



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 PM UTC

PDB ID : 2ANT / pdb_00002ant
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

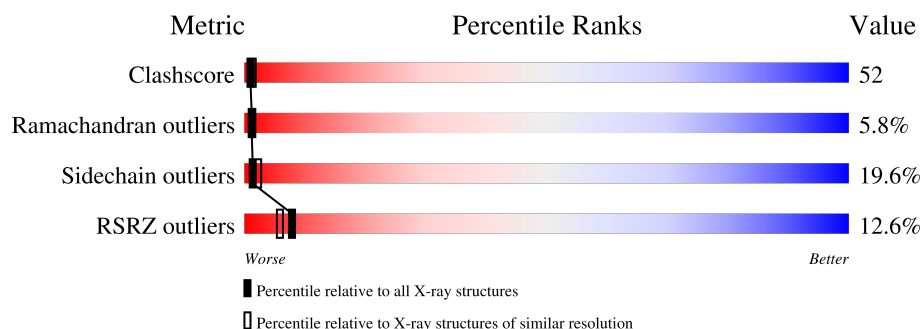
1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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](#)

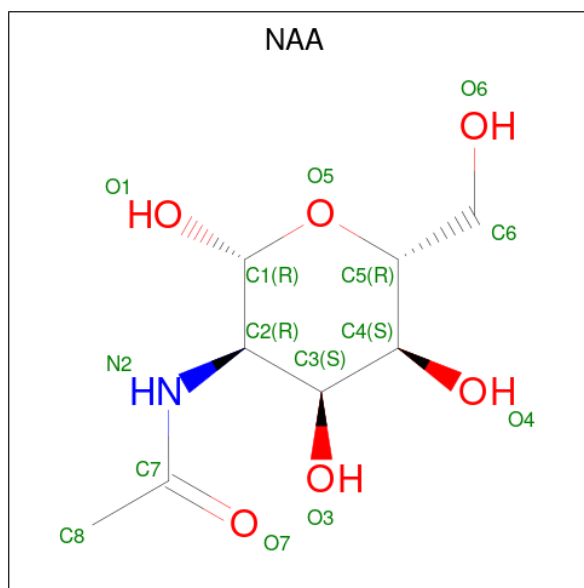
There are 3 unique types of molecules in this entry. The entry contains 6636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-acetamido-2-deoxy-beta-D-allopyranose (CCD ID: 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		

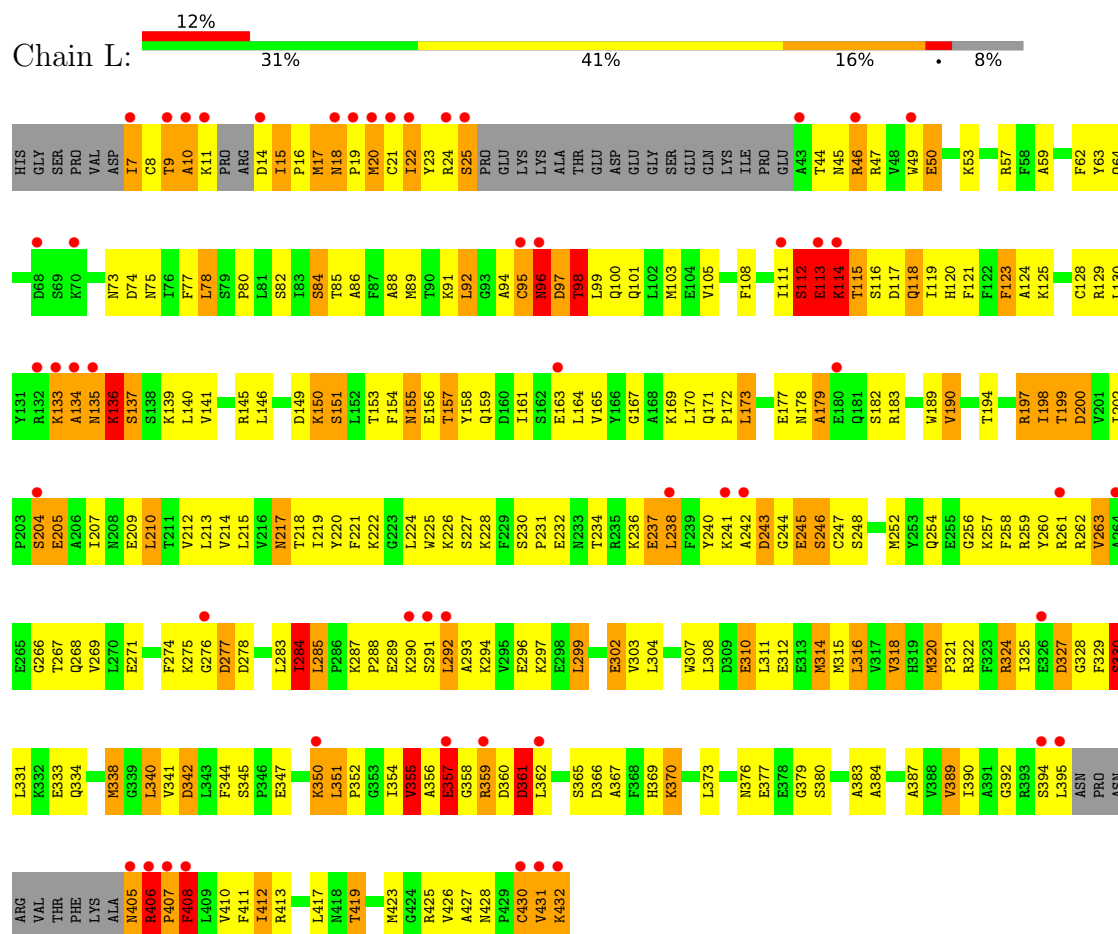
- Molecule 3 is water.

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

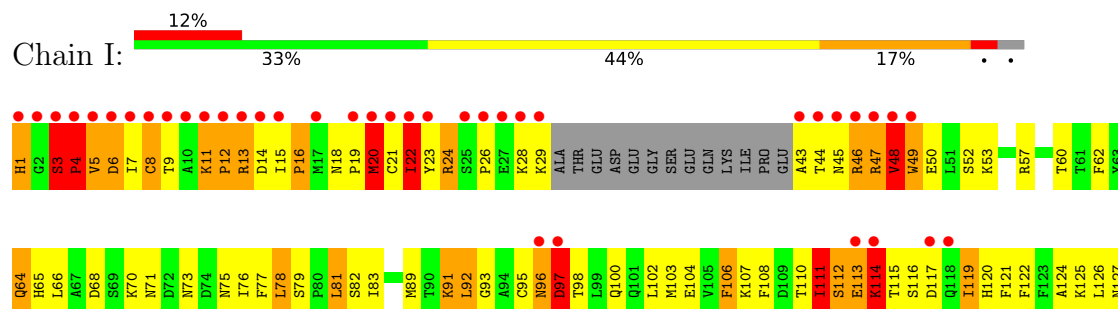
3 Residue-property plots [i](#)

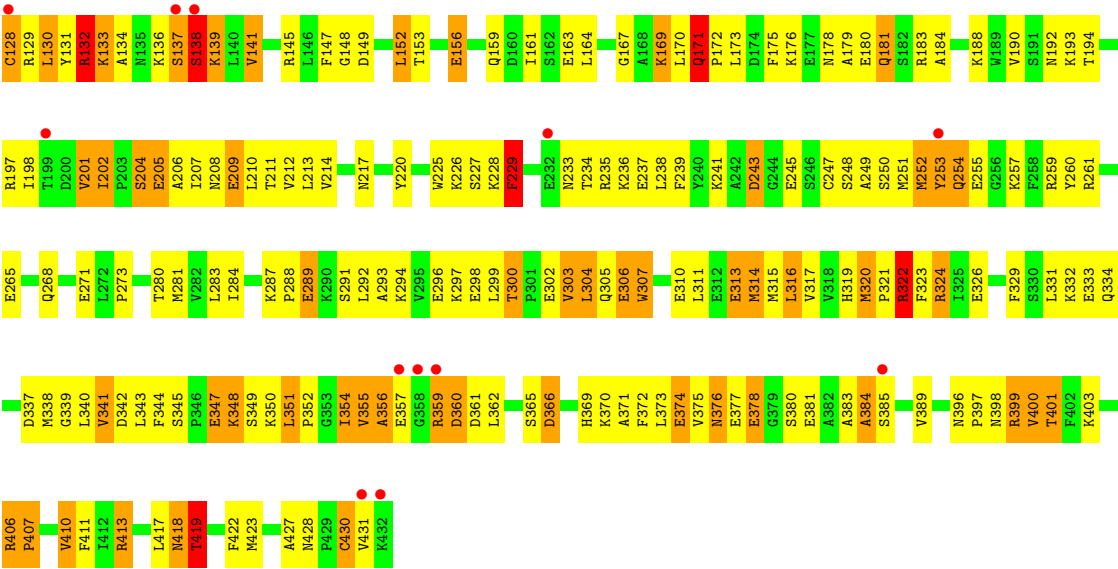
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: ANTITHROMBIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.41Å 98.31Å 90.41Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	26.90 – 2.60 26.90 – 2.62	Depositor EDS
% Data completeness (in resolution range)	74.0 (26.90-2.60) 78.0 (26.90-2.62)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.63Å)	Xtriage
Refinement program	TNT 5D	Depositor
R, R_{free}	0.217 , 0.290 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 97.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6636	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.95	0/3415	1.60	39/4608 (0.8%)
1	L	0.94	2/3240 (0.1%)	1.70	44/4367 (1.0%)
All	All	0.95	2/6655 (0.0%)	1.65	83/8975 (0.9%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	406	ARG	C-O	6.54	1.32	1.24
1	L	407	PRO	N-CD	5.17	1.54	1.47

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	406	ARG	CA-C-N	20.18	145.06	119.84
1	L	406	ARG	C-N-CA	20.18	145.06	119.84
1	L	406	ARG	C-N-CD	-15.87	59.94	125.00
1	L	135	ASN	N-CA-C	12.76	137.97	110.80
1	I	8	CYS	N-CA-C	-12.03	98.25	113.16
1	L	134	ALA	CA-C-N	11.36	143.24	121.54
1	L	134	ALA	C-N-CA	11.36	143.24	121.54
1	I	97	ASP	CA-CB-CG	-11.17	101.43	112.60
1	I	331	LEU	N-CA-C	10.81	123.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	407	PRO	CA-N-CD	-10.30	97.57	112.00
1	L	135	ASN	CA-C-N	10.12	140.86	121.54
1	L	135	ASN	C-N-CA	10.12	140.86	121.54
1	L	408	PHE	N-CA-C	10.09	132.29	110.80
1	L	407	PRO	N-CA-CB	9.22	112.93	103.25
1	I	13	ARG	N-CA-C	-8.93	102.55	113.97
1	L	407	PRO	CA-C-N	8.58	137.94	121.54
1	L	407	PRO	C-N-CA	8.58	137.94	121.54
1	I	111	ILE	CA-C-N	-8.51	111.39	122.79
1	I	111	ILE	C-N-CA	-8.51	111.39	122.79
1	I	48	VAL	N-CA-C	-8.28	104.63	112.83
1	L	135	ASN	CA-C-O	8.20	132.24	120.51
1	I	171	GLN	N-CA-C	8.04	124.00	109.44
1	L	155	ASN	CA-CB-CG	7.83	120.43	112.60
1	I	137	SER	N-CA-C	7.58	121.50	110.28
1	L	112	SER	N-CA-C	7.56	120.82	109.25
1	L	18	ASN	C-N-CD	-6.70	97.55	125.00
1	L	112	SER	N-CA-CB	6.60	120.63	109.87
1	I	3	SER	C-N-CD	-6.57	98.05	125.00
1	L	345	SER	N-CA-C	6.54	118.34	109.24
1	L	178	ASN	N-CA-C	6.52	118.26	110.44
1	I	252	MET	CA-C-N	6.47	132.55	121.29
1	I	252	MET	C-N-CA	6.47	132.55	121.29
1	L	135	ASN	O-C-N	6.46	131.18	122.59
1	L	200	ASP	CA-CB-CG	6.43	119.03	112.60
1	I	114	LYS	N-CA-C	6.32	124.25	110.80
1	I	360	ASP	N-CA-C	6.26	117.36	108.54
1	I	3	SER	N-CA-C	6.23	123.57	109.81
1	L	318	VAL	CB-CA-C	-6.19	102.50	110.98
1	L	98	THR	N-CA-C	-6.19	104.61	111.36
1	I	8	CYS	CA-C-N	6.11	133.20	121.54
1	I	8	CYS	C-N-CA	6.11	133.20	121.54
1	I	137	SER	CA-C-N	6.01	133.03	121.54
1	I	137	SER	C-N-CA	6.01	133.03	121.54
1	I	375	VAL	N-CA-C	5.98	116.54	108.17
1	I	139	LYS	N-CA-C	5.94	118.66	110.35
1	I	139	LYS	CB-CA-C	5.93	118.99	109.61
1	L	357	GLU	N-CA-C	5.91	118.16	108.52
1	L	136	LYS	N-CA-C	5.87	123.31	110.80
1	L	413	ARG	N-CA-C	5.82	118.70	109.50
1	L	347	GLU	N-CA-C	5.82	117.70	111.36
1	L	355	VAL	N-CA-CB	5.76	117.90	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	4	PRO	N-CA-CB	5.71	109.25	103.25
1	I	112	SER	N-CA-C	5.68	117.18	109.11
1	I	98	THR	N-CA-C	-5.64	105.04	111.07
1	I	322	ARG	N-CA-C	-5.53	103.09	110.55
1	I	226	LYS	N-CA-C	-5.49	105.45	111.82
1	I	229	PHE	N-CA-C	-5.48	102.42	110.52
1	I	407	PRO	N-CA-CB	5.48	107.92	103.32
1	L	351	LEU	CA-C-N	5.45	125.80	119.47
1	L	351	LEU	C-N-CA	5.45	125.80	119.47
1	I	356	ALA	N-CA-C	5.43	117.83	110.88
1	I	106	PHE	CA-CB-CG	-5.40	108.40	113.80
1	I	419	THR	CA-CB-OG1	5.37	117.66	109.60
1	I	141	VAL	N-CA-C	5.35	115.66	108.17
1	I	64	GLN	CA-C-N	5.33	128.20	120.79
1	I	64	GLN	C-N-CA	5.33	128.20	120.79
1	L	299	LEU	N-CA-C	5.31	117.87	109.96
1	I	413	ARG	N-CA-C	5.29	118.20	109.85
1	I	114	LYS	CA-C-N	5.22	130.76	122.62
1	I	114	LYS	C-N-CA	5.22	130.76	122.62
1	L	237	GLU	CA-C-N	5.21	131.50	121.54
1	L	237	GLU	C-N-CA	5.21	131.50	121.54
1	L	135	ASN	CB-CA-C	-5.19	100.08	110.42
1	I	112	SER	CB-CA-C	5.19	119.66	111.72
1	L	278	ASP	N-CA-C	-5.13	106.85	113.01
1	L	88	ALA	N-CA-C	-5.11	105.79	111.36
1	L	237	GLU	N-CA-C	5.10	115.89	108.14
1	L	179	ALA	N-CA-C	5.10	117.23	111.11
1	L	226	LYS	N-CA-C	-5.08	105.86	111.71
1	L	330	SER	N-CA-C	-5.05	104.20	110.41
1	L	133	LYS	N-CA-C	5.01	121.48	110.80
1	L	45	ASN	N-CA-C	-5.01	106.43	112.54
1	L	284	ILE	N-CA-CB	5.01	118.51	112.10

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	354	10
1	L	3181	0	3184	328	10
2	I	14	0	12	1	0
2	L	14	0	12	2	0
3	I	42	0	0	11	0
3	L	37	0	0	8	0
All	All	6636	0	6565	680	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 52.

All (680) 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:I:314:MET:HE1	1:I:400:VAL:HG13	1.27	1.16
1:L:355:VAL:HG13	1:L:359:ARG:HD2	1.31	1.08
1:L:252:MET:HE3	1:L:322:ARG:HB2	1.30	1.07
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:I:5:VAL:HG21	1:I:133:LYS:HZ3	1.32	0.91
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:L:252:MET:HE3	1:L:322:ARG:CB	2.01	0.90
1:I:5:VAL:HG21	1:I:133:LYS:NZ	1.86	0.89
1:L:86:ALA:HA	1:L:89:MET:HE3	1.52	0.89
1:L:283:LEU:HD13	1:L:408:PHE:HZ	1.35	0.89
1:I:62:PHE:HA	1:I:338:MET:HE1	1.56	0.88
1:L:179:ALA:HB1	1:L:207:ILE:HG22	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:314:MET:CE	1:I:400:VAL:HG13	2.04	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:252:MET:HE1	1:L:376:ASN:HA	1.57	0.86
1:L:355:VAL:N	1:L:359:ARG:HD3	1.91	0.86
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: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:HG2	1:I:406:ARG:HH11	1.45	0.80
1:L:73:ASN:HB3	1:L:405:ASN:N	1.96	0.80
1:I:23:TYR:HB2	1:I:100:GLN:HE22	1.46	0.80
1:L:252:MET:HE1	1:L:376:ASN:CA	2.12	0.79
1:I:75:ASN:ND2	1:I:427:ALA:N	2.29	0.79
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:L:62:PHE:HA	1:L:338:MET:CE	2.13	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:I:314:MET:HE2	1:I:315:MET:O	1.84	0.78
1:L:24:ARG:HB3	1:L:114:LYS:CE	2.14	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:53:LYS:HZ3	1:I:57:ARG:NH2	1.80	0.78
1:I:153:THR:H	1:I:356:ALA:CB	1.97	0.78
1:L:324:ARG:O	1:L:431:VAL:HG11	1.84	0.77
1:L:101:GLN:O	1:L:105:VAL:HG23	1.85	0.77
1:I:47:ARG:HD2	1:I:122:PHE:CE1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:LYS:HZ3	1:I:57:ARG:HH12	1.32	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: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:I:47:ARG:NH2	1:I:125:LYS:HZ1	1.85	0.75
1:L:20:MET:HB3	3:L:504:HOH:O	1.87	0.75
1:L:262:ARG:HE	1:L:266:GLY:HA2	1.53	0.74
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: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:L:53:LYS:O	1:L:57:ARG:HG3	1.89	0.73
1:L:252:MET:HE2	1:L:377:GLU:CD	2.14	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:L:252:MET:HE1	1:L:376:ASN:C	2.14	0.73
1:I:50:GLU:C	1:I:111:ILE:HD11	2.14	0.73
1:L:237:GLU:HG3	1:L:238:LEU:N	2.04	0.72
1:I:316:LEU:HG	1:I:400:VAL:HG22	1.71	0.72
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:HE1	1:L:377:GLU:N	2.04	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:L:238:LEU:HD21	1:L:240:TYR:HE2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:PRO:HG2	1:I:117:ASP:OD2	1.89	0.71
1:L:113:GLU:O	1:L:115:THR:HG22	1.91	0.71
1:I:236:LYS:HA	1:I:249:ALA:O	1.91	0.71
1:I:334:GLN:O	1:I:338:MET:HG3	1.90	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:L:59:ALA:O	1:L:423:MET:HE1	1.91	0.69
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: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
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:85:THR:O	1:L:89:MET:HG3	1.93	0.68
1:L:355:VAL:CG1	1:L:359:ARG:HH11	2.07	0.68
1:I:352:PRO:O	1:I:355:VAL:HG23	1.94	0.67
1:L:62:PHE:HA	1:L:338:MET:HE2	1.74	0.67
1:I:126:LEU:HD11	1:I:419:THR:HG21	1.77	0.67
1:I:103:MET:HE2	1:I:116:SER:HB3	1.76	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:47:ARG:HH21	1:I:125:LYS:HZ1	1.42	0.67
1:L:8:CYS:O	1:L:10:ALA:N	2.28	0.67
1:L:137:SER:OG	1:L:276:GLY:HA2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:VAL:CG2	1:I:132:ARG:HG2	2.23	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:I:376:ASN:C	1:I:376:ASN:HD22	2.03	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:HD2	1:I:399:ARG:N	2.11	0.66
1:I:152:LEU:HA	1:I:356:ALA:CB	2.21	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:111:ILE:HG23	1:I:112:SER:N	2.10	0.65
1:L:358:GLY:O	1:L:360:ASP:N	2.30	0.65
1:I:95:CYS:HB2	1:I:352:PRO:CG	2.26	0.65
1:L:261:ARG:HH11	1:L:312:GLU:HG3	1.61	0.65
1:I:53:LYS:NZ	1:I:57:ARG:NH2	2.44	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:62:PHE:HA	1:L:338:MET:HE1	1.79	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: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:18:ASN:OD1	1:I:19:PRO:HD2	1.96	0.64
1:I:108:PHE:HB3	1:I:119:ILE:CD1	2.28	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:I:281:MET:CE	1:I:283:LEU:HD21	2.28	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:47:ARG:NH2	1:I:125:LYS:NZ	2.46	0.64
1:I:97:ASP:HB3	3:I:527:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:PRO:HB3	1:I:15:ILE:HD12	1.80	0.63
1:I:204:SER:C	1:I:205:GLU:HG3	2.24	0.63
1:I:204:SER:O	1:I:205:GLU:HG3	1.99	0.63
1:I:334:GLN:HE21	1:I:338:MET:CE	2.12	0.63
1:I:18:ASN:CG	1:I:19:PRO:HD2	2.23	0.63
1:L:236:LYS:HG2	1:L:248:SER:OG	1.97	0.63
1:L:213:LEU:HG	1:L:214:VAL:N	2.13	0.63
1:I:396:ASN:OD1	1:I:397:PRO:HD2	1.98	0.63
1:L:287:LYS:CG	1:L:288:PRO:HD2	2.28	0.63
1:I:208:ASN:OD1	1:I:210:LEU:HB2	1.99	0.62
1:I:292:LEU:O	1:I:296:GLU:HG3	1.98	0.62
1:L:103:MET:HE1	1:L:119:ILE:HD11	1.80	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:L:224:LEU:HB3	1:L:275:LYS:HD2	1.82	0.62
1:I:5:VAL:N	1:I:132:ARG:HB2	2.15	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:204:SER:C	1:L:205:GLU:HG2	2.25	0.61
1:L:269:VAL:HG22	1:L:284:ILE:HG13	1.81	0.61
1:L:18:ASN:CA	1:L:161:ILE:HD11	2.29	0.61
1:L:124:ALA:HB2	1:L:165:VAL:HG13	1.82	0.61
1:L:159:GLN:HE21	1:L:170:LEU:HD22	1.65	0.61
1:L:238:LEU:HD21	1:L:240:TYR:CE2	2.34	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
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:16:PRO:HA	1:L:17:MET:HE3	1.82	0.60
1:L:252:MET:CE	1:L:376:ASN:HA	2.27	0.60
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:L:261:ARG:NE	1:L:310:GLU:HG2	2.17	0.60
1:I:24:ARG:O	1:I:24:ARG:HG3	2.02	0.60
1:L:163:GLU:O	1:L:167:GLY:HA2	2.02	0.60
1:I:26:PRO:HG2	1:I:29:LYS:C	2.27	0.60
1:I:334:GLN:NE2	1:I:338:MET:HE3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:252:MET:CE	1:L:322:ARG:HB2	2.20	0.60
1:I:281:MET:HE1	1:I:323:PHE:HZ	1.66	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:224:LEU:HB2	1:L:275:LYS:HD2	1.84	0.59
1:L:359:ARG:HG3	1:L:362:LEU:HD12	1.83	0.59
1:L:7:ILE:HG21	1:L:121:PHE:CD1	2.37	0.59
1:L:159:GLN:NE2	1:L:170:LEU:HD22	2.15	0.59
1:I:306:GLU:O	1:I:310:GLU:HG3	2.02	0.59
1:I:340:LEU:HD21	1:I:343:LEU:HD23	1.84	0.59
1:I:6:ASP:CG	1:I:7:ILE:H	2.11	0.59
1:I:281:MET:HE2	1:I:283:LEU:HD21	1.83	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:334:GLN:HE21	1:I:338:MET:HE3	1.68	0.59
1:L:329:PHE:HD2	1:L:330:SER:O	1.86	0.58
1:I:93:GLY:O	1:I:352:PRO:HD2	2.03	0.58
1:I:131:TYR:O	1:I:132:ARG:HB3	2.01	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: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:NH1	1:L:47:ARG:HG2	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
1:L:73:ASN:HD22	1:L:242:ALA:HB2	1.69	0.57
1:L:111:ILE:HD11	1:L:119:ILE:CD1	2.34	0.57
1:L:365:SER:OG	1:L:389:VAL:HG22	2.05	0.57
1:I:233:ASN:HB2	1:I:253:TYR:CB	2.35	0.57
1:L:14:ASP:CG	1:L:15:ILE:H	2.12	0.57
1:L:314:MET:HG3	1:L:315:MET:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PRO:HA	1:I:132:ARG:HA	1.87	0.57
1:I:356:ALA:O	1:I:357:GLU:HG2	2.05	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:137:SER:HB2	1:L:275:LYS:C	2.30	0.57
1:L:322:ARG:NH1	1:L:376:ASN:HB2	2.18	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:14:ASP:O	1:I:15:ILE:HG13	2.05	0.56
1:I:359:ARG:NH1	1:I:359:ARG:HG3	2.19	0.56
1:L:293:ALA:HB1	1:L:297:LYS:HZ1	1.69	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:359:ARG:HG2	1:I:361:ASP:OD1	2.06	0.56
1:I:141:VAL:CG1	1:I:193:LYS:HD3	2.36	0.56
1:I:156:GLU:OE2	2:I:500:NAA:N2	2.38	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:L:183:ARG:HB2	1:L:207:ILE:HD12	1.87	0.55
1:I:12:PRO:HB2	1:I:15:ILE:HB	1.87	0.55
1:L:299:LEU:CD2	1:L:304:LEU:HD21	2.36	0.55
1:L:316:LEU:C	1:L:316:LEU:HD23	2.31	0.55
1:I:11:LYS:HD2	1:I:11:LYS:O	2.05	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:113:GLU:C	1:I:114:LYS:HG3	2.31	0.55
1:I:108:PHE:HB3	1:I:119:ILE:HD11	1.89	0.55
1:I:175:PHE:HD2	1:I:211:THR:O	1.90	0.55
1:I:253:TYR:CG	1:I:254:GLN:N	2.74	0.55
1:L:75:ASN:OD1	1:L:427:ALA:N	2.28	0.55
1:L:419:THR:HG22	3:L:501:HOH:O	2.06	0.55
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:I:43:ALA:N	1:I:125:LYS:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:229:PHE:CD2	1:I:252:MET:HB3	2.42	0.54
1:I:121:PHE:HZ	1:I:125:LYS:HZ1	1.53	0.54
1:L:80:PRO:HG3	1:L:423:MET:HE2	1.89	0.54
1:L:173:LEU:CD1	1:L:182:SER:HA	2.36	0.54
1:L:190:VAL:O	1:L:194:THR:HG23	2.08	0.54
1:I:233:ASN:HB2	1:I:253:TYR:HB2	1.89	0.54
1:L:96:ASN:O	1:L:97:ASP:HB2	2.06	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:348:LYS:NZ	3:I:528:HOH:O	2.30	0.54
1:I:314:MET:HE1	1:I:400:VAL:H	1.72	0.54
1:I:5:VAL:HG23	1:I:133:LYS:N	2.22	0.54
1:I:289:GLU:CD	1:I:289:GLU:H	2.14	0.54
1:L:44:THR:CG2	1:L:47:ARG:HG2	2.37	0.54
1:L:103:MET:SD	1:L:108:PHE:HB2	2.47	0.54
1:L:361:ASP:C	1:L:362:LEU:HG	2.33	0.54
1:I:252:MET:SD	1:I:377:GLU:HG3	2.48	0.54
1:I:354:ILE:O	1:I:356:ALA:N	2.41	0.54
1:L:137:SER:HB2	1:L:276:GLY:CA	2.38	0.53
1:I:136:LYS:HA	1:I:136:LYS:HE2	1.90	0.53
1:I:159:GLN:CG	1:I:170:LEU:HD12	2.39	0.53
1:I:248:SER:O	1:I:430:CYS:HB3	2.09	0.53
1:I:350:LYS:C	1:I:352:PRO:HD3	2.34	0.53
1:I:48:VAL:CG2	1:I:126:LEU:HB2	2.38	0.53
1:L:9:THR:HG22	1:L:9:THR:O	2.09	0.53
1:I:198:ILE:HG23	1:I:370:LYS:HZ2	1.71	0.53
1:I:359:ARG:HG3	1:I:359:ARG:HH11	1.74	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:I:77:PHE:CE2	1:I:371:ALA:HB1	2.43	0.52
1:L:44:THR:HG22	1:L:44:THR:O	2.09	0.52
1:L:145:ARG:HG3	1:L:169:LYS:O	2.09	0.52
1:L:173:LEU:HD13	1:L:182:SER:HA	1.91	0.52
1:L:260:TYR:CG	1:L:261:ARG:N	2.77	0.52
1:L:125:LYS:O	1:L:129:ARG:HG3	2.09	0.52
1:L:370:LYS:O	1:L:384:ALA:HA	2.09	0.52
1:I:1:HIS:H2	1:I:8:CYS:HA	1.72	0.52
1:I:129:ARG:CG	1:I:417:LEU:HD11	2.35	0.52
1:I:345:SER:HG	1:I:348:LYS:HB2	1.74	0.52
1:L:341:VAL:HG23	1:L:342:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:ARG:NH1	1:L:171:GLN:OE1	2.42	0.52
1:I:3:SER:OG	1:I:127:ASN:O	2.28	0.52
1:I:83:ILE:HD13	1:I:217:ASN:ND2	2.21	0.52
1:I:83:ILE:CD1	1:I:217:ASN:HD21	2.22	0.52
1:I:132:ARG:O	1:I:132:ARG:HD3	2.10	0.52
1:I:300:THR:HG23	1:I:303:VAL:CG2	2.40	0.52
1:L:7:ILE:HD11	1:L:16:PRO:CG	2.40	0.52
1:L:242:ALA:C	1:L:244:GLY:H	2.18	0.52
1:L:283:LEU:HD22	1:L:408:PHE:CZ	2.45	0.52
1:L:94:ALA:HB1	1:L:98:THR:HG22	1.90	0.52
1:L:269:VAL:HG22	1:L:284:ILE:CG1	2.40	0.52
1:I:281:MET:CE	1:I:320:MET:HE1	2.39	0.52
1:L:431:VAL:HB	1:L:432:LYS:HE2	1.91	0.51
1:L:78:LEU:HD22	1:L:78:LEU:C	2.35	0.51
1:L:231:PRO:O	1:L:234:THR:OG1	2.29	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:111:ILE:HD11	1:L:119:ILE:HD13	1.92	0.51
1:L:116:SER:O	1:L:119:ILE:HG12	2.10	0.51
1:L:134:ALA:O	3:L:519:HOH:O	2.19	0.51
1:L:200:ASP:OD1	1:L:370:LYS:HD2	2.10	0.51
1:I:229:PHE:HA	1:I:253:TYR:CE1	2.45	0.51
1:L:11:LYS:O	1:L:164:LEU:HD11	2.11	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:417:LEU:HB2	1:I:419:THR:HG23	1.92	0.51
1:L:238:LEU:HD11	1:L:240:TYR:HE2	1.75	0.51
1:I:1:HIS:H1	1:I:8:CYS:C	2.18	0.51
1:I:13:ARG:HA	1:I:121:PHE:CE1	2.45	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:24:ARG:HB3	1:L:114:LYS:CD	2.41	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:I:180:GLU:N	3:I:508:HOH:O	2.43	0.51
1:I:304:LEU:HD21	1:I:411:PHE:CZ	2.46	0.51
1:L:63:TYR:HB2	1:L:423:MET:HE3	1.93	0.51
1:I:3:SER:N	1:I:4:PRO:CD	2.74	0.51
1:I:83:ILE:HD11	1:I:369:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:198:ILE:HD12	1:L:370:LYS:O	2.12	0.51
1:I:4:PRO:O	1:I:6:ASP:OD1	2.29	0.51
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:L:62:PHE:CA	1:L:338:MET:HE1	2.40	0.50
1:L:405:ASN:O	1:L:427:ALA:O	2.29	0.50
1:I:1:HIS:CG	1:I:9:THR:HG23	2.45	0.50
1:L:283:LEU:HD11	1:L:320:MET:HE1	1.94	0.50
1:L:238:LEU:HD11	1:L:240:TYR:CZ	2.46	0.50
1:L:327:ASP:O	1:L:370:LYS:HA	2.11	0.50
1:L:357:GLU:OE1	1:I:245:GLU:HG3	2.10	0.50
1:I:359:ARG:HG3	1:I:360:ASP:H	1.75	0.50
1:L:331:LEU:HA	1:L:334:GLN:OE1	2.10	0.50
1:L:73:ASN:ND2	1:L:242:ALA:HB2	2.27	0.50
1:L:179:ALA:O	1:L:182:SER:HB2	2.12	0.50
1:I:234:THR:HA	1:I:251:MET:O	2.12	0.50
1:L:77:PHE:HB2	1:L:325:ILE:HD11	1.94	0.50
1:L:237:GLU:CG	1:L:238:LEU:H	2.21	0.50
1:L:351:LEU:HD12	1:L:362:LEU:O	2.11	0.50
1:I:89:MET:O	1:I:92:LEU:HB2	2.12	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:L:99:LEU:HD12	1:L:99:LEU:O	2.12	0.49
1:L:190:VAL:HG22	1:L:218:THR:CG2	2.41	0.49
1:I:127:ASN:O	1:I:130:LEU:N	2.45	0.49
1:L:62:PHE:CB	1:L:338:MET:HE1	2.42	0.49
1:L:252:MET:HE3	1:L:322:ARG:CG	2.41	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:L:263:VAL:HG23	1:L:267:THR:HB	1.95	0.49
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.95	0.49
1:I:147:PHE:O	1:I:213:LEU:HA	2.13	0.49
1:L:139:LYS:O	1:L:221:PHE:HA	2.13	0.49
1:L:287:LYS:HG2	1:L:288:PRO:HD2	1.94	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:L:115:THR:HG23	1:L:118:GLN:HB2	1.93	0.48
1:I:7:ILE:C	1:I:9:THR:H	2.07	0.48
1:L:355:VAL:HG12	1:L:359:ARG:NH1	2.26	0.48

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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:227:SER:CB	1:I:254:GLN:HE22	2.26	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:255:GLU:HA	1:I:316:LEU:O	2.14	0.48
1:I:359:ARG:HH11	1:I:359:ARG:CG	2.27	0.48
1:L:194:THR:O	1:L:197:ARG:HB2	2.13	0.48
1:L:257:LYS:HG2	1:L:315:MET:HG2	1.94	0.48
1:I:9:THR:HG21	1:I:164:LEU:CD1	2.44	0.48
1:I:236:LYS:C	1:I:237:GLU:HG2	2.38	0.48
1:L:7:ILE:HD12	1:L:7:ILE:O	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:48:VAL:HG21	1:I:126:LEU:HB2	1.96	0.47
1:I:106:PHE:HB2	1:I:108:PHE:CE2	2.49	0.47
1:I:283:LEU:CD2	1:I:410:VAL:HG22	2.44	0.47
1:L:252:MET:HE2	1:L:377:GLU:OE1	2.13	0.47
1:L:263:VAL:N	1:L:267:THR:O	2.44	0.47
1:L:287:LYS:HG3	1:L:288:PRO:HD2	1.95	0.47
1:I:5:VAL:HG23	1:I:132:ARG:HB2	1.96	0.47
1:I:50:GLU:OE1	1:I:112:SER:OG	2.31	0.47
1:L:97:ASP:HA	1:L:100:GLN:HB3	1.96	0.47
1:L:431:VAL:HG12	1:L:432:LYS:NZ	2.29	0.47
1:I:287:LYS:HG3	1:I:289:GLU:HG2	1.96	0.47
1:I:145:ARG:HG3	1:I:169:LYS:O	2.14	0.47
1:I:281:MET:HE3	1:I:410:VAL:HG22	1.97	0.47
1:I:300:THR:HG23	1:I:303:VAL:CB	2.43	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:62:PHE:CD1	1:L:338:MET:CE	2.98	0.47
1:L:91:LYS:HE3	1:L:120:HIS:CE1	2.50	0.47
1:L:354:ILE:HG22	1:L:359:ARG:NH1	2.29	0.47
1:I:1:HIS:H1	1:I:8:CYS:CA	2.27	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: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:L:350:LYS:HB3	1:L:350:LYS:HE2	1.66	0.47
1:I:260:TYR:CG	1:I:261:ARG:N	2.83	0.47
1:I:373:LEU:HD12	1:I:374:GLU:N	2.29	0.47
1:L:59:ALA:C	1:L:423:MET:HE1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:225:TRP:CD1	1:L:379:GLY:HA2	2.50	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:299:LEU:HD22	1:L:304:LEU:HD11	1.97	0.46
1:L:64:GLN:NE2	1:L:299:LEU:O	2.48	0.46
1:L:112:SER:O	1:L:113:GLU:HB2	2.15	0.46
1:L:419:THR:HA	3:L:501:HOH:O	2.15	0.46
1:I:281:MET:HE1	1:I:323:PHE:CZ	2.49	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:I:209:GLU:CD	1:I:209:GLU:H	2.22	0.46
1:L:238:LEU:CD2	1:L:240:TYR:HE2	2.26	0.46
1:L:354:ILE:CG2	1:L:359:ARG:NH1	2.79	0.46
1:I:299:LEU:C	1:I:300:THR:HG22	2.40	0.46
1:L:355:VAL:CG1	1:L:359:ARG:NH1	2.77	0.46
1:I:149:ASP:OD2	1:I:176:LYS:HE3	2.16	0.46
1:I:212:VAL:HG21	1:I:362:LEU:HD23	1.98	0.46
1:I:250:SER:O	1:I:321:PRO:HA	2.16	0.46
1:I:329:PHE:N	1:I:369:HIS:O	2.46	0.46
1:I:359:ARG:NH1	1:I:360:ASP:N	2.42	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:L:95:CYS:HB2	1:L:352:PRO:HG3	1.97	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:I:152:LEU:CA	1:I:356:ALA:HB1	2.28	0.46
1:L:17:MET:SD	1:L:17:MET:N	2.88	0.45
1:L:62:PHE:HD1	1:L:338:MET:CE	2.29	0.45
1:L:290:LYS:CG	1:L:291:SER:N	2.80	0.45
1:I:112:SER:C	1:I:113:GLU:HG3	2.41	0.45
1:I:349:SER:OG	1:I:362:LEU:O	2.31	0.45
1:I:50:GLU:CD	1:I:112:SER:HG	2.23	0.45
1:I:108:PHE:O	1:I:111:ILE:HB	2.16	0.45
1:L:241:LYS:CG	1:L:405:ASN:HB3	2.47	0.45
1:L:428:ASN:ND2	1:L:430:CYS:SG	2.89	0.45
1:L:428:ASN:O	1:L:431:VAL:HG13	2.17	0.45
1:I:418:ASN:HD22	1:I:418:ASN:HA	1.48	0.45
1:L:183:ARG:NH1	1:L:202:ILE:O	2.45	0.45
1:L:256:GLY:O	1:L:316:LEU:HD22	2.16	0.45
1:I:53:LYS:CE	1:I:57:ARG:NH1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:ILE:HG23	1:I:112:SER:H	1.81	0.45
1:I:350:LYS:O	1:I:352:PRO:HD3	2.17	0.45
1:I:410:VAL:O	1:I:423:MET:HA	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:CD1	1:I:120:HIS:CE1	2.99	0.45
1:I:92:LEU:HD13	1:I:120:HIS:CE1	2.52	0.45
1:L:46:ARG:CG	1:L:47:ARG:NH1	2.79	0.45
1:L:408:PHE:CD2	1:L:426:VAL:HB	2.47	0.45
1:I:3:SER:OG	1:I:131:TYR:O	2.27	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:L:145:ARG:HB2	1:L:189:TRP:CH2	2.52	0.44
1:L:213:LEU:HG	1:L:214:VAL:H	1.82	0.44
1:L:149:ASP:C	1:L:151:SER:H	2.25	0.44
1:I:110:THR:O	1:I:111:ILE:O	2.35	0.44
1:I:273:PRO:HB3	1:I:280:THR:HG22	1.99	0.44
1:I:316:LEU:CG	1:I:400:VAL:HG22	2.44	0.44
1:L:199:THR:O	1:L:200:ASP:OD1	2.35	0.44
1:L:293:ALA:HB1	1:L:297:LYS:HE3	1.99	0.44
1:I:138:SER:O	1:I:138:SER:OG	2.30	0.44
1:L:46:ARG:O	1:L:50:GLU:HB2	2.17	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:215:LEU:O	1:L:387:ALA:HA	2.18	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:18:ASN:CB	1:L:161:ILE:HD11	2.47	0.44
1:L:259:ARG:NH1	1:L:271:GLU:OE1	2.51	0.44
1:L:408:PHE:HB3	1:L:426:VAL:O	2.18	0.44
1:I:20:MET:O	1:I:22:ILE:HG12	2.17	0.44
1:I:103:MET:CE	1:I:116:SER:HB3	2.45	0.44
1:L:150:LYS:NZ	1:I:70:LYS:O	2.42	0.44
1:I:81:LEU:HD11	1:I:130:LEU:HD21	2.00	0.44
1:I:92:LEU:HA	1:I:92:LEU:HD12	1.65	0.44
1:I:305:GLN:OE1	1:I:305:GLN:HA	2.18	0.44
1:L:248:SER:O	1:L:430:CYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:302:GLU:H	1:L:302:GLU:HG2	1.23	0.43
1:I:239:PHE:O	1:I:247:CYS:N	2.51	0.43
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.99	0.43
1:I:332:LYS:HE3	1:I:344:PHE:HB3	2.00	0.43
1:I:362:LEU:HD23	1:I:362:LEU:HA	1.80	0.43
1:I:147:PHE:HB2	1:I:214:VAL:HG12	1.99	0.43
1:I:292:LEU:HD22	1:I:407:PRO:HB2	2.00	0.43
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.53	0.43
1:L:146:LEU:HD21	1:L:215:LEU:HD23	2.00	0.43
1:L:333:GLU:H	1:L:333:GLU:CD	2.20	0.43
1:L:417:LEU:HA	1:L:417:LEU:HD23	1.72	0.43
1:I:178:ASN:HB3	1:I:181:GLN:HB3	1.99	0.43
1:I:179:ALA:HB1	1:I:207:ILE:HG22	2.00	0.43
1:L:412:ILE:N	3:L:534:HOH:O	2.51	0.43
1:I:46:ARG:HA	1:I:49:TRP:HB2	1.99	0.43
1:I:130:LEU:HD13	1:I:417:LEU:HD12	2.00	0.43
1:L:432:LYS:CD	1:L:432:LYS:N	2.80	0.43
1:I:129:ARG:O	1:I:129:ARG:HG3	2.09	0.43
1:I:152:LEU:CD1	1:I:362:LEU:HD21	2.47	0.43
1:I:265:GLU:O	1:I:287:LYS:HD3	2.19	0.43
1:I:281:MET:HE2	1:I:320:MET:HE1	1.99	0.43
1:I:281:MET:HE3	1:I:283:LEU:HD21	1.98	0.43
1:L:257:LYS:HG2	1:L:315:MET:SD	2.58	0.43
1:L:283:LEU:HD11	1:L:320:MET:CE	2.48	0.43
1:L:410:VAL:HG12	1:L:411:PHE:N	2.33	0.43
1:I:5:VAL:O	1:I:6:ASP:O	2.36	0.43
1:I:107:LYS:HB3	1:I:110:THR:HG21	2.00	0.43
1:I:281:MET:HE3	1:I:410:VAL:CG2	2.48	0.43
1:L:316:LEU:HD23	1:L:316:LEU:O	2.19	0.43
1:L:365:SER:CB	1:L:392:GLY:H	2.32	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:340:LEU:HD13	1:L:344:PHE:CE1	2.54	0.43
1:I:1:HIS:H1	1:I:8:CYS:HA	1.81	0.43
1:L:241:LYS:HB3	1:L:405:ASN:HB3	2.01	0.43
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:L:293:ALA:HB1	1:L:297:LYS:HZ2	1.79	0.42
1:I:52:SER:HB2	1:I:418:ASN:O	2.20	0.42
1:L:209:GLU:C	1:L:210:LEU:HD23	2.44	0.42

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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:HD2	1:I:197:ARG:HA	1.74	0.42
1:L:258:PHE:CD1	1:L:316:LEU:CD2	3.01	0.42
1:L:304:LEU:HD23	1:L:307:TRP:CZ3	2.54	0.42
1:I:288:PRO:HD3	1:I:406:ARG:NH2	2.34	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:I:19:PRO:O	1:I:20:MET:SD	2.77	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:L:47:ARG:HD3	1:L:50:GLU:OE1	2.20	0.42
1:L:91:LYS:NZ	1:L:120:HIS:HE1	2.17	0.42
1:I:5:VAL:CG2	1:I:133:LYS:HB3	2.50	0.42
1:I:97:ASP:CG	3:I:537:HOH:O	2.62	0.42
1:I:243:ASP:O	1:I:245:GLU:HG2	2.20	0.42
1:I:342:ASP:OD2	1:I:348:LYS:NZ	2.30	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:65:HIS:CD2	1:I:338:MET:HE2	2.55	0.42
1:L:224:LEU:HA	1:L:224:LEU:HD23	1.81	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:230:SER:OG	1:L:232:GLU:HG2	2.19	0.41
1:L:320:MET:HA	1:L:321:PRO:HD3	1.93	0.41
1:I:229:PHE:CD2	1:I:253:TYR:O	2.73	0.41
1:I:307:TRP:O	1:I:311:LEU:HD13	2.20	0.41
1:I:326:GLU:HG2	1:I:372:PHE:CD2	2.54	0.41
1:I:281:MET:HE1	1:I:320:MET:HE1	2.03	0.41
1:L:101:GLN:OE1	1:L:342:ASP:HB2	2.19	0.41
1:L:220:TYR:CD1	1:L:220:TYR:C	2.97	0.41
1:L:308:LEU:HD23	1:L:311:LEU:HD11	2.02	0.41
1:I:13:ARG:HA	1:I:13:ARG:HD3	1.62	0.41
1:I:107:LYS:HB3	1:I:110:THR:CG2	2.50	0.41
1:L:324:ARG:HA	1:L:373:LEU:O	2.21	0.41
1:L:362:LEU:HB3	1:L:390:ILE:CG2	2.50	0.41
1:L:7:ILE:HA	1:L:11:LYS:O	2.20	0.41
1:L:183:ARG:CA	1:L:207:ILE:HD12	2.51	0.41
1:I:44:THR:CG2	1:I:47:ARG:HG2	2.48	0.41
1:I:70:LYS:CE	1:I:76:ILE:HG12	2.51	0.41
1:I:77:PHE:CD2	1:I:371:ALA:HB1	2.55	0.41
1:L:7:ILE:CD1	1:L:16:PRO:CG	2.99	0.41

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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:219:ILE:O	1:L:383:ALA:HA	2.21	0.41
1:L:329:PHE:CE2	1:L:331:LEU:HD23	2.56	0.41
1:L:242:ALA:C	1:L:244:GLY:N	2.78	0.41
1:L:290:LYS:CE	1:L:294:LYS:HD2	2.50	0.41
1:I:65:HIS:NE2	1:I:337:ASP:OD2	2.46	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: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:260:TYR:HE1	1:L:268:GLN:HB3	1.86	0.41
1:L:315:MET:HE3	1:L:315:MET:HB3	1.96	0.41
1:I:428:ASN:OD1	1:I:430:CYS:SG	2.79	0.41
1:L:62:PHE:HB2	1:L:338:MET:HE1	2.03	0.41
1:L:103:MET:SD	1:L:108:PHE:CB	3.08	0.41
1:L:247:CYS:HB2	1:L:430:CYS:HB2	1.90	0.41
1:I:53:LYS:NZ	1:I:57:ARG:CZ	2.81	0.41
1:I:53:LYS:CE	1:I:57:ARG:CZ	2.99	0.41
1:I:141:VAL:HB	1:I:220:TYR:HB3	2.01	0.41
1:I:173:LEU:HB2	1:I:175:PHE:CE1	2.56	0.41
1:I:183:ARG:CA	1:I:207:ILE:HD12	2.51	0.41
1:I:280:THR:OG1	1:I:413:ARG:NH1	2.54	0.41
1:I:299:LEU:O	1:I:300:THR:HG22	2.21	0.41
1:I:400:VAL:HG23	1:I:401:THR:N	2.35	0.41
1:L:130:LEU:HD22	1:L:140:LEU:HD21	2.02	0.41
1:I:188:LYS:O	1:I:192:ASN:ND2	2.54	0.41
1:I:239:PHE:CZ	1:I:406:ARG:C	2.99	0.41
1:L:137:SER:CB	1:L:276:GLY:CA	2.99	0.40
1:L:159:GLN:HE21	1:L:170:LEU:HD13	1.86	0.40
1:L:274:PHE:CZ	1:L:380:SER:HB3	2.55	0.40
1:I:132:ARG:HD3	1:I:132:ARG:C	2.46	0.40
1:I:152:LEU:N	1:I:152:LEU:HD23	2.35	0.40
1:L:252:MET:CE	1:L:377:GLU:N	2.81	0.40
1:I:28:LYS:HA	1:I:28:LYS:HD3	1.78	0.40
1:I:347:GLU:H	1:I:347:GLU:HG2	1.44	0.40
1:L:241:LYS:CB	1:L:405:ASN:HB3	2.52	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
1:I:11:LYS:N	1:I:12:PRO:CD	2.83	0.40
1:I:284:ILE:CD1	1:I:411:PHE:HE1	2.26	0.40
1:L:405:ASN:O	1:L:406:ARG:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:I:413:ARG:HH11	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	1
1	L	390/432 (90%)	342 (88%)	25 (6%)	23 (6%)	1	1
All	All	805/864 (93%)	695 (86%)	63 (8%)	47 (6%)	1	1

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	9	THR

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Mol	Chain	Res	Type
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

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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%)	298 (80%)	74 (20%)	1	2
1	L	353/383 (92%)	285 (81%)	68 (19%)	1	2
All	All	725/766 (95%)	583 (80%)	142 (20%)	1	2

All (142) 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	22	ILE
1	L	25	SER
1	L	46	ARG
1	L	50	GLU
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

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Mol	Chain	Res	Type
1	L	123	PHE
1	L	136	LYS
1	L	137	SER
1	L	151	SER
1	L	156	GLU
1	L	157	THR
1	L	173	LEU
1	L	177	GLU
1	L	190	VAL
1	L	197	ARG
1	L	198	ILE
1	L	199	THR
1	L	205	GLU
1	L	210	LEU
1	L	217	ASN
1	L	222	LYS
1	L	227	SER
1	L	238	LEU
1	L	243	ASP
1	L	246	SER
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	338	MET
1	L	340	LEU
1	L	342	ASP
1	L	350	LYS
1	L	355	VAL
1	L	357	GLU
1	L	361	ASP
1	L	370	LYS

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Mol	Chain	Res	Type
1	L	389	VAL
1	L	405	ASN
1	L	408	PHE
1	L	412	ILE
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	119	ILE
1	I	128	CYS
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	152	LEU
1	I	156	GLU
1	I	169	LYS
1	I	171	GLN
1	I	181	GLN
1	I	201	VAL
1	I	202	ILE
1	I	204	SER
1	I	205	GLU

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Mol	Chain	Res	Type
1	I	209	GLU
1	I	229	PHE
1	I	235	ARG
1	I	253	TYR
1	I	268	GLN
1	I	289	GLU
1	I	300	THR
1	I	302	GLU
1	I	303	VAL
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	320	MET
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	400	VAL
1	I	401	THR
1	I	406	ARG
1	I	410	VAL
1	I	418	ASN
1	I	419	THR
1	I	430	CYS
1	I	431	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	45	ASN
1	L	120	HIS
1	L	135	ASN
1	L	159	GLN
1	L	178	ASN
1	L	217	ASN
1	L	233	ASN
1	L	254	GLN
1	L	336	GLN
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	178	ASN
1	I	217	ASN
1	I	254	GLN
1	I	268	GLN
1	I	319	HIS
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 oligosaccharides 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	L	500	-	14,14,15	1.02	1 (7%)	17,19,21	3.89	13 (76%)
2	NAA	I	500	-	14,14,15	1.05	1 (7%)	17,19,21	4.39	13 (76%)

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	L	500	-	1/1/5/7	3/6/23/26	0/1/1/1
2	NAA	I	500	-	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	500	NAA	C7-N2	3.44	1.45	1.34
2	I	500	NAA	C7-N2	3.33	1.45	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	500	NAA	C1-C2-N2	10.75	127.38	110.43
2	L	500	NAA	C1-C2-N2	-6.81	99.69	110.43
2	I	500	NAA	C1-O5-C5	-6.24	103.83	112.19
2	L	500	NAA	O5-C5-C6	5.71	118.77	107.66
2	L	500	NAA	O5-C1-C2	5.33	119.53	111.29
2	L	500	NAA	O3-C3-C2	4.99	119.76	109.40
2	I	500	NAA	O4-C4-C5	4.82	121.19	109.32
2	I	500	NAA	O5-C1-C2	4.81	118.73	111.29
2	L	500	NAA	O4-C4-C5	4.67	120.83	109.32
2	I	500	NAA	O5-C5-C6	4.48	116.39	107.66
2	L	500	NAA	O4-C4-C3	4.46	120.88	110.38
2	I	500	NAA	O3-C3-C2	4.45	118.64	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	500	NAA	O5-C5-C4	4.32	121.35	110.83
2	L	500	NAA	C3-C4-C5	4.30	118.03	110.23
2	I	500	NAA	O4-C4-C3	4.27	120.45	110.38
2	I	500	NAA	O5-C5-C4	3.91	120.35	110.83
2	I	500	NAA	O3-C3-C4	3.81	119.36	110.38
2	L	500	NAA	O3-C3-C4	3.43	118.47	110.38
2	I	500	NAA	C8-C7-N2	-3.23	110.76	116.12
2	L	500	NAA	C4-C3-C2	3.08	115.53	111.02
2	I	500	NAA	C3-C4-C5	2.95	115.58	110.23
2	L	500	NAA	C8-C7-N2	-2.92	111.28	116.12
2	L	500	NAA	O6-C6-C5	2.80	120.88	111.33
2	I	500	NAA	O6-C6-C5	2.51	119.88	111.33
2	I	500	NAA	C2-N2-C7	-2.40	119.68	122.90
2	L	500	NAA	C2-N2-C7	-2.31	119.80	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	L	500	NAA	C4

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	500	NAA	C8-C7-N2-C2
2	I	500	NAA	O7-C7-N2-C2
2	L	500	NAA	O7-C7-N2-C2
2	I	500	NAA	O5-C5-C6-O6
2	L	500	NAA	C4-C5-C6-O6
2	I	500	NAA	C8-C7-N2-C2
2	I	500	NAA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	500	NAA	2	0
2	I	500	NAA	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	419/432 (96%)	0.55	51 (12%) 8 6	26, 47, 121, 162	0
1	L	398/432 (92%)	0.67	52 (13%) 7 5	27, 54, 121, 136	0
All	All	817/864 (94%)	0.61	103 (12%) 8 6	26, 49, 121, 162	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	3	SER	7.0
1	I	2	GLY	6.3
1	L	7	ILE	6.3
1	I	253	TYR	5.6
1	L	406	ARG	5.5
1	I	7	ILE	5.2
1	L	407	PRO	5.0
1	I	1	HIS	5.0
1	I	4	PRO	4.9
1	I	20	MET	4.9
1	I	5	VAL	4.7
1	I	21	CYS	4.6
1	I	10	ALA	4.4
1	I	357	GLU	4.4
1	I	43	ALA	4.3
1	I	49	TRP	4.2
1	L	113	GLU	4.2
1	I	9	THR	4.2
1	L	238	LEU	4.2
1	I	19	PRO	4.2
1	I	6	ASP	4.1
1	L	19	PRO	4.1
1	L	241	LYS	4.0
1	I	29	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	26	PRO	4.0
1	L	25	SER	3.9
1	L	96	ASN	3.9
1	L	20	MET	3.8
1	L	95	CYS	3.7
1	I	13	ARG	3.7
1	L	357	GLU	3.7
1	I	138	SER	3.6
1	I	25	SER	3.6
1	L	405	ASN	3.5
1	L	70	LYS	3.5
1	L	292	LEU	3.4
1	I	45	ASN	3.4
1	I	46	ARG	3.4
1	I	23	TYR	3.3
1	I	8	CYS	3.3
1	L	291	SER	3.3
1	I	27	GLU	3.3
1	I	385	SER	3.3
1	L	114	LYS	3.3
1	I	44	THR	3.2
1	L	68	ASP	3.1
1	I	47	ARG	3.1
1	L	359	ARG	3.1
1	I	199	THR	3.0
1	L	163	GLU	3.0
1	L	10	ALA	3.0
1	L	408	PHE	3.0
1	I	12	PRO	2.9
1	I	117	ASP	2.9
1	I	358	GLY	2.9
1	L	431	VAL	2.9
1	I	96	ASN	2.8
1	L	21	CYS	2.8
1	I	14	ASP	2.8
1	I	48	VAL	2.8
1	L	134	ALA	2.7
1	L	132	ARG	2.7
1	I	15	ILE	2.7
1	L	362	LEU	2.6
1	L	46	ARG	2.6
1	L	18	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	395	LEU	2.6
1	L	261	ARG	2.6
1	I	432	LYS	2.6
1	L	242	ALA	2.6
1	I	17	MET	2.5
1	I	28	LYS	2.5
1	I	232	GLU	2.5
1	I	97	ASP	2.5
1	I	359	ARG	2.5
1	I	114	LYS	2.4
1	I	128	CYS	2.4
1	L	180	GLU	2.4
1	L	326	GLU	2.4
1	L	432	LYS	2.4
1	L	9	THR	2.4
1	L	290	LYS	2.4
1	I	431	VAL	2.4
1	L	430	CYS	2.3
1	I	22	ILE	2.3
1	L	49	TRP	2.3
1	I	113	GLU	2.2
1	I	118	GLN	2.2
1	L	204	SER	2.2
1	L	276	GLY	2.2
1	L	111	ILE	2.2
1	L	24	ARG	2.2
1	I	11	LYS	2.2
1	L	22	ILE	2.1
1	L	135	ASN	2.1
1	I	137	SER	2.1
1	L	43	ALA	2.1
1	L	264	ALA	2.1
1	L	394	SER	2.0
1	L	350	LYS	2.0
1	L	14	ASP	2.0
1	L	11	LYS	2.0
1	L	133	LYS	2.0

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 [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	NAA	I	500	14/15	0.83	0.28	2,69,398,468	1
2	NAA	L	500	14/15	0.86	0.24	2,99,518,652	1

6.5 Other polymers [i](#)

There are no such residues in this entry.