69
1:I:351:LEU:HG	3:I:526:HOH:O	1.90	0.69
1:I:93:GLY:HA3	3:I:520:HOH:O	1.92	0.69
1:L:234:THR:HG21	1:L:377:GLU:OE2	1.93	0.69
1:L:115:THR:CG2	1:L:118:GLN:HB2	2.24	0.69
1:L:245:GLU:HG2	1:L:246:SER:N	2.08	0.69
1:L:7:ILE:CG1	1:L:16:PRO:HG2	2.23	0.68
1:I:50:GLU:O	1:I:111:ILE:HD11	1.94	0.68
1:I:293:ALA:O	1:I:297:LYS:HG3	1.93	0.68
1:I:5:VAL:HG21	1:I:133:LYS:HZ3	1.55	0.68
1:L:137:SER:HB2	1:L:276:GLY:N	2.08	0.68
1:L:224:LEU:CB	1:L:275:LYS:HD2	2.23	0.68
1:I:190:VAL:O	1:I:194:THR:HG23	1.92	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:50:GLU:C	1:I:111:ILE:HD11	2.14	0.68
1:L:359:ARG:HG3	1:L:362:LEU:CD1	2.23	0.68
1:I:3:SER:HB3	1:I:131:TYR:HB2	1.76	0.68
1:L:157:THR:HG21	2:L:500:NAA:H83	1.75	0.68
1:I:202:ILE:HG22	1:I:206:ALA:HB3	1.76	0.68
1:I:233:ASN:CB	1:I:253:TYR:HB2	2.23	0.68
1:L:355:VAL:CG1	1:L:359:ARG:HH11	2.07	0.68
1:L:85:THR:O	1:L:89:MET:HG3	1.93	0.68
1:I:352:PRO:O	1:I:355:VAL:HG23	1.94	0.67
1:I:126:LEU:HD11	1:I:419:THR:HG21	1.77	0.67
1:I:227:SER:OG	1:I:254:GLN:NE2	2.27	0.67
1:L:78:LEU:CD2	1:L:80:PRO:HD3	2.24	0.67
1:I:5:VAL:CG2	1:I:132:ARG:HG2	2.23	0.67
1:L:137:SER:OG	1:L:276:GLY:HA2	1.95	0.67
1:L:8:CYS:O	1:L:10:ALA:N	2.28	0.67
1:L:355:VAL:H	1:L:359:ARG:CD	2.02	0.66
1:I:53:LYS:HZ3	1:I:57:ARG:CZ	2.07	0.66
1:L:228:LYS:HB2	1:L:377:GLU:O	1.94	0.66
1:L:292:LEU:HD12	1:L:293:ALA:N	2.11	0.66
1:I:291:SER:OG	1:I:294:LYS:HG3	1.96	0.66
1:L:18:ASN:OD1	1:L:117:ASP:HB2	1.96	0.66
1:L:299:LEU:HD21	1:L:304:LEU:HD21	1.76	0.66
1:L:150:LYS:HG3	1:L:172:PRO:HB2	1.78	0.66
1:I:1:HIS:HB3	1:I:164:LEU:O	1.96	0.66
1:I:399:ARG:N	1:I:399:ARG:HD2	2.11	0.66
1:I:152:LEU:HA	1:I:356:ALA:CB	2.21	0.65
1:I:111:ILE:HG23	1:I:112:SER:N	2.10	0.65
1:L:322:ARG:HH11	1:L:376:ASN:HB2	1.61	0.65
1:I:20:MET:O	1:I:22:ILE:N	2.29	0.65
1:I:95:CYS:HB2	1:I:352:PRO:CG	2.26	0.65
1:L:358:GLY:O	1:L:360:ASP:N	2.30	0.65
1:I:53:LYS:NZ	1:I:57:ARG:NH2	2.44	0.65
1:L:261:ARG:HH11	1:L:312:GLU:HG3	1.61	0.65
1:I:238:LEU:HA	1:I:247:CYS:O	1.96	0.65
1:L:155:ASN:OD1	2:L:500:NAA:N2	2.29	0.65
1:I:153:THR:H	1:I:356:ALA:HB2	1.62	0.65
1:L:46:ARG:HG2	1:L:47:ARG:NH1	2.10	0.65
1:L:432:LYS:H	1:L:432:LYS:CD	2.08	0.65
1:I:284:ILE:HD12	1:I:411:PHE:CE1	2.32	0.65
1:I:153:THR:H	1:I:356:ALA:HB1	1.62	0.64
1:I:47:ARG:NH2	1:I:125:LYS:NZ	2.46	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:VAL:HB	1:I:401:THR:HB	1.80	0.64
1:L:354:ILE:HB	1:L:359:ARG:NE	2.12	0.64
1:I:108:PHE:HB3	1:I:119:ILE:CD1	2.28	0.64
1:I:18:ASN:OD1	1:I:19:PRO:HD2	1.96	0.64
1:L:252:MET:CE	1:L:376:ASN:HA	2.27	0.64
1:I:53:LYS:NZ	1:I:57:ARG:HH12	1.95	0.64
1:L:20:MET:O	1:L:22:ILE:HD12	1.98	0.64
1:I:233:ASN:HB3	1:I:253:TYR:HB2	1.78	0.64
1:L:241:LYS:HE3	1:L:247:CYS:SG	2.38	0.64
1:L:260:TYR:OH	1:L:268:GLN:HG2	1.97	0.64
1:I:1:HIS:N	1:I:8:CYS:HA	2.12	0.64
1:I:281:MET:CE	1:I:283:LEU:HD21	2.28	0.64
1:I:97:ASP:HB3	3:I:527:HOH:O	1.97	0.63
1:I:121:PHE:HZ	1:I:125:LYS:HZ1	1.46	0.63
1:I:12:PRO:HB3	1:I:15:ILE:HD12	1.80	0.63
1:L:24:ARG:HD3	1:L:114:LYS:HE3	1.80	0.63
1:L:287:LYS:O	1:L:290:LYS:HB3	1.97	0.63
1:I:334:GLN:HE21	1:I:338:MET:CE	2.12	0.63
1:I:204:SER:O	1:I:205:GLU:HG3	1.99	0.63
1:L:236:LYS:HG2	1:L:248:SER:OG	1.97	0.63
1:I:396:ASN:OD1	1:I:397:PRO:HD2	1.98	0.63
1:L:213:LEU:HG	1:L:214:VAL:N	2.13	0.63
1:L:287:LYS:CG	1:L:288:PRO:HD2	2.28	0.63
1:I:292:LEU:O	1:I:296:GLU:HG3	1.98	0.62
1:I:208:ASN:OD1	1:I:210:LEU:HB2	1.99	0.62
1:I:44:THR:HG21	1:I:47:ARG:HG2	1.82	0.62
1:I:317:VAL:HG12	1:I:319:HIS:CE1	2.34	0.62
1:I:5:VAL:N	1:I:132:ARG:HB2	2.15	0.62
1:L:224:LEU:HB3	1:L:275:LYS:HD2	1.82	0.62
1:L:292:LEU:O	1:L:296:GLU:HG3	1.99	0.62
1:L:408:PHE:HD2	1:L:426:VAL:HB	1.65	0.62
1:I:300:THR:HG23	1:I:303:VAL:HB	1.81	0.62
1:I:152:LEU:HD11	1:I:362:LEU:HD21	1.81	0.61
1:L:269:VAL:HG22	1:L:284:ILE:HG13	1.81	0.61
1:L:159:GLN:HE21	1:L:170:LEU:HD22	1.65	0.61
1:L:124:ALA:HB2	1:L:165:VAL:HG13	1.82	0.61
1:L:18:ASN:CA	1:L:161:ILE:HD11	2.29	0.61
1:L:238:LEU:HD21	1:L:240:TYR:CE2	2.34	0.61
1:I:376:ASN:C	1:I:376:ASN:HD22	2.03	0.61
1:I:396:ASN:HD21	1:I:398:ASN:HB2	1.65	0.61
1:I:1:HIS:ND1	1:I:9:THR:HG23	2.15	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:ARG:HA	1:L:114:LYS:HB2	1.82	0.61
1:I:257:LYS:HA	1:I:314:MET:O	2.01	0.61
1:L:252:MET:HE2	1:L:322:ARG:HB2	1.82	0.61
1:L:303:VAL:HA	3:L:531:HOH:O	2.01	0.60
1:L:7:ILE:HD11	1:L:16:PRO:HG3	1.83	0.60
1:I:24:ARG:O	1:I:24:ARG:HG3	2.02	0.60
1:L:261:ARG:NE	1:L:310:GLU:HG2	2.17	0.60
1:L:163:GLU:O	1:L:167:GLY:HA2	2.02	0.60
1:L:82:SER:OG	1:L:217:ASN:ND2	2.35	0.60
1:I:66:LEU:HA	3:I:525:HOH:O	2.01	0.60
1:I:340:LEU:HD21	1:I:343:LEU:CD2	2.32	0.60
1:I:29:LYS:HA	1:I:110:THR:HA	1.83	0.59
1:I:183:ARG:CB	1:I:207:ILE:HD12	2.32	0.59
1:I:197:ARG:HH22	1:I:324:ARG:NH2	1.99	0.59
1:L:359:ARG:HG3	1:L:362:LEU:HD12	1.83	0.59
1:L:224:LEU:HB2	1:L:275:LYS:HD2	1.84	0.59
1:L:159:GLN:NE2	1:L:170:LEU:HD22	2.15	0.59
1:L:7:ILE:HG21	1:L:121:PHE:CD1	2.37	0.59
1:I:340:LEU:HD21	1:I:343:LEU:HD23	1.84	0.59
1:I:306:GLU:O	1:I:310:GLU:HG3	2.02	0.59
1:L:44:THR:HG22	1:L:47:ARG:HG2	1.85	0.59
1:L:74:ASP:O	1:L:425:ARG:HD2	2.03	0.59
1:L:365:SER:HB3	1:L:392:GLY:H	1.68	0.59
1:I:204:SER:C	1:I:205:GLU:HG3	2.24	0.59
1:I:131:TYR:O	1:I:132:ARG:HB3	2.01	0.58
1:I:93:GLY:O	1:I:352:PRO:HD2	2.03	0.58
1:L:329:PHE:HD2	1:L:330:SER:O	1.86	0.58
1:I:18:ASN:CG	1:I:19:PRO:HD2	2.23	0.58
1:I:241:LYS:HE2	1:I:247:CYS:HB2	1.85	0.58
1:L:283:LEU:CD1	1:L:408:PHE:HZ	2.11	0.58
1:I:47:ARG:NH2	1:I:125:LYS:HZ1	2.00	0.58
1:I:3:SER:N	1:I:4:PRO:HD3	2.17	0.58
1:L:210:LEU:HD23	1:L:210:LEU:N	2.19	0.58
1:L:25:SER:H	1:L:114:LYS:HB3	1.67	0.58
1:I:228:LYS:HD3	1:I:378:GLU:HG2	1.86	0.58
1:L:47:ARG:HG2	1:L:47:ARG:NH1	2.17	0.58
1:L:158:TYR:CZ	1:L:354:ILE:HG23	2.38	0.58
1:L:254:GLN:NE2	1:L:258:PHE:HZ	2.02	0.58
1:L:259:ARG:NH2	1:L:311:LEU:HB2	2.18	0.58
1:L:258:PHE:CD1	1:L:316:LEU:HD21	2.39	0.57
1:L:95:CYS:HB2	1:L:352:PRO:CG	2.34	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:111:ILE:HD11	1:L:119:ILE:CD1	2.34	0.57
1:L:73:ASN:HD22	1:L:242:ALA:HB2	1.69	0.57
1:I:233:ASN:HB2	1:I:253:TYR:CB	2.35	0.57
1:L:365:SER:OG	1:L:389:VAL:HG22	2.05	0.57
1:I:356:ALA:O	1:I:357:GLU:HG2	2.05	0.57
1:I:4:PRO:HA	1:I:132:ARG:HA	1.87	0.57
1:L:314:MET:HG3	1:L:315:MET:N	2.19	0.57
1:I:197:ARG:NH2	1:I:372:PHE:HZ	2.01	0.57
1:L:50:GLU:CB	1:L:111:ILE:HG22	2.15	0.57
1:L:322:ARG:NH1	1:L:376:ASN:HB2	2.18	0.57
1:L:204:SER:C	1:L:205:GLU:HG2	2.25	0.57
1:I:257:LYS:HE3	1:I:313:GLU:HB3	1.87	0.57
1:L:293:ALA:HB1	1:L:297:LYS:CE	2.34	0.56
1:I:359:ARG:HG3	1:I:359:ARG:NH1	2.19	0.56
1:I:14:ASP:O	1:I:15:ILE:HG13	2.05	0.56
1:L:80:PRO:HG3	1:L:423:MET:HE2	1.86	0.56
1:I:359:ARG:HG2	1:I:361:ASP:OD1	2.06	0.56
1:I:49:TRP:HE3	1:I:49:TRP:O	1.89	0.56
1:I:339:GLY:O	1:I:341:VAL:HG22	2.05	0.56
1:I:156:GLU:OE2	2:I:500:NAA:N2	2.38	0.56
1:I:141:VAL:CG1	1:I:193:LYS:HD3	2.36	0.56
1:I:271:GLU:OE2	1:I:413:ARG:NH1	2.33	0.56
1:I:53:LYS:NZ	1:I:57:ARG:NH1	2.52	0.56
1:I:12:PRO:HB2	1:I:15:ILE:HB	1.87	0.55
1:L:183:ARG:HB2	1:L:207:ILE:HD12	1.87	0.55
1:I:26:PRO:HG2	1:I:29:LYS:C	2.27	0.55
1:I:11:LYS:HD2	1:I:11:LYS:O	2.05	0.55
1:L:299:LEU:CD2	1:L:304:LEU:HD21	2.36	0.55
1:I:121:PHE:CZ	1:I:125:LYS:HE3	2.40	0.55
1:I:1:HIS:NE2	1:I:124:ALA:HB1	2.22	0.55
1:I:197:ARG:HD3	3:I:538:HOH:O	2.06	0.55
1:L:7:ILE:HG13	1:L:121:PHE:HE1	1.71	0.55
1:L:263:VAL:HG11	1:L:307:TRP:CD1	2.42	0.55
1:I:70:LYS:HE3	1:I:76:ILE:HG12	1.89	0.55
1:I:108:PHE:HB3	1:I:119:ILE:HD11	1.89	0.55
1:I:253:TYR:CG	1:I:254:GLN:N	2.74	0.55
1:I:175:PHE:HD2	1:I:211:THR:O	1.90	0.55
1:L:75:ASN:OD1	1:L:427:ALA:N	2.28	0.55
1:L:96:ASN:O	1:L:97:ASP:HB2	2.06	0.55
1:L:419:THR:HG22	3:L:501:HOH:O	2.06	0.55
1:I:43:ALA:N	1:I:125:LYS:O	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ASP:OD1	1:I:7:ILE:N	2.40	0.55
1:I:7:ILE:HG13	1:I:7:ILE:O	2.05	0.55
1:L:49:TRP:O	1:L:53:LYS:HG3	2.07	0.55
1:L:141:VAL:HA	3:L:527:HOH:O	2.06	0.55
1:L:212:VAL:HG21	1:L:362:LEU:HD21	1.89	0.54
1:I:229:PHE:CD2	1:I:252:MET:HB3	2.42	0.54
1:I:6:ASP:CG	1:I:7:ILE:H	2.11	0.54
1:L:173:LEU:CD1	1:L:182:SER:HA	2.36	0.54
1:I:233:ASN:HB2	1:I:253:TYR:HB2	1.89	0.54
1:L:190:VAL:O	1:L:194:THR:HG23	2.08	0.54
1:L:141:VAL:HG12	3:L:527:HOH:O	2.07	0.54
1:I:79:SER:HB2	1:I:422:PHE:CD1	2.43	0.54
1:I:5:VAL:HG23	1:I:133:LYS:N	2.22	0.54
1:L:103:MET:SD	1:L:108:PHE:HB2	2.47	0.54
1:L:44:THR:CG2	1:L:47:ARG:HG2	2.37	0.54
1:I:354:ILE:O	1:I:356:ALA:N	2.41	0.54
1:I:252:MET:SD	1:I:377:GLU:HG3	2.48	0.54
1:L:137:SER:HB2	1:L:276:GLY:CA	2.38	0.53
1:I:136:LYS:HE2	1:I:136:LYS:HA	1.90	0.53
1:I:248:SER:O	1:I:430:CYS:HB3	2.09	0.53
1:L:260:TYR:CG	1:L:261:ARG:N	2.77	0.53
1:I:159:GLN:CG	1:I:170:LEU:HD12	2.39	0.53
1:I:48:VAL:CG2	1:I:126:LEU:HB2	2.38	0.53
1:I:198:ILE:HG23	1:I:370:LYS:HZ2	1.71	0.53
1:L:9:THR:O	1:L:9:THR:HG22	2.09	0.53
1:I:359:ARG:HG3	1:I:359:ARG:HH11	1.74	0.53
1:L:341:VAL:HG23	1:L:342:ASP:N	2.24	0.53
1:L:268:GLN:OE1	1:L:285:LEU:HD12	2.09	0.53
1:I:365:SER:O	1:I:366:ASP:HB2	2.09	0.53
1:L:108:PHE:O	1:L:111:ILE:HG12	2.08	0.53
1:L:14:ASP:CG	1:L:15:ILE:H	2.12	0.53
1:I:77:PHE:CE2	1:I:371:ALA:HB1	2.43	0.52
1:L:44:THR:O	1:L:44:THR:HG22	2.09	0.52
1:L:173:LEU:HD13	1:L:182:SER:HA	1.91	0.52
1:L:145:ARG:HG3	1:L:169:LYS:O	2.09	0.52
1:L:125:LYS:O	1:L:129:ARG:HG3	2.09	0.52
1:I:129:ARG:CG	1:I:417:LEU:HD11	2.35	0.52
1:I:1:HIS:H2	1:I:8:CYS:HA	1.72	0.52
1:L:137:SER:HB2	1:L:275:LYS:C	2.30	0.52
1:L:370:LYS:O	1:L:384:ALA:HA	2.09	0.52
1:I:132:ARG:HD3	1:I:132:ARG:O	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:SER:OG	1:I:127:ASN:O	2.28	0.52
1:I:83:ILE:CD1	1:I:217:ASN:HD21	2.22	0.52
1:I:83:ILE:HD13	1:I:217:ASN:ND2	2.21	0.52
1:I:300:THR:HG23	1:I:303:VAL:CG2	2.40	0.52
1:L:145:ARG:NH1	1:L:171:GLN:OE1	2.42	0.52
1:L:283:LEU:HD22	1:L:408:PHE:CZ	2.45	0.52
1:L:7:ILE:HD11	1:L:16:PRO:CG	2.40	0.52
1:L:269:VAL:HG22	1:L:284:ILE:CG1	2.40	0.52
1:L:94:ALA:HB1	1:L:98:THR:HG22	1.90	0.52
1:L:431:VAL:HB	1:L:432:LYS:HE2	1.91	0.51
1:I:148:GLY:HA2	1:I:212:VAL:O	2.10	0.51
1:I:202:ILE:HG22	1:I:206:ALA:CB	2.40	0.51
1:L:116:SER:O	1:L:119:ILE:HG12	2.10	0.51
1:L:111:ILE:HD11	1:L:119:ILE:HD13	1.92	0.51
1:L:231:PRO:O	1:L:234:THR:OG1	2.29	0.51
1:I:229:PHE:HA	1:I:253:TYR:CE1	2.45	0.51
1:L:200:ASP:OD1	1:L:370:LYS:HD2	2.10	0.51
1:L:134:ALA:O	3:L:519:HOH:O	2.19	0.51
1:I:417:LEU:HB2	1:I:419:THR:HG23	1.92	0.51
1:L:11:LYS:O	1:L:164:LEU:HD11	2.11	0.51
1:L:252:MET:HE1	1:L:377:GLU:H	1.73	0.51
1:I:23:TYR:CG	1:I:24:ARG:N	2.78	0.51
1:I:95:CYS:HB2	1:I:352:PRO:HG3	1.91	0.51
1:I:13:ARG:HA	1:I:121:PHE:CE1	2.45	0.51
1:L:238:LEU:HD11	1:L:240:TYR:HE2	1.75	0.51
1:I:378:GLU:OE2	1:I:384:ALA:HB3	2.10	0.51
1:L:25:SER:N	1:L:114:LYS:HD2	2.26	0.51
1:I:190:VAL:HB	1:I:201:VAL:HG21	1.92	0.51
1:I:197:ARG:HH21	1:I:372:PHE:HZ	1.59	0.51
1:L:238:LEU:HD11	1:L:240:TYR:OH	2.11	0.51
1:I:100:GLN:O	1:I:104:GLU:HG3	2.11	0.51
1:L:24:ARG:HB3	1:L:114:LYS:CD	2.41	0.51
1:I:304:LEU:HD21	1:I:411:PHE:CZ	2.46	0.51
1:I:180:GLU:N	3:I:508:HOH:O	2.43	0.51
1:I:3:SER:N	1:I:4:PRO:CD	2.74	0.51
1:L:252:MET:HE3	1:L:322:ARG:HB2	1.93	0.51
1:I:83:ILE:HD11	1:I:369:HIS:CD2	2.45	0.51
1:L:316:LEU:HD23	1:L:316:LEU:C	2.31	0.51
1:I:4:PRO:O	1:I:6:ASP:OD1	2.29	0.51
1:L:293:ALA:HB1	1:L:297:LYS:HZ1	1.75	0.51
1:L:198:ILE:HD12	1:L:370:LYS:O	2.12	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:LYS:CA	1:I:110:THR:HA	2.42	0.50
1:I:197:ARG:NE	1:I:372:PHE:CZ	2.79	0.50
1:I:1:HIS:CG	1:I:9:THR:HG23	2.45	0.50
1:L:62:PHE:CD1	1:L:338:MET:HE1	2.47	0.50
1:L:405:ASN:O	1:L:427:ALA:O	2.29	0.50
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.76	0.50
1:I:359:ARG:HG3	1:I:360:ASP:H	1.75	0.50
1:L:238:LEU:HD11	1:L:240:TYR:CZ	2.46	0.50
1:L:357:GLU:OE1	1:I:245:GLU:HG3	2.10	0.50
1:L:327:ASP:O	1:L:370:LYS:HA	2.11	0.50
1:L:331:LEU:HA	1:L:334:GLN:OE1	2.10	0.50
1:I:113:GLU:C	1:I:114:LYS:HG3	2.31	0.50
1:L:179:ALA:O	1:L:182:SER:HB2	2.12	0.50
1:L:73:ASN:ND2	1:L:242:ALA:HB2	2.27	0.50
1:I:234:THR:HA	1:I:251:MET:O	2.12	0.50
1:L:351:LEU:HD12	1:L:362:LEU:O	2.11	0.50
1:L:237:GLU:CG	1:L:238:LEU:H	2.21	0.50
1:L:77:PHE:HB2	1:L:325:ILE:HD11	1.94	0.50
1:I:89:MET:O	1:I:92:LEU:HB2	2.12	0.50
1:I:103:MET:HE2	1:I:116:SER:HB3	1.94	0.50
1:L:408:PHE:O	1:L:425:ARG:HA	2.12	0.50
1:I:141:VAL:HG11	1:I:193:LYS:HD3	1.94	0.50
1:I:127:ASN:O	1:I:130:LEU:N	2.45	0.49
1:L:190:VAL:HG22	1:L:218:THR:CG2	2.41	0.49
1:L:99:LEU:HD12	1:L:99:LEU:O	2.12	0.49
1:I:259:ARG:HB3	1:I:311:LEU:HB3	1.94	0.49
1:L:158:TYR:CD2	1:L:354:ILE:HG23	2.48	0.49
1:I:13:ARG:HD2	1:I:121:PHE:CZ	2.48	0.49
1:I:16:PRO:HA	1:I:161:ILE:CD1	2.37	0.49
1:I:289:GLU:CD	1:I:289:GLU:H	2.14	0.49
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.95	0.49
1:L:263:VAL:HG23	1:L:267:THR:HB	1.95	0.49
1:I:147:PHE:O	1:I:213:LEU:HA	2.13	0.49
1:L:361:ASP:C	1:L:362:LEU:HG	2.33	0.49
1:L:287:LYS:HG2	1:L:288:PRO:HD2	1.94	0.49
1:L:139:LYS:O	1:L:221:PHE:HA	2.13	0.49
1:L:366:ASP:OD1	1:L:367:ALA:N	2.42	0.49
1:I:53:LYS:HE2	1:I:57:ARG:CZ	2.43	0.49
1:I:47:ARG:HH21	1:I:125:LYS:HZ1	1.61	0.48
1:L:115:THR:HG23	1:L:118:GLN:HB2	1.93	0.48
1:L:355:VAL:HG12	1:L:359:ARG:NH1	2.26	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:THR:HG21	1:L:118:GLN:HB2	1.96	0.48
1:I:350:LYS:C	1:I:352:PRO:HD3	2.34	0.48
1:I:227:SER:CB	1:I:254:GLN:HE22	2.26	0.48
1:L:293:ALA:HB1	1:L:297:LYS:HZ2	1.74	0.48
1:I:163:GLU:O	1:I:167:GLY:HA2	2.12	0.48
1:I:396:ASN:O	1:I:399:ARG:NE	2.46	0.48
1:I:359:ARG:HH11	1:I:359:ARG:CG	2.27	0.48
1:I:255:GLU:HA	1:I:316:LEU:O	2.14	0.48
1:I:9:THR:HG21	1:I:164:LEU:CD1	2.44	0.48
1:L:257:LYS:HG2	1:L:315:MET:HG2	1.94	0.48
1:L:194:THR:O	1:L:197:ARG:HB2	2.13	0.48
1:L:7:ILE:O	1:L:7:ILE:HD12	2.14	0.48
1:L:84:SER:HB3	1:L:123:PHE:HZ	1.79	0.48
1:L:359:ARG:CD	1:L:362:LEU:HD13	2.43	0.47
1:I:106:PHE:HB2	1:I:108:PHE:CE2	2.49	0.47
1:I:48:VAL:HG21	1:I:126:LEU:HB2	1.96	0.47
1:I:283:LEU:CD2	1:I:410:VAL:HG22	2.44	0.47
1:L:263:VAL:N	1:L:267:THR:O	2.44	0.47
1:I:50:GLU:OE1	1:I:112:SER:OG	2.31	0.47
1:I:5:VAL:HG23	1:I:132:ARG:HB2	1.96	0.47
1:L:287:LYS:HG3	1:L:288:PRO:HD2	1.95	0.47
1:L:431:VAL:HG12	1:L:432:LYS:NZ	2.29	0.47
1:L:97:ASP:HA	1:L:100:GLN:HB3	1.96	0.47
1:I:287:LYS:HG3	1:I:289:GLU:HG2	1.96	0.47
1:I:300:THR:HG23	1:I:303:VAL:CB	2.43	0.47
1:I:145:ARG:HG3	1:I:169:LYS:O	2.14	0.47
1:I:334:GLN:HE21	1:I:338:MET:HE1	1.79	0.47
1:I:83:ILE:HD11	1:I:369:HIS:CG	2.50	0.47
1:I:198:ILE:HG12	1:I:370:LYS:NZ	2.30	0.47
1:L:354:ILE:HG22	1:L:359:ARG:NH1	2.29	0.47
1:I:103:MET:CE	1:I:116:SER:HB3	2.45	0.47
1:I:1:HIS:H1	1:I:8:CYS:CA	2.27	0.47
1:L:62:PHE:CD1	1:L:338:MET:CE	2.98	0.47
1:I:348:LYS:NZ	3:I:528:HOH:O	2.30	0.47
1:L:91:LYS:HE3	1:L:120:HIS:CE1	2.50	0.47
1:I:171:GLN:NE2	1:I:172:PRO:O	2.46	0.47
1:I:43:ALA:N	1:I:129:ARG:HB3	2.29	0.47
1:L:78:LEU:HD22	1:L:78:LEU:C	2.35	0.47
1:L:103:MET:O	1:L:108:PHE:N	2.48	0.47
1:L:183:ARG:HA	1:L:207:ILE:HD12	1.97	0.47
1:I:373:LEU:HD12	1:I:374:GLU:N	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:TYR:CG	1:I:261:ARG:N	2.83	0.47
1:L:350:LYS:HB3	1:L:350:LYS:HE2	1.66	0.47
1:I:1:HIS:H1	1:I:8:CYS:C	2.18	0.46
1:I:153:THR:HA	3:I:514:HOH:O	2.14	0.46
1:I:197:ARG:NH2	1:I:324:ARG:NH2	2.62	0.46
1:L:225:TRP:CD1	1:L:379:GLY:HA2	2.50	0.46
1:L:299:LEU:HD22	1:L:304:LEU:HD11	1.97	0.46
1:L:112:SER:O	1:L:113:GLU:HB2	2.15	0.46
1:L:64:GLN:NE2	1:L:299:LEU:O	2.48	0.46
1:L:419:THR:HA	3:L:501:HOH:O	2.15	0.46
1:I:75:ASN:HD22	1:I:427:ALA:N	1.99	0.46
1:I:92:LEU:CD1	1:I:120:HIS:NE2	2.79	0.46
1:L:354:ILE:CG2	1:L:359:ARG:NH1	2.79	0.46
1:L:238:LEU:CD2	1:L:240:TYR:HE2	2.26	0.46
1:I:334:GLN:NE2	1:I:338:MET:HE3	2.31	0.46
1:L:242:ALA:C	1:L:244:GLY:H	2.18	0.46
1:L:355:VAL:CG1	1:L:359:ARG:NH1	2.77	0.46
1:I:212:VAL:HG21	1:I:362:LEU:HD23	1.98	0.46
1:I:359:ARG:NH1	1:I:360:ASP:N	2.42	0.46
1:I:329:PHE:N	1:I:369:HIS:O	2.46	0.46
1:I:149:ASP:OD2	1:I:176:LYS:HE3	2.16	0.46
1:I:250:SER:O	1:I:321:PRO:HA	2.16	0.46
1:I:15:ILE:N	1:I:16:PRO:CD	2.76	0.46
1:I:229:PHE:HA	1:I:253:TYR:CD1	2.50	0.46
1:I:152:LEU:CA	1:I:356:ALA:HB1	2.28	0.46
1:L:238:LEU:CD1	1:L:240:TYR:CE2	2.99	0.46
1:L:245:GLU:HG2	1:L:246:SER:H	1.78	0.46
1:L:331:LEU:HD21	1:L:369:HIS:HB2	1.97	0.46
1:L:95:CYS:HB2	1:L:352:PRO:HG3	1.97	0.46
1:L:62:PHE:HD1	1:L:338:MET:CE	2.29	0.45
1:L:86:ALA:HA	1:L:89:MET:HE2	1.97	0.45
1:L:290:LYS:CG	1:L:291:SER:N	2.80	0.45
1:L:17:MET:N	1:L:17:MET:SD	2.88	0.45
1:I:108:PHE:O	1:I:111:ILE:HB	2.16	0.45
1:L:252:MET:HE3	1:L:322:ARG:CB	2.46	0.45
1:I:334:GLN:NE2	1:I:338:MET:CE	2.79	0.45
1:L:241:LYS:CG	1:L:405:ASN:HB3	2.47	0.45
1:L:428:ASN:O	1:L:431:VAL:HG13	2.17	0.45
1:L:428:ASN:ND2	1:L:430:CYS:SG	2.89	0.45
1:I:418:ASN:HA	1:I:418:ASN:HD22	1.48	0.45
1:L:183:ARG:NH1	1:L:202:ILE:O	2.45	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:256:GLY:O	1:L:316:LEU:HD22	2.16	0.45
1:I:111:ILE:HG23	1:I:112:SER:H	1.81	0.45
1:I:53:LYS:CE	1:I:57:ARG:NH1	2.80	0.45
1:I:410:VAL:O	1:I:423:MET:HA	2.17	0.45
1:I:350:LYS:O	1:I:352:PRO:HD3	2.17	0.45
1:L:258:PHE:HD1	1:L:316:LEU:CD2	2.30	0.45
1:L:92:LEU:HD13	1:L:120:HIS:CE1	2.51	0.45
1:L:137:SER:CB	1:L:276:GLY:HA2	2.47	0.45
1:I:92:LEU:HD13	1:I:120:HIS:CE1	2.52	0.45
1:I:92:LEU:CD1	1:I:120:HIS:CE1	2.99	0.45
1:L:46:ARG:CG	1:L:47:ARG:NH1	2.79	0.45
1:I:3:SER:OG	1:I:131:TYR:O	2.27	0.45
1:L:408:PHE:CD2	1:L:426:VAL:HB	2.47	0.45
1:I:79:SER:HB2	1:I:422:PHE:CE1	2.52	0.45
1:I:169:LYS:HB3	3:I:519:HOH:O	2.16	0.45
1:L:46:ARG:HD2	1:L:50:GLU:OE2	2.17	0.44
1:I:225:TRP:HD1	1:I:377:GLU:O	2.00	0.44
1:I:380:SER:O	1:I:381:GLU:HB2	2.16	0.44
1:I:281:MET:HE1	1:I:323:PHE:HZ	1.81	0.44
1:L:213:LEU:HG	1:L:214:VAL:H	1.82	0.44
1:L:145:ARG:HB2	1:L:189:TRP:CH2	2.52	0.44
1:I:110:THR:O	1:I:111:ILE:O	2.35	0.44
1:I:316:LEU:CG	1:I:400:VAL:HG22	2.44	0.44
1:I:273:PRO:HB3	1:I:280:THR:HG22	1.99	0.44
1:L:293:ALA:HB1	1:L:297:LYS:HE3	1.99	0.44
1:L:199:THR:O	1:L:200:ASP:OD1	2.35	0.44
1:I:138:SER:OG	1:I:138:SER:O	2.30	0.44
1:L:46:ARG:O	1:L:50:GLU:HB2	2.17	0.44
1:L:238:LEU:CG	1:L:240:TYR:CE2	3.00	0.44
1:I:284:ILE:CD1	1:I:411:PHE:CE1	3.00	0.44
1:L:215:LEU:O	1:L:387:ALA:HA	2.18	0.44
1:L:95:CYS:HB2	1:L:352:PRO:CD	2.48	0.44
1:L:190:VAL:HG12	1:L:198:ILE:O	2.17	0.44
1:L:408:PHE:HB3	1:L:426:VAL:O	2.18	0.44
1:L:18:ASN:CB	1:L:161:ILE:HD11	2.47	0.44
1:I:20:MET:O	1:I:22:ILE:HG12	2.17	0.44
1:L:259:ARG:NH1	1:L:271:GLU:OE1	2.51	0.44
1:I:81:LEU:HD11	1:I:130:LEU:HD21	2.00	0.44
1:L:150:LYS:NZ	1:I:70:LYS:O	2.42	0.44
1:I:92:LEU:HD12	1:I:92:LEU:HA	1.65	0.44
1:I:305:GLN:OE1	1:I:305:GLN:HA	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:362:LEU:HA	1:I:362:LEU:HD23	1.80	0.43
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.99	0.43
1:L:248:SER:O	1:L:430:CYS:HB3	2.18	0.43
1:I:239:PHE:O	1:I:247:CYS:N	2.51	0.43
1:L:302:GLU:HG2	1:L:302:GLU:H	1.23	0.43
1:I:332:LYS:HE3	1:I:344:PHE:HB3	2.00	0.43
1:L:62:PHE:HA	1:L:338:MET:HE1	1.97	0.43
1:I:292:LEU:HD22	1:I:407:PRO:HB2	2.00	0.43
1:I:147:PHE:HB2	1:I:214:VAL:HG12	1.99	0.43
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.53	0.43
1:I:179:ALA:HB1	1:I:207:ILE:HG22	2.00	0.43
1:L:146:LEU:HD21	1:L:215:LEU:HD23	2.00	0.43
1:I:178:ASN:HB3	1:I:181:GLN:HB3	1.99	0.43
1:L:417:LEU:HA	1:L:417:LEU:HD23	1.72	0.43
1:I:130:LEU:HD13	1:I:417:LEU:HD12	2.00	0.43
1:I:334:GLN:HE21	1:I:338:MET:HE3	1.84	0.43
1:I:46:ARG:HA	1:I:49:TRP:HB2	1.99	0.43
1:L:412:ILE:N	3:L:534:HOH:O	2.51	0.43
1:I:236:LYS:C	1:I:237:GLU:HG2	2.38	0.43
1:I:152:LEU:CD1	1:I:362:LEU:HD21	2.47	0.43
1:I:129:ARG:O	1:I:129:ARG:HG3	2.09	0.43
1:L:432:LYS:N	1:L:432:LYS:CD	2.80	0.43
1:I:265:GLU:O	1:I:287:LYS:HD3	2.19	0.43
1:I:209:GLU:CD	1:I:209:GLU:H	2.22	0.43
1:I:107:LYS:HB3	1:I:110:THR:HG21	2.00	0.43
1:I:5:VAL:O	1:I:6:ASP:O	2.36	0.43
1:L:283:LEU:HD11	1:L:320:MET:CE	2.48	0.43
1:L:257:LYS:HG2	1:L:315:MET:SD	2.58	0.43
1:L:410:VAL:HG12	1:L:411:PHE:N	2.33	0.43
1:I:78:LEU:HB3	1:I:329:PHE:CZ	2.54	0.43
1:I:190:VAL:CB	1:I:201:VAL:HG21	2.48	0.43
1:I:324:ARG:HD3	1:I:326:GLU:OE2	2.19	0.43
1:L:365:SER:CB	1:L:392:GLY:H	2.32	0.43
1:L:316:LEU:HD23	1:L:316:LEU:O	2.19	0.43
1:I:1:HIS:H1	1:I:8:CYS:HA	1.81	0.43
1:L:340:LEU:HD13	1:L:344:PHE:CE1	2.54	0.43
1:L:241:LYS:HB3	1:L:405:ASN:HB3	2.01	0.43
1:I:136:LYS:HZ3	1:I:136:LYS:HB3	1.84	0.42
1:L:154:PHE:HB2	1:L:159:GLN:NE2	2.35	0.42
1:L:285:LEU:N	1:L:285:LEU:HD23	2.33	0.42
1:I:52:SER:HB2	1:I:418:ASN:O	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:PRO:HB3	1:I:15:ILE:CD1	2.49	0.42
1:I:197:ARG:HA	1:I:197:ARG:HD2	1.74	0.42
1:L:258:PHE:CD1	1:L:316:LEU:CD2	3.01	0.42
1:I:288:PRO:HD3	1:I:406:ARG:NH2	2.34	0.42
1:I:281:MET:HE3	1:I:410:VAL:CG2	2.49	0.42
1:L:304:LEU:HD23	1:L:307:TRP:CZ3	2.54	0.42
1:I:116:SER:O	1:I:119:ILE:HG13	2.20	0.42
1:I:314:MET:SD	1:I:400:VAL:HG13	2.60	0.42
1:I:19:PRO:O	1:I:20:MET:SD	2.77	0.42
1:L:333:GLU:HG2	1:L:334:GLN:NE2	2.34	0.42
1:L:410:VAL:CG1	1:L:411:PHE:N	2.82	0.42
1:L:47:ARG:HD3	1:L:50:GLU:OE1	2.20	0.42
1:I:5:VAL:CG2	1:I:133:LYS:HB3	2.50	0.42
1:I:342:ASP:OD2	1:I:348:LYS:NZ	2.30	0.42
1:L:91:LYS:NZ	1:L:120:HIS:HE1	2.17	0.42
1:I:243:ASP:O	1:I:245:GLU:HG2	2.20	0.42
1:L:124:ALA:O	1:L:128:CYS:HB2	2.20	0.42
1:L:153:THR:HG22	1:L:356:ALA:HB3	2.01	0.42
1:I:75:ASN:HD21	1:I:427:ALA:N	2.15	0.42
1:I:236:LYS:HD3	1:I:249:ALA:O	2.19	0.42
1:L:224:LEU:HD23	1:L:224:LEU:HA	1.81	0.42
1:L:320:MET:HA	1:L:321:PRO:HD3	1.93	0.41
1:I:307:TRP:O	1:I:311:LEU:HD13	2.20	0.41
1:I:229:PHE:CD2	1:I:253:TYR:O	2.73	0.41
1:I:326:GLU:HG2	1:I:372:PHE:CD2	2.54	0.41
1:L:230:SER:OG	1:L:232:GLU:HG2	2.19	0.41
1:L:62:PHE:CB	1:L:338:MET:HE1	2.50	0.41
1:I:107:LYS:HB3	1:I:110:THR:CG2	2.50	0.41
1:I:13:ARG:HD3	1:I:13:ARG:HA	1.62	0.41
1:L:101:GLN:OE1	1:L:342:ASP:HB2	2.19	0.41
1:L:308:LEU:HD23	1:L:311:LEU:HD11	2.02	0.41
1:L:362:LEU:HB3	1:L:390:ILE:CG2	2.50	0.41
1:L:324:ARG:HA	1:L:373:LEU:O	2.21	0.41
1:I:281:MET:HE1	1:I:320:MET:HE1	2.02	0.41
1:I:299:LEU:C	1:I:300:THR:HG22	2.40	0.41
1:I:114:LYS:HZ3	1:I:122:PHE:HE2	1.68	0.41
1:I:44:THR:CG2	1:I:47:ARG:HG2	2.48	0.41
1:L:183:ARG:CA	1:L:207:ILE:HD12	2.51	0.41
1:L:7:ILE:HA	1:L:11:LYS:O	2.20	0.41
1:I:77:PHE:CD2	1:I:371:ALA:HB1	2.55	0.41
1:I:70:LYS:CE	1:I:76:ILE:HG12	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ASN:HB3	1:L:158:TYR:HB3	2.03	0.41
1:L:7:ILE:CD1	1:L:16:PRO:CG	2.99	0.41
1:L:329:PHE:CE2	1:L:331:LEU:HD23	2.56	0.41
1:L:219:ILE:O	1:L:383:ALA:HA	2.21	0.41
1:L:103:MET:HE1	1:L:108:PHE:HB3	2.03	0.41
1:I:65:HIS:NE2	1:I:337:ASP:OD2	2.46	0.41
1:L:290:LYS:CE	1:L:294:LYS:HD2	2.50	0.41
1:I:383:ALA:O	1:I:384:ALA:HB2	2.20	0.41
1:L:23:TYR:N	1:L:116:SER:OG	2.50	0.41
1:I:428:ASN:OD1	1:I:430:CYS:SG	2.79	0.41
1:L:260:TYR:HE1	1:L:268:GLN:HB3	1.86	0.41
1:L:92:LEU:HD13	1:L:120:HIS:CD2	2.55	0.41
1:L:146:LEU:HB3	1:L:213:LEU:HD11	2.03	0.41
1:L:103:MET:SD	1:L:108:PHE:CB	3.08	0.41
1:I:112:SER:C	1:I:113:GLU:HG3	2.41	0.41
1:I:400:VAL:HG23	1:I:401:THR:N	2.35	0.41
1:I:53:LYS:CE	1:I:57:ARG:CZ	2.99	0.41
1:I:53:LYS:NZ	1:I:57:ARG:CZ	2.81	0.41
1:L:247:CYS:HB2	1:L:430:CYS:HB2	1.90	0.41
1:I:183:ARG:CA	1:I:207:ILE:HD12	2.51	0.41
1:I:299:LEU:O	1:I:300:THR:HG22	2.21	0.41
1:I:141:VAL:HB	1:I:220:TYR:HB3	2.01	0.41
1:I:280:THR:OG1	1:I:413:ARG:NH1	2.54	0.41
1:I:173:LEU:HB2	1:I:175:PHE:CE1	2.56	0.41
1:I:89:MET:HE2	1:I:144:ASN:ND2	2.35	0.41
1:I:50:GLU:CD	1:I:112:SER:HG	2.23	0.41
1:I:188:LYS:O	1:I:192:ASN:ND2	2.54	0.41
1:L:130:LEU:HD22	1:L:140:LEU:HD21	2.02	0.41
1:L:159:GLN:HE21	1:L:170:LEU:HD13	1.86	0.40
1:I:152:LEU:HD23	1:I:152:LEU:N	2.35	0.40
1:L:137:SER:CB	1:L:276:GLY:CA	2.99	0.40
1:L:274:PHE:CZ	1:L:380:SER:HB3	2.55	0.40
1:I:347:GLU:H	1:I:347:GLU:HG2	1.44	0.40
1:I:28:LYS:HA	1:I:28:LYS:HD3	1.78	0.40
1:I:111:ILE:CG2	1:I:112:SER:N	2.80	0.40
1:I:11:LYS:N	1:I:12:PRO:CD	2.83	0.40
1:I:65:HIS:CG	1:I:338:MET:HE3	2.56	0.40
1:L:241:LYS:CB	1:L:405:ASN:HB3	2.52	0.40
1:I:284:ILE:CD1	1:I:411:PHE:HE1	2.26	0.40
1:L:328:GLY:O	1:L:329:PHE:HB3	2.20	0.40
1:L:394:SER:O	1:L:395:LEU:HB2	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:252:MET:HE1	1:L:377:GLU:OE1	2.21	0.40
1:L:405:ASN:O	1:L:406:ARG:O	2.39	0.40
1:I:241:LYS:HE3	1:I:245:GLU:O	2.20	0.40
1:I:5:VAL:HG22	1:I:132:ARG:CG	2.45	0.40
1:I:413:ARG:HH11	1:I:413:ARG:CG	2.34	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.







Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:261:ARG:NH2	1:I:13:ARG:CB[1_554]	1.31	0.89
1:L:310:GLU:OE2	1:I:47:ARG:NH2[1_554]	1.54	0.66
1:L:261:ARG:NH1	1:I:13:ARG:CB[1_554]	1.59	0.61
1:L:261:ARG:CZ	1:I:13:ARG:CB[1_554]	1.60	0.60
1:L:261:ARG:NH2	1:I:13:ARG:CG[1_554]	1.83	0.37
1:L:310:GLU:CD	1:I:47:ARG:NH2[1_554]	2.00	0.20
1:L:261:ARG:CZ	1:I:13:ARG:CG[1_554]	2.02	0.18
1:L:310:GLU:OE2	1:I:47:ARG:CZ[1_554]	2.13	0.07
1:L:261:ARG:NH1	1:I:13:ARG:CG[1_554]	2.14	0.06
1:L:310:GLU:OE1	1:I:47:ARG:NH2[1_554]	2.18	0.02

## 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	415/432 (96%)	353 (85%)	38 (9%)	24 (6%)		
1	L	390/432 (90%)	342 (88%)	25 (6%)	23 (6%)		
All	All	805/864 (93%)	695 (86%)	63 (8%)	47 (6%)		

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	9	THR
1	L	19	PRO
1	L	97	ASP
1	L	113	GLU
1	L	133	LYS
1	L	135	ASN
1	L	136	LYS
1	L	245	GLU
1	L	406	ARG
1	L	407	PRO
1	L	431	VAL
1	I	3	SER
1	I	4	PRO
1	I	5	VAL
1	I	6	ASP
1	I	11	LYS
1	I	12	PRO
1	I	16	PRO
1	I	21	CYS
1	I	22	ILE
1	I	97	ASP
1	I	111	ILE
1	I	113	GLU
1	I	138	SER
1	I	254	GLN
1	L	96	ASN
1	L	115	THR
1	L	277	ASP
1	L	359	ARG
1	I	20	MET
1	I	46	ARG
1	I	96	ASN
1	I	128	CYS
1	I	132	ARG
1	L	114	LYS
1	L	204	SER
1	L	361	ASP
1	I	114	LYS
1	I	243	ASP
1	I	355	VAL
1	L	150	LYS
1	I	384	ALA
1	L	10	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	243	ASP
1	L	408	PHE
1	I	366	ASP
1	L	263	VAL

### 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	372/383 (97%)	303 (82%)	69 (18%)	2	3
1	L	353/383 (92%)	288 (82%)	65 (18%)	2	3
All	All	725/766 (95%)	591 (82%)	134 (18%)	2	3

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ILE
1	L	15	ILE
1	L	17	MET
1	L	20	MET
1	L	21	CYS
1	L	25	SER
1	L	46	ARG
1	L	78	LEU
1	L	84	SER
1	L	92	LEU
1	L	95	CYS
1	L	96	ASN
1	L	98	THR
1	L	112	SER
1	L	113	GLU
1	L	114	LYS
1	L	118	GLN
1	L	123	PHE
1	L	128	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	136	LYS
1	L	137	SER
1	L	151	SER
1	L	155	ASN
1	L	156	GLU
1	L	157	THR
1	L	173	LEU
1	L	177	GLU
1	L	197	ARG
1	L	199	THR
1	L	205	GLU
1	L	210	LEU
1	L	227	SER
1	L	235	ARG
1	L	238	LEU
1	L	243	ASP
1	L	246	SER
1	L	261	ARG
1	L	277	ASP
1	L	284	ILE
1	L	285	LEU
1	L	289	GLU
1	L	292	LEU
1	L	302	GLU
1	L	310	GLU
1	L	314	MET
1	L	316	LEU
1	L	318	VAL
1	L	320	MET
1	L	324	ARG
1	L	327	ASP
1	L	330	SER
1	L	340	LEU
1	L	342	ASP
1	L	350	LYS
1	L	355	VAL
1	L	357	GLU
1	L	362	LEU
1	L	370	LYS
1	L	389	VAL
1	L	405	ASN
1	L	408	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	L	413	ARG
1	L	419	THR
1	L	430	CYS
1	L	432	LYS
1	I	1	HIS
1	I	3	SER
1	I	20	MET
1	I	22	ILE
1	I	24	ARG
1	I	47	ARG
1	I	48	VAL
1	I	49	TRP
1	I	68	ASP
1	I	78	LEU
1	I	81	LEU
1	I	82	SER
1	I	91	LYS
1	I	92	LEU
1	I	96	ASN
1	I	111	ILE
1	I	114	LYS
1	I	115	THR
1	I	128	CYS
1	I	129	ARG
1	I	130	LEU
1	I	132	ARG
1	I	133	LYS
1	I	137	SER
1	I	138	SER
1	I	139	LYS
1	I	158	TYR
1	I	169	LYS
1	I	171	GLN
1	I	201	VAL
1	I	202	ILE
1	I	204	SER
1	I	205	GLU
1	I	209	GLU
1	I	225	TRP
1	I	229	PHE
1	I	235	ARG
1	I	253	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	260	TYR
1	I	262	ARG
1	I	268	GLN
1	I	300	THR
1	I	302	GLU
1	I	304	LEU
1	I	306	GLU
1	I	307	TRP
1	I	313	GLU
1	I	314	MET
1	I	316	LEU
1	I	322	ARG
1	I	324	ARG
1	I	333	GLU
1	I	341	VAL
1	I	347	GLU
1	I	348	LYS
1	I	351	LEU
1	I	354	ILE
1	I	359	ARG
1	I	374	GLU
1	I	376	ASN
1	I	378	GLU
1	I	385	SER
1	I	389	VAL
1	I	399	ARG
1	I	401	THR
1	I	406	ARG
1	I	418	ASN
1	I	419	THR
1	I	430	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	120	HIS
1	L	135	ASN
1	L	159	GLN
1	L	178	ASN
1	L	217	ASN
1	L	254	GLN
1	L	336	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	428	ASN
1	I	45	ASN
1	I	75	ASN
1	I	100	GLN
1	I	118	GLN
1	I	127	ASN
1	I	159	GLN
1	I	171	GLN
1	I	217	ASN
1	I	233	ASN
1	I	254	GLN
1	I	268	GLN
1	I	319	HIS
1	I	334	GLN
1	I	376	ASN
1	I	396	ASN
1	I	418	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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	NAA	I	500	1	14,14,15	0.93	1 (7%)	15,19,21	3.45	10 (66%)
2	NAA	L	500	1	14,14,15	0.89	1 (7%)	15,19,21	4.36	11 (73%)

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	NAA	I	500	1	-	0/6/23/26	0/1/1/1
2	NAA	L	500	1	2/2/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	NAA	C7-N2	2.81	1.45	1.34
2	L	500	NAA	C7-N2	2.89	1.45	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	500	NAA	C3-C2-N2	-11.08	84.03	110.56
2	I	500	NAA	C1-O5-C5	-6.63	103.83	112.25
2	I	500	NAA	C8-C7-N2	-2.79	110.76	116.11
2	I	500	NAA	C2-N2-C7	-2.61	119.68	123.04
2	L	500	NAA	C8-C7-N2	-2.52	111.28	116.11
2	L	500	NAA	C2-N2-C7	-2.52	119.80	123.04
2	I	500	NAA	O6-C6-C5	2.59	119.88	111.33
2	L	500	NAA	C4-C3-C2	2.77	115.53	111.23
2	L	500	NAA	O6-C6-C5	2.89	120.88	111.33
2	I	500	NAA	C3-C4-C5	3.09	115.58	110.20
2	L	500	NAA	O3-C3-C4	3.61	118.47	110.34
2	I	500	NAA	O3-C3-C4	4.01	119.36	110.34
2	I	500	NAA	O5-C5-C6	4.18	116.39	107.35
2	L	500	NAA	O4-C4-C5	4.37	120.83	109.24
2	L	500	NAA	C3-C4-C5	4.49	118.03	110.20
2	I	500	NAA	O4-C4-C3	4.49	120.45	110.34
2	I	500	NAA	O4-C4-C5	4.51	121.19	109.24
2	L	500	NAA	O4-C4-C3	4.68	120.88	110.34
2	I	500	NAA	O3-C3-C2	4.81	118.64	109.11
2	L	500	NAA	O5-C5-C6	5.28	118.77	107.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	500	NAA	O3-C3-C2	5.37	119.76	109.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	L	500	NAA	C4
2	L	500	NAA	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	500	NAA	1	0
2	L	500	NAA	2	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<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	419/432 (96%)	0.22	42 (10%)	9 6	26, 47, 121, 162	0
1	L	398/432 (92%)	0.25	37 (9%)	11 7	27, 54, 121, 136	0
All	All	817/864 (94%)	0.23	79 (9%)	10 6	26, 49, 121, 162	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	6	ASP	10.1
1	I	26	PRO	9.9
1	I	4	PRO	8.4
1	I	20	MET	8.4
1	I	27	GLU	7.4
1	I	3	SER	7.4
1	L	432	LYS	6.9
1	I	29	LYS	6.4
1	I	7	ILE	6.2
1	L	10	ALA	5.7
1	I	25	SER	5.6
1	L	134	ALA	5.4
1	I	43	ALA	5.2
1	I	19	PRO	4.8
1	I	5	VAL	4.6
1	I	117	ASP	4.5
1	I	135	ASN	4.4
1	I	2	GLY	4.3
1	L	291	SER	4.3
1	L	133	LYS	4.3
1	L	114	LYS	4.3
1	I	28	LYS	4.3
1	I	10	ALA	4.2
1	I	14	ASP	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	432	LYS	3.8
1	I	49	TRP	3.7
1	L	242	ALA	3.6
1	I	46	ARG	3.6
1	I	385	SER	3.5
1	I	9	THR	3.4
1	L	243	ASP	3.4
1	I	11	LYS	3.3
1	I	13	ARG	3.3
1	L	289	GLU	3.3
1	L	7	ILE	3.3
1	I	44	THR	3.2
1	L	135	ASN	3.2
1	L	113	GLU	3.2
1	I	23	TYR	3.1
1	I	22	ILE	3.1
1	L	357	GLU	3.0
1	I	8	CYS	3.0
1	L	68	ASP	3.0
1	L	406	ARG	2.9
1	I	115	THR	2.9
1	L	46	ARG	2.9
1	L	14	ASP	2.9
1	I	253	TYR	2.9
1	I	137	SER	2.8
1	L	261	ARG	2.8
1	L	19	PRO	2.8
1	I	133	LYS	2.8
1	L	16	PRO	2.8
1	L	245	GLU	2.7
1	I	21	CYS	2.7
1	L	24	ARG	2.7
1	I	17	MET	2.6
1	I	1	HIS	2.6
1	L	49	TRP	2.5
1	L	244	GLY	2.5
1	L	20	MET	2.5
1	L	15	ILE	2.5
1	L	241	LYS	2.5
1	L	358	GLY	2.4
1	L	132	ARG	2.4
1	L	25	SER	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	69	SER	2.2
1	I	204	SER	2.2
1	I	116	SER	2.2
1	I	18	ASN	2.2
1	I	12	PRO	2.1
1	I	359	ARG	2.1
1	I	431	VAL	2.1
1	L	359	ARG	2.1
1	L	405	ASN	2.1
1	L	209	GLU	2.1
1	L	431	VAL	2.1
1	L	96	ASN	2.0
1	L	294	LYS	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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(Å <sup>2</sup> )	Q<0.9
2	NAA	I	500	14/15	0.89	0.19	0.44	2,69,398,468	1
2	NAA	L	500	14/15	0.93	0.23	-0.33	2,99,518,652	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.