



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2020 – 02:36 am BST

PDB ID : 2I6B
Title : Human Adenosine Kinase in Complex with An Acetylinic Inhibitor
Authors : Muchmore, S.W.
Deposited on : 2006-08-28
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

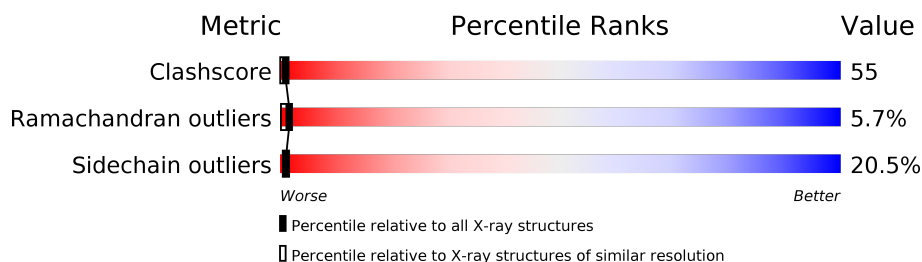
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	

2 Entry composition [i](#)

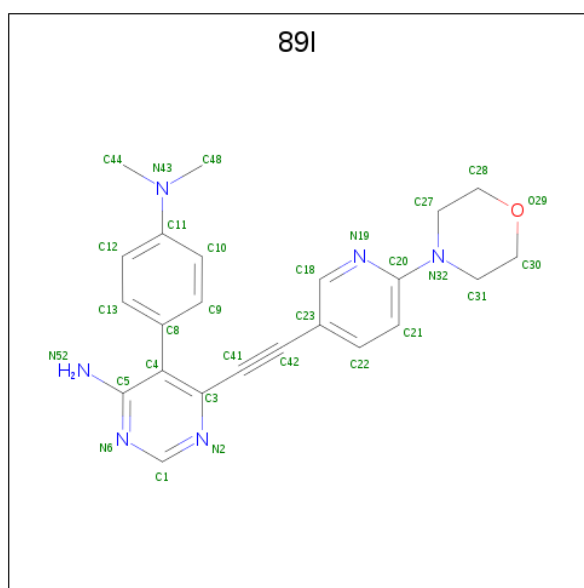
There are 3 unique types of molecules in this entry. The entry contains 5447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2587	1645	438	491	13			
1	B	326	Total	C	N	O	S	0	0	0
			2564	1629	435	487	13			

- Molecule 2 is 5-[4-(DIMETHYLAMINO)PHENYL]-6-[(6-MORPHOLIN-4-YLPYRIDIN-3-YL)ETHYNYL]PYRIMIDIN-4-AMINE (three-letter code: 89I) (formula: C₂₃H₂₄N₆O).



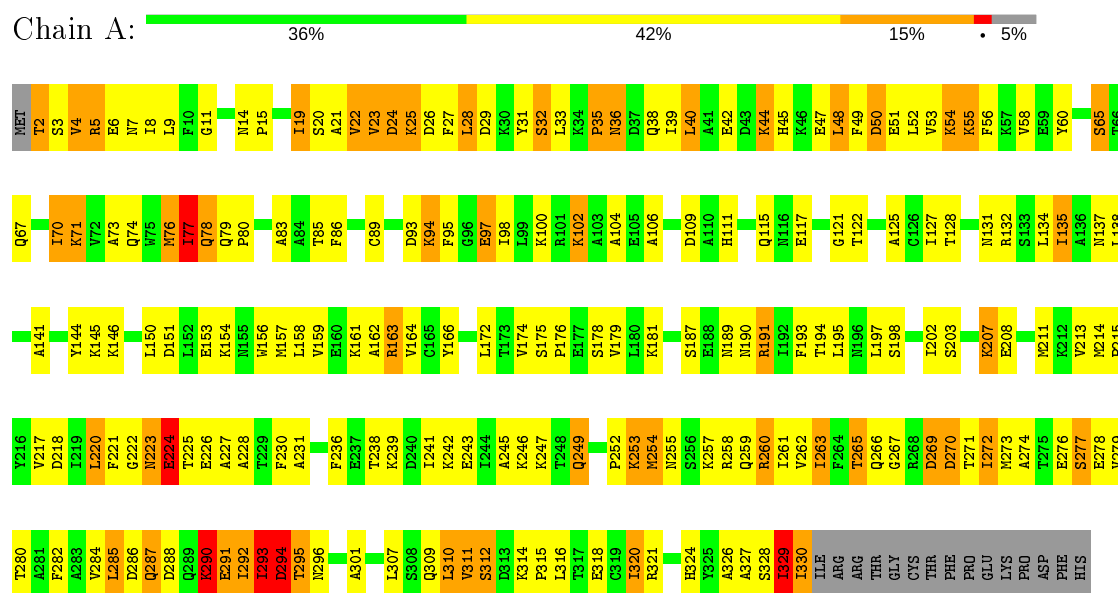
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total 124	O 124	0	0
3	B	112	Total 112	O 112	0	0

3 Residue-property plots

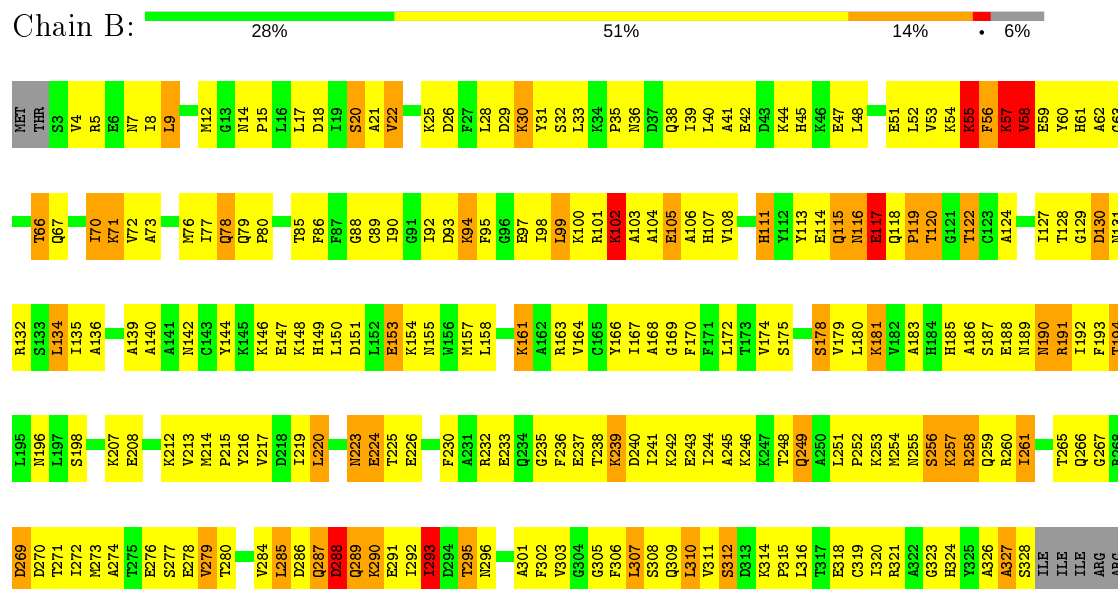
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Adenosine kinase



- Molecule 1: Adenosine kinase



THR
GLY
CYS
THR
PHE
PRO
GLU
LYS
PRO
ASP
PHE
HIS

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.18 Å 58.20 Å 89.21 Å 90.00° 107.54° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (50.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER	Depositor
R, R_{free}	0.221 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5447	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 89I

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/2636	0.87	5/3555 (0.1%)
1	B	0.64	0/2613	0.86	5/3523 (0.1%)
All	All	0.68	0/5249	0.87	10/7078 (0.1%)

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	B	1	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	MET	C-N-CA	8.54	143.04	121.70
1	B	56	PHE	N-CA-C	7.09	130.14	111.00
1	B	120	THR	O-C-N	-7.01	111.29	123.20
1	B	220	LEU	CA-CB-CG	6.60	130.48	115.30
1	B	172	LEU	CA-CB-CG	6.38	129.98	115.30
1	A	40	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	294	ASP	O-C-N	-6.16	112.84	122.70
1	A	329	ILE	N-CA-C	-6.13	94.46	111.00
1	A	22	VAL	O-C-N	-5.81	113.40	122.70
1	B	120	THR	CA-C-N	5.28	126.75	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	56	PHE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	ASN	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2587	0	2576	265	1
1	B	2564	0	2547	301	1
2	A	30	0	24	5	0
2	B	30	0	24	6	0
3	A	124	0	0	19	0
3	B	112	0	0	15	0
All	All	5447	0	5171	570	1

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 55.

All (570) 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:A:290:LYS:HB3	1:A:293:ILE:CG2	1.48	1.42
1:A:290:LYS:CB	1:A:293:ILE:HG23	1.56	1.36
1:A:290:LYS:O	1:A:293:ILE:HG12	1.26	1.27
1:A:290:LYS:HZ3	1:A:292:ILE:CB	1.56	1.18
1:A:73:ALA:O	1:A:77:ILE:HG13	1.01	1.16
1:B:7:ASN:HD22	1:B:161:LYS:NZ	1.43	1.15
1:A:73:ALA:O	1:A:77:ILE:CG1	1.95	1.14
1:B:22:VAL:HG23	1:B:57:LYS:HD2	1.26	1.12
1:A:290:LYS:NZ	1:A:292:ILE:HB	1.65	1.12
1:A:21:ALA:HB2	1:A:58:VAL:HG12	1.32	1.11
1:A:290:LYS:HZ3	1:A:292:ILE:HB	1.15	1.07
1:B:79:GLN:HG3	1:B:80:PRO:HA	1.30	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:HG23	1:A:4:VAL:HG23	1.38	1.05
1:B:194:THR:HG22	1:B:219:ILE:HB	1.39	1.04
1:B:276:GLU:HG3	3:B:603:HOH:O	1.58	1.02
1:B:42:GLU:H	1:B:45:HIS:HD2	1.02	1.01
1:A:23:VAL:HG21	1:A:28:LEU:HD21	1.40	0.98
1:B:284:VAL:HG22	1:B:324:HIS:HE1	1.26	0.97
1:B:284:VAL:HG22	1:B:324:HIS:CE1	1.98	0.97
1:A:121:GLY:O	1:A:122:THR:HG22	1.63	0.97
1:B:7:ASN:HD22	1:B:161:LYS:HZ2	1.09	0.97
1:A:79:GLN:HG3	1:A:80:PRO:HA	1.49	0.94
1:B:94:LYS:HD3	1:B:98:ILE:HD11	1.48	0.94
1:A:25:LYS:HA	1:A:28:LEU:HG	1.50	0.94
1:A:290:LYS:CE	1:A:292:ILE:HB	1.98	0.93
1:A:259:GLN:HG2	1:A:276:GLU:HB2	1.48	0.92
1:A:121:GLY:C	1:A:122:THR:CG2	2.38	0.91
1:B:119:PRO:O	1:B:140:ALA:HB2	1.70	0.91
1:B:223:ASN:HD21	1:B:226:GLU:HG3	1.35	0.90
1:A:23:VAL:HG13	3:A:570:HOH:O	1.71	0.89
1:A:290:LYS:NZ	1:A:292:ILE:CB	2.26	0.89
1:B:22:VAL:CG2	1:B:57:LYS:HD2	2.02	0.88
1:A:35:PRO:O	1:A:131:ASN:HB3	1.72	0.88
1:A:35:PRO:HB2	1:A:131:ASN:ND2	1.88	0.88
1:B:273:MET:SD	1:B:316:LEU:HD13	2.15	0.86
1:B:290:LYS:HZ3	1:B:292:ILE:HB	1.41	0.86
1:B:20:SER:O	1:B:58:VAL:HA	1.76	0.86
1:A:320:ILE:O	1:A:324:HIS:HD2	1.59	0.85
1:B:102:LYS:HG3	3:B:531:HOH:O	1.77	0.85
1:A:290:LYS:CG	1:A:293:ILE:HG23	2.07	0.85
1:B:42:GLU:H	1:B:45:HIS:CD2	1.93	0.85
1:A:290:LYS:NZ	1:A:292:ILE:CG2	2.40	0.85
1:B:290:LYS:HB3	1:B:293:ILE:HG23	1.59	0.84
1:A:121:GLY:C	1:A:122:THR:HG23	1.97	0.84
1:A:42:GLU:H	1:A:45:HIS:HD2	1.25	0.83
1:B:180:LEU:CD2	1:B:213:VAL:HG22	2.08	0.83
1:B:79:GLN:CG	1:B:80:PRO:HA	2.07	0.83
1:B:290:LYS:NZ	1:B:292:ILE:HB	1.93	0.83
1:A:23:VAL:CG2	1:A:28:LEU:HD21	2.08	0.82
1:B:285:LEU:H	1:B:285:LEU:HD12	1.43	0.82
1:B:194:THR:CG2	1:B:219:ILE:HB	2.09	0.82
1:A:290:LYS:HB3	1:A:293:ILE:HG23	0.83	0.81
1:B:9:LEU:HD21	1:B:70:ILE:HD12	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:SER:OG	1:B:255:ASN:HB2	1.80	0.81
1:A:175:SER:O	1:A:179:VAL:HG23	1.80	0.81
1:B:192:ILE:HD13	1:B:310:LEU:HD11	1.61	0.81
1:A:320:ILE:O	1:A:324:HIS:CD2	2.34	0.81
1:B:163:ARG:NH1	1:B:191:ARG:NH1	2.29	0.80
1:A:121:GLY:O	1:A:122:THR:CG2	2.30	0.80
1:A:20:SER:HA	1:A:125:ALA:HB3	1.64	0.80
1:B:296:ASN:HB3	3:B:609:HOH:O	1.80	0.80
1:B:180:LEU:HD23	1:B:213:VAL:HG22	1.62	0.80
1:A:153:GLU:O	1:A:157:MET:HG3	1.81	0.79
1:B:90:ILE:CD1	1:B:114:GLU:HG2	2.12	0.79
1:A:213:VAL:O	1:A:217:VAL:HG23	1.82	0.79
1:B:312:SER:HB2	3:B:608:HOH:O	1.82	0.79
1:A:290:LYS:CB	1:A:293:ILE:CG2	2.35	0.78
1:B:7:ASN:ND2	1:B:161:LYS:NZ	2.27	0.78
1:A:21:ALA:HB2	1:A:58:VAL:CG1	2.11	0.78
1:A:253:LYS:HE2	1:A:255:ASN:HB3	1.65	0.78
1:B:189:ASN:HB2	1:B:191:ARG:HE	1.48	0.78
1:B:47:GLU:O	1:B:51:GLU:HG2	1.83	0.78
1:B:59:GLU:HA	3:B:560:HOH:O	1.84	0.78
1:A:42:GLU:H	1:A:45:HIS:CD2	2.01	0.77
1:A:79:GLN:CG	1:A:80:PRO:HA	2.15	0.77
1:B:116:ASN:O	1:B:118:GLN:N	2.18	0.77
1:B:94:LYS:O	1:B:98:ILE:HD12	1.84	0.77
1:B:290:LYS:CG	1:B:293:ILE:HG23	2.14	0.77
1:A:290:LYS:O	1:A:293:ILE:CG1	2.22	0.77
1:B:290:LYS:CB	1:B:293:ILE:HG23	2.15	0.77
1:B:290:LYS:HD2	1:B:292:ILE:H	1.49	0.76
1:B:22:VAL:HB	1:B:57:LYS:CE	2.16	0.76
1:A:14:ASN:HD21	1:A:174:VAL:HG21	1.51	0.76
2:B:500:89I:N52	3:B:585:HOH:O	2.19	0.76
1:B:22:VAL:O	1:B:57:LYS:HE2	1.85	0.76
1:B:62:ALA:O	1:B:71:LYS:HE3	1.86	0.75
1:A:135:ILE:N	1:A:135:ILE:HD12	2.01	0.75
1:B:66:THR:HG23	1:B:168:ALA:H	1.50	0.75
1:A:271:THR:C	1:A:272:ILE:HD13	2.07	0.75
1:B:58:VAL:HG23	1:B:60:TYR:CE1	2.22	0.75
1:A:284:VAL:HG13	1:A:324:HIS:ND1	2.01	0.74
1:A:197:LEU:HD12	1:A:222:GLY:HA3	1.68	0.74
1:A:290:LYS:HZ1	1:A:292:ILE:CG2	2.01	0.74
1:B:58:VAL:HG23	1:B:60:TYR:HE1	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLN:HA	1:B:80:PRO:O	1.88	0.74
1:A:2:THR:HG22	1:A:3:SER:N	2.02	0.73
1:B:308:SER:O	1:B:311:VAL:HG12	1.87	0.73
1:A:32:SER:O	1:A:33:LEU:HD23	1.88	0.73
1:B:94:LYS:HD3	1:B:98:ILE:CD1	2.17	0.72
1:A:328:SER:HB3	1:A:330:ILE:HD12	1.71	0.72
1:A:290:LYS:NZ	1:A:292:ILE:HG22	2.04	0.72
1:B:7:ASN:ND2	1:B:161:LYS:HZ2	1.87	0.72
1:B:175:SER:OG	1:B:178:SER:HB3	1.90	0.72
1:A:117:GLU:HB2	3:A:514:HOH:O	1.90	0.72
1:A:162:ALA:HB2	3:A:574:HOH:O	1.90	0.72
1:A:326:ALA:O	1:A:328:SER:HA	1.88	0.72
1:B:9:LEU:HD11	1:B:307:LEU:HD13	1.73	0.71
1:B:70:ILE:HG22	1:B:71:LYS:N	2.04	0.71
1:A:224:GLU:OE2	1:A:225:THR:HG23	1.90	0.71
1:A:269:ASP:HA	3:A:518:HOH:O	1.90	0.71
1:A:132:ARG:HB2	3:A:619:HOH:O	1.90	0.71
1:B:292:ILE:N	1:B:292:ILE:HD12	2.06	0.71
1:A:312:SER:HB2	1:A:314:LYS:HZ2	1.56	0.71
1:B:79:GLN:HG3	1:B:80:PRO:CA	2.14	0.71
1:B:189:ASN:CB	1:B:191:ARG:HE	2.04	0.70
1:B:285:LEU:H	1:B:285:LEU:CD1	2.02	0.70
1:B:170:PHE:CZ	2:B:500:89I:H13	2.25	0.70
1:A:254:MET:HG3	1:A:255:ASN:N	2.05	0.70
1:A:74:GLN:HA	1:A:77:ILE:HB	1.73	0.70
1:B:129:GLY:O	1:B:130:ASP:HB2	1.89	0.70
1:A:60:TYR:O	1:A:102:LYS:HG2	1.92	0.70
1:B:223:ASN:ND2	1:B:226:GLU:HG3	2.05	0.70
1:B:286:ASP:HB3	1:B:288:ASP:OD1	1.91	0.70
1:B:90:ILE:CG2	1:B:99:LEU:HD12	2.22	0.70
1:A:25:LYS:HG2	1:A:29:ASP:OD2	1.92	0.70
1:B:153:GLU:O	1:B:157:MET:HG3	1.91	0.70
1:B:55:LYS:HG3	1:B:56:PHE:CE1	2.27	0.70
1:A:307:LEU:O	1:A:311:VAL:HG12	1.91	0.69
1:B:285:LEU:HD13	1:B:324:HIS:HB3	1.75	0.69
1:A:218:ASP:O	1:A:260:ARG:HB2	1.93	0.69
1:A:328:SER:CB	1:A:330:ILE:HD12	2.23	0.69
1:A:223:ASN:ND2	1:A:226:GLU:H	1.91	0.69
1:A:249:GLN:HB3	1:A:262:VAL:HG21	1.74	0.69
1:B:290:LYS:HG3	1:B:293:ILE:N	2.08	0.69
1:A:273:MET:SD	1:A:316:LEU:HD13	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:HD22	1:A:161:LYS:NZ	1.91	0.68
1:A:290:LYS:HZ3	1:A:292:ILE:CG2	2.04	0.68
1:B:14:ASN:HD21	1:B:174:VAL:HG21	1.56	0.68
1:B:93:ASP:OD2	1:B:95:PHE:HB2	1.94	0.68
1:B:7:ASN:HD22	1:B:161:LYS:HZ1	1.42	0.68
1:A:249:GLN:NE2	1:A:260:ARG:O	2.28	0.67
1:A:290:LYS:HZ3	1:A:292:ILE:CA	2.08	0.67
1:B:223:ASN:ND2	1:B:226:GLU:H	1.91	0.67
1:B:92:ILE:HD12	1:B:116:ASN:OD1	1.93	0.67
1:A:278:GLU:HG2	1:A:279:VAL:N	2.09	0.67
1:A:285:LEU:HD22	1:A:324:HIS:HB3	1.76	0.67
1:A:265:THR:HG23	1:A:267:GLY:H	1.59	0.67
1:A:287:GLN:NE2	1:A:287:GLN:N	2.42	0.67
1:A:290:LYS:HB3	1:A:293:ILE:HG21	1.69	0.67
1:B:90:ILE:HD11	1:B:114:GLU:HG2	1.75	0.67
1:A:272:ILE:N	1:A:272:ILE:HD13	2.10	0.67
1:A:79:GLN:HG3	1:A:80:PRO:CA	2.25	0.67
1:A:330:ILE:HG23	3:A:561:HOH:O	1.96	0.66
1:B:214:MET:O	1:B:214:MET:HG3	1.95	0.66
1:A:146:LYS:NZ	1:A:151:ASP:OD1	2.28	0.66
1:B:151:ASP:OD2	1:B:181:LYS:HE2	1.95	0.66
1:A:20:SER:CA	1:A:125:ALA:HB3	2.26	0.66
1:B:167:ILE:HD12	1:B:179:VAL:HG13	1.78	0.66
1:A:261:ILE:HG22	1:A:263:ILE:CD1	2.24	0.66
1:B:38:GLN:HG2	1:B:134:LEU:HD12	1.77	0.65
1:A:329:ILE:HG12	1:A:329:ILE:O	1.94	0.65
1:B:238:THR:C	1:B:239:LYS:HD2	2.16	0.65
1:B:56:PHE:C	1:B:57:LYS:HG2	2.17	0.65
1:B:285:LEU:N	1:B:285:LEU:HD12	2.10	0.65
1:B:153:GLU:HG2	1:B:157:MET:CE	2.26	0.65
1:A:290:LYS:HE2	1:A:292:ILE:HB	1.77	0.65
1:B:318:GLU:OE2	1:B:321:ARG:HD3	1.97	0.65
1:B:95:PHE:HB3	1:B:120:THR:HG21	1.78	0.65
1:A:198:SER:HB2	1:A:202:ILE:CD1	2.26	0.65
1:A:259:GLN:HA	1:A:259:GLN:HE21	1.62	0.65
1:B:9:LEU:HD11	1:B:307:LEU:CD1	2.26	0.65
1:B:153:GLU:HG2	1:B:157:MET:HE3	1.77	0.65
1:A:20:SER:HB3	1:A:125:ALA:HB3	1.79	0.64
1:A:31:TYR:OH	1:A:47:GLU:HB3	1.97	0.64
1:B:115:GLN:NE2	1:B:117:GLU:HB2	2.13	0.64
1:B:166:TYR:CZ	1:B:303:VAL:HG11	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HG23	1:A:266:GLN:N	2.12	0.64
1:A:277:SER:OG	1:A:278:GLU:N	2.31	0.64
1:A:154:LYS:HG2	3:A:524:HOH:O	1.98	0.64
1:B:290:LYS:HG3	1:B:293:ILE:HG23	1.78	0.64
1:B:9:LEU:HD12	1:B:164:VAL:HG12	1.79	0.64
1:A:7:ASN:HD22	1:A:161:LYS:HZ2	1.46	0.64
1:A:249:GLN:HB3	1:A:262:VAL:CG2	2.27	0.63
1:A:259:GLN:NE2	1:A:259:GLN:HA	2.13	0.63
1:B:219:ILE:HG12	1:B:261:ILE:HD13	1.80	0.63
1:B:290:LYS:O	1:B:293:ILE:HG12	1.99	0.63
1:B:239:LYS:HD2	1:B:239:LYS:N	2.13	0.62
1:B:5:ARG:HE	1:B:8:ILE:HD13	1.64	0.62
1:A:28:LEU:N	1:A:28:LEU:HD23	2.15	0.62
1:B:22:VAL:HB	1:B:57:LYS:HE2	1.82	0.62
1:B:111:HIS:HB2	3:B:580:HOH:O	1.99	0.62
1:B:38:GLN:CG	1:B:134:LEU:HD12	2.29	0.62
1:A:312:SER:HB2	1:A:314:LYS:NZ	2.14	0.62
1:B:73:ALA:O	1:B:77:ILE:HG13	2.00	0.62
1:B:314:LYS:NZ	3:B:608:HOH:O	2.32	0.62
1:B:240:ASP:O	1:B:243:GLU:N	2.30	0.61
1:B:265:THR:HG23	1:B:266:GLN:N	2.13	0.61
1:A:50:ASP:HB3	1:A:54:LYS:HZ1	1.64	0.61
1:A:7:ASN:ND2	1:A:161:LYS:NZ	2.49	0.61
1:A:285:LEU:HD22	1:A:324:HIS:CB	2.31	0.61
1:B:89:CYS:SG	1:B:113:TYR:HD2	2.23	0.60
1:B:187:SER:HB2	3:B:601:HOH:O	2.00	0.60
1:B:94:LYS:CD	1:B:98:ILE:HD11	2.28	0.60
1:B:223:ASN:HD22	1:B:223:ASN:C	2.04	0.60
1:A:65:SER:OG	2:A:500:89I:N6	2.34	0.60
1:A:23:VAL:HG21	1:A:28:LEU:CD2	2.23	0.60
1:B:180:LEU:HD21	1:B:213:VAL:HG22	1.84	0.60
1:B:146:LYS:NZ	1:B:151:ASP:OD1	2.34	0.60
1:B:271:THR:O	1:B:272:ILE:HD13	2.02	0.60
1:B:60:TYR:CD2	1:B:98:ILE:HG21	2.36	0.60
1:B:150:LEU:HD23	1:B:181:LYS:HD3	1.83	0.60
1:B:163:ARG:NH1	1:B:191:ARG:HH11	1.99	0.60
1:A:290:LYS:HG3	1:A:293:ILE:HG23	1.82	0.59
1:A:2:THR:HG23	1:A:4:VAL:CG2	2.23	0.59
1:B:53:VAL:HG13	1:B:60:TYR:OH	2.02	0.59
1:B:271:THR:HG21	1:B:320:ILE:HD11	1.82	0.59
1:B:9:LEU:CD1	1:B:307:LEU:HD13	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HB2	1:B:260:ARG:HH12	1.68	0.59
1:A:50:ASP:O	1:A:54:LYS:NZ	2.28	0.59
1:B:290:LYS:HZ2	1:B:292:ILE:C	2.05	0.59
1:B:90:ILE:HG21	1:B:99:LEU:HD12	1.83	0.59
1:A:292:ILE:HG22	1:A:292:ILE:O	2.01	0.59
1:A:270:ASP:H	1:A:284:VAL:HG23	1.67	0.58
1:A:104:ALA:C	1:A:106:ALA:H	2.06	0.58
1:A:224:GLU:HG3	1:A:266:GLN:HA	1.84	0.58
1:A:214:MET:N	1:A:215:PRO:CD	2.66	0.58
1:A:211:MET:O	1:A:215:PRO:HD3	2.03	0.58
1:A:190:ASN:HD21	1:A:257:LYS:HB2	1.69	0.58
1:B:119:PRO:HD2	1:B:139:ALA:HB1	1.85	0.58
1:A:287:GLN:HE21	1:A:287:GLN:N	2.00	0.58
1:A:2:THR:CG2	1:A:4:VAL:HG23	2.23	0.58
1:B:21:ALA:HB1	1:B:57:LYS:HG3	1.86	0.58
1:A:23:VAL:HG23	1:A:24:ASP:N	2.17	0.58
1:B:7:ASN:HD22	1:B:161:LYS:CE	2.14	0.58
1:A:20:SER:CB	1:A:125:ALA:HB3	2.33	0.58
1:A:270:ASP:N	1:A:284:VAL:HG23	2.19	0.58
1:A:50:ASP:O	1:A:54:LYS:HD3	2.04	0.58
1:A:9:LEU:HD12	1:A:164:VAL:HG12	1.86	0.57
1:B:40:LEU:HD11	2:B:500:89I:C21	2.35	0.57
1:A:20:SER:O	1:A:58:VAL:HG12	2.05	0.57
1:A:225:THR:O	1:A:228:ALA:HB3	2.05	0.57
1:B:251:LEU:HB2	1:B:260:ARG:NH1	2.19	0.57
1:A:292:ILE:CD1	1:A:292:ILE:N	2.67	0.57
1:B:261:ILE:HD12	1:B:261:ILE:N	2.19	0.57
1:B:285:LEU:O	1:B:287:GLN:NE2	2.35	0.57
1:B:100:LYS:NZ	1:B:114:GLU:OE1	2.38	0.57
1:B:163:ARG:HH11	1:B:191:ARG:NH1	2.01	0.57
1:B:323:GLY:O	1:B:327:ALA:HB2	2.04	0.57
1:B:104:ALA:C	1:B:106:ALA:H	2.09	0.56
1:B:269:ASP:O	1:B:270:ASP:HB2	2.04	0.56
1:B:144:TYR:OH	1:B:150:LEU:HB2	2.04	0.56
1:A:224:GLU:O	1:A:227:ALA:HB3	2.06	0.56
1:B:18:ASP:OD2	1:B:63:GLY:HA3	2.05	0.56
1:B:9:LEU:HD21	1:B:70:ILE:CD1	2.34	0.56
1:A:284:VAL:HG12	1:A:285:LEU:N	2.21	0.56
1:A:27:PHE:CE1	1:A:51:GLU:HG3	2.41	0.56
1:A:31:TYR:HE2	1:A:51:GLU:OE2	1.88	0.55
1:B:55:LYS:HD2	3:B:554:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:VAL:HG23	1:B:80:PRO:HD2	1.88	0.55
1:A:328:SER:HB2	1:A:330:ILE:N	2.21	0.55
1:A:247:LYS:HG2	3:A:590:HOH:O	2.06	0.55
1:A:266:GLN:HB3	1:A:269:ASP:O	2.07	0.55
1:A:294:ASP:O	1:A:296:ASN:N	2.39	0.55
1:A:301:ALA:CB	1:A:330:ILE:HD11	2.37	0.55
1:A:27:PHE:HE1	1:A:51:GLU:HG3	1.71	0.55
1:B:320:ILE:O	1:B:320:ILE:HG23	2.07	0.55
1:B:265:THR:HG23	1:B:267:GLY:H	1.72	0.55
1:A:15:PRO:HD2	1:A:141:ALA:CB	2.37	0.55
1:B:259:GLN:HG3	1:B:260:ARG:H	1.72	0.54
1:A:2:THR:CG2	1:A:3:SER:N	2.71	0.54
1:A:67:GLN:O	1:A:71:LYS:HG3	2.08	0.54
1:B:217:VAL:HG12	1:B:217:VAL:O	2.06	0.54
1:B:183:ALA:O	1:B:216:TYR:HB3	2.07	0.54
1:B:33:LEU:HD13	1:B:135:ILE:HD11	1.88	0.54
1:A:290:LYS:HD2	1:A:292:ILE:H	1.73	0.54
1:A:23:VAL:HA	1:A:56:PHE:CE2	2.42	0.54
1:B:77:ILE:HG22	1:B:77:ILE:O	2.07	0.54
1:A:290:LYS:CG	1:A:293:ILE:CG2	2.80	0.54
1:B:163:ARG:HH11	1:B:191:ARG:HH11	1.56	0.54
1:B:8:ILE:O	1:B:8:ILE:HG13	2.08	0.54
1:A:5:ARG:O	1:A:8:ILE:HB	2.08	0.54
1:B:255:ASN:OD1	1:B:258:ARG:HG3	2.08	0.54
1:B:60:TYR:O	1:B:61:HIS:HD2	1.91	0.54
1:A:290:LYS:HG3	1:A:293:ILE:CG2	2.38	0.54
1:A:6:GLU:HA	1:A:83:ALA:HA	1.89	0.54
1:B:103:ALA:O	1:B:106:ALA:HB3	2.08	0.54
1:A:26:ASP:HB3	3:A:543:HOH:O	2.08	0.53
1:B:292:ILE:O	1:B:292:ILE:HG22	2.08	0.53
1:A:7:ASN:ND2	1:A:161:LYS:HZ1	2.07	0.53
1:B:295:THR:HG23	3:B:507:HOH:O	2.09	0.53
1:A:49:PHE:HZ	1:A:137:ASN:HB2	1.73	0.53
1:A:19:ILE:HG22	1:A:19:ILE:O	2.08	0.53
1:B:186:ALA:CB	1:B:193:PHE:HB2	2.38	0.53
1:A:174:VAL:HA	3:A:616:HOH:O	2.09	0.53
1:A:15:PRO:HD2	1:A:141:ALA:HB2	1.89	0.53
1:B:224:GLU:HG3	1:B:266:GLN:HA	1.91	0.53
1:A:223:ASN:HD22	1:A:223:ASN:C	2.12	0.53
1:B:155:ASN:HD22	1:B:155:ASN:N	2.06	0.53
1:A:190:ASN:CG	1:A:255:ASN:HD21	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ILE:CG1	1:B:261:ILE:HD13	2.38	0.53
1:B:53:VAL:O	1:B:53:VAL:HG12	2.09	0.53
1:B:9:LEU:CD2	1:B:70:ILE:HD12	2.35	0.53
1:A:109:ASP:CG	1:A:111:HIS:HE1	2.11	0.53
1:A:207:LYS:HD3	3:A:582:HOH:O	2.08	0.53
1:B:163:ARG:CZ	1:B:191:ARG:HD3	2.39	0.53
1:B:235:GLY:O	1:B:236:PHE:HD1	1.92	0.53
1:A:53:VAL:HG12	1:A:53:VAL:O	2.10	0.52
1:B:22:VAL:HB	1:B:57:LYS:HE3	1.90	0.52
1:A:11:GLY:HA3	1:A:70:ILE:HD13	1.91	0.52
1:A:294:ASP:O	1:A:295:THR:C	2.47	0.52
1:A:3:SER:HA	3:A:549:HOH:O	2.09	0.52
1:B:154:LYS:HE2	1:B:155:ASN:HD21	1.74	0.52
1:B:230:PHE:HE2	1:B:248:THR:HG1	1.56	0.52
1:B:273:MET:HE3	1:B:316:LEU:HD12	1.91	0.52
1:B:104:ALA:O	1:B:106:ALA:N	2.43	0.52
1:A:135:ILE:CD1	1:A:135:ILE:N	2.72	0.52
1:B:314:LYS:HB3	1:B:315:PRO:CD	2.39	0.52
1:A:223:ASN:HD21	1:A:226:GLU:H	1.58	0.52
1:B:101:ARG:HG2	1:B:105:GLU:OE1	2.09	0.52
1:B:192:ILE:CD1	1:B:310:LEU:HD11	2.38	0.52
1:B:310:LEU:HG	1:B:310:LEU:O	2.08	0.52
1:B:190:ASN:ND2	1:B:255:ASN:HD21	2.07	0.52
1:B:48:LEU:HD21	1:B:135:ILE:HD13	1.92	0.52
1:A:128:THR:OG1	1:A:131:ASN:OD1	2.27	0.52
1:A:135:ILE:H	1:A:135:ILE:HD12	1.75	0.52
1:A:314:LYS:HB3	1:A:315:PRO:HD2	1.90	0.52
1:B:12:MET:O	1:B:167:ILE:HG23	2.10	0.52
1:B:278:GLU:CG	1:B:279:VAL:H	2.22	0.52
1:B:94:LYS:O	1:B:97:GLU:N	2.43	0.51
1:A:109:ASP:OD1	1:A:111:HIS:HE1	1.93	0.51
1:A:290:LYS:HZ3	1:A:292:ILE:C	2.12	0.51
1:B:287:GLN:N	1:B:287:GLN:NE2	2.58	0.51
1:A:31:TYR:HD2	3:A:605:HOH:O	1.92	0.51
1:B:271:THR:CG2	1:B:320:ILE:HD11	2.40	0.51
1:B:291:GLU:HB3	1:B:292:ILE:HD12	1.92	0.51
1:B:39:ILE:C	1:B:39:ILE:HD12	2.31	0.51
1:A:163:ARG:NH2	3:A:594:HOH:O	2.44	0.51
1:A:20:SER:HB3	1:A:125:ALA:CB	2.41	0.51
1:A:261:ILE:HG22	1:A:263:ILE:HD13	1.90	0.51
1:B:290:LYS:HG3	1:B:293:ILE:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:ND2	1:A:255:ASN:HD21	2.08	0.51
1:B:22:VAL:HG22	3:B:598:HOH:O	2.11	0.51
1:B:115:GLN:HE21	1:B:117:GLU:HB2	1.73	0.51
1:B:189:ASN:O	1:B:191:ARG:HG2	2.10	0.51
1:A:48:LEU:CD2	1:A:135:ILE:HG12	2.40	0.51
1:B:9:LEU:HD12	1:B:164:VAL:CG1	2.40	0.51
1:A:292:ILE:CG2	1:A:292:ILE:O	2.59	0.50
1:A:50:ASP:HB3	1:A:54:LYS:NZ	2.27	0.50
1:B:163:ARG:HH12	1:B:191:ARG:CZ	2.24	0.50
1:B:38:GLN:C	2:B:500:89I:H481	2.31	0.50
1:A:162:ALA:O	1:A:163:ARG:HD2	2.11	0.50
1:A:50:ASP:C	1:A:54:LYS:HZ3	2.13	0.50
1:B:89:CYS:HG	1:B:113:TYR:HD2	1.60	0.50
1:B:57:LYS:H	1:B:58:VAL:HG13	1.76	0.50
1:A:318:GLU:OE2	1:A:321:ARG:HD3	2.12	0.50
1:B:163:ARG:HH12	1:B:191:ARG:NH1	2.08	0.50
1:B:236:PHE:O	1:B:237:GLU:HB2	2.12	0.50
1:B:108:VAL:O	1:B:108:VAL:HG12	2.12	0.50
1:B:142:ASN:HD22	1:B:174:VAL:HG22	1.77	0.50
1:B:292:ILE:N	1:B:292:ILE:CD1	2.75	0.50
1:A:51:GLU:HB2	1:A:55:LYS:HZ1	1.77	0.49
1:B:5:ARG:CG	1:B:8:ILE:HD13	2.41	0.49
1:A:9:LEU:CD1	1:A:164:VAL:HG12	2.42	0.49
1:B:276:GLU:HA	3:B:603:HOH:O	2.11	0.49
1:B:256:SER:O	1:B:257:LYS:O	2.30	0.49
1:B:225:THR:CG2	3:B:607:HOH:O	2.60	0.49
1:A:78:GLN:O	1:A:78:GLN:HG3	2.13	0.49
1:B:42:GLU:N	1:B:45:HIS:HD2	1.88	0.49
1:B:58:VAL:CG2	1:B:60:TYR:HE1	2.22	0.49
1:B:5:ARG:HE	1:B:8:ILE:CD1	2.25	0.49
1:A:93:ASP:OD2	1:A:95:PHE:HB2	2.12	0.49
1:A:241:ILE:CG2	1:A:242:LYS:N	2.75	0.48
1:A:301:ALA:CB	1:A:330:ILE:CD1	2.91	0.48
1:B:285:LEU:HD13	1:B:324:HIS:CB	2.42	0.48
1:B:15:PRO:HG3	1:B:88:GLY:HA3	1.94	0.48
1:A:286:ASP:C	1:A:287:GLN:HE21	2.17	0.48
1:A:320:ILE:HG23	1:A:320:ILE:O	2.13	0.48
1:B:213:VAL:O	1:B:213:VAL:HG12	2.12	0.48
1:A:291:GLU:O	1:A:291:GLU:HG3	2.13	0.48
1:A:42:GLU:N	1:A:45:HIS:HD2	2.03	0.48
1:B:127:ILE:HA	1:B:131:ASN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:HG3	1:B:155:ASN:ND2	2.29	0.48
1:A:151:ASP:OD2	1:A:181:LYS:HE2	2.14	0.48
1:A:51:GLU:HB2	1:A:55:LYS:NZ	2.28	0.48
1:B:38:GLN:HB3	2:B:500:89I:H483	1.95	0.48
1:B:163:ARG:NH1	1:B:191:ARG:CZ	2.76	0.48
1:B:302:PHE:HA	1:B:323:GLY:O	2.13	0.48
1:A:138:LEU:HD11	2:A:500:89I:C42	2.44	0.48
1:B:153:GLU:OE1	1:B:154:LYS:HA	2.14	0.48
1:A:203:SER:HG	1:A:230:PHE:HD1	1.61	0.48
1:A:314:LYS:HB3	1:A:315:PRO:CD	2.44	0.48
1:A:243:GLU:O	1:A:246:LYS:HB3	2.14	0.47
1:A:36:ASN:ND2	3:A:619:HOH:O	2.46	0.47
1:B:7:ASN:HB2	1:B:161:LYS:HZ2	1.78	0.47
1:A:310:LEU:O	1:A:310:LEU:HG	2.14	0.47
1:B:31:TYR:OH	1:B:47:GLU:HB3	2.14	0.47
1:B:52:LEU:C	1:B:54:LYS:H	2.17	0.47
1:A:223:ASN:CB	1:A:265:THR:HG22	2.45	0.47
1:A:284:VAL:HG12	1:A:285:LEU:H	1.79	0.47
1:B:89:CYS:SG	1:B:113:TYR:CD2	3.06	0.47
1:B:104:ALA:C	1:B:106:ALA:N	2.68	0.47
1:B:273:MET:HE1	1:B:316:LEU:HB3	1.96	0.47
1:B:290:LYS:HD2	1:B:292:ILE:N	2.24	0.47
1:A:23:VAL:HA	1:A:56:PHE:HE2	1.78	0.47
1:B:90:ILE:HG22	1:B:120:THR:OG1	2.15	0.47
1:A:23:VAL:HG12	1:A:56:PHE:CE2	2.49	0.47
1:A:292:ILE:N	1:A:292:ILE:HD12	2.30	0.47
1:A:231:ALA:HB1	1:A:236:PHE:HB2	1.97	0.47
1:A:131:ASN:O	1:A:132:ARG:HG2	2.15	0.47
1:A:11:GLY:O	1:A:86:PHE:HA	2.15	0.47
1:A:172:LEU:HD23	1:A:179:VAL:HG21	1.97	0.47
1:A:312:SER:CB	1:A:314:LYS:NZ	2.78	0.46
1:A:49:PHE:CZ	1:A:137:ASN:HB2	2.49	0.46
1:B:302:PHE:HE1	1:B:324:HIS:NE2	2.13	0.46
1:A:278:GLU:CG	1:A:279:VAL:N	2.78	0.46
1:B:190:ASN:ND2	1:B:257:LYS:HD2	2.31	0.46
1:B:25:LYS:O	1:B:25:LYS:HG2	2.16	0.46
1:B:293:ILE:HD12	1:B:295:THR:OG1	2.15	0.46
1:B:39:ILE:HD12	1:B:39:ILE:O	2.15	0.46
1:B:54:LYS:O	1:B:56:PHE:N	2.48	0.46
1:A:50:ASP:OD2	1:A:50:ASP:N	2.49	0.46
1:A:53:VAL:HG13	1:A:60:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:O	1:A:98:ILE:HG13	2.15	0.46
1:B:127:ILE:HG13	1:B:132:ARG:HG2	1.98	0.46
1:B:66:THR:CG2	1:B:168:ALA:H	2.25	0.46
1:B:58:VAL:CG2	1:B:60:TYR:CE1	2.95	0.46
1:A:156:TRP:CE3	1:A:159:VAL:HG21	2.51	0.46
1:A:97:GLU:HA	3:A:617:HOH:O	2.15	0.46
1:B:213:VAL:O	1:B:217:VAL:HG23	2.16	0.46
1:B:292:ILE:H	1:B:292:ILE:HD12	1.81	0.46
1:B:90:ILE:CG2	1:B:99:LEU:CD1	2.94	0.46
1:A:33:LEU:HA	3:A:622:HOH:O	2.16	0.46
1:B:119:PRO:O	1:B:140:ALA:CB	2.55	0.45
1:B:273:MET:HE3	1:B:316:LEU:CD1	2.45	0.45
1:A:150:LEU:HD11	1:A:156:TRP:HZ3	1.82	0.45
1:B:214:MET:N	1:B:215:PRO:HD2	2.32	0.45
1:B:26:ASP:O	1:B:30:LYS:HG2	2.16	0.45
1:B:7:ASN:ND2	1:B:161:LYS:HZ1	2.06	0.45
1:A:190:ASN:ND2	1:A:257:LYS:HD2	2.32	0.45
1:B:12:MET:CE	1:B:150:LEU:HD13	2.45	0.45
1:B:98:ILE:O	1:B:98:ILE:HG22	2.16	0.45
1:A:259:GLN:CA	1:A:259:GLN:HE21	2.25	0.45
2:A:500:89I:H272	2:A:500:89I:H21	1.66	0.45
1:B:186:ALA:HB2	1:B:193:PHE:HB2	1.97	0.45
1:A:166:TYR:HB2	1:A:194:THR:OG1	2.17	0.45
1:A:245:ALA:HB1	1:A:274:ALA:HB2	1.99	0.45
1:B:261:ILE:HD12	1:B:261:ILE:H	1.80	0.45
1:A:241:ILE:HG23	1:A:242:LYS:N	2.32	0.45
1:A:218:ASP:OD1	1:A:258:ARG:HD2	2.17	0.45
1:B:241:ILE:CG2	1:B:242:LYS:N	2.80	0.45
1:B:248:THR:O	1:B:251:LEU:HD12	2.16	0.45
1:B:44:LYS:HE2	1:B:45:HIS:CE1	2.51	0.45
1:B:77:ILE:CG1	1:B:308:SER:HB2	2.47	0.45
1:A:162:ALA:C	1:A:163:ARG:HD2	2.38	0.44
1:A:249:GLN:CB	1:A:262:VAL:CG2	2.95	0.44
1:B:30:LYS:HG2	1:B:30:LYS:H	1.52	0.44
1:A:28:LEU:O	1:A:32:SER:N	2.50	0.44
1:B:72:VAL:O	1:B:76:MET:HG2	2.18	0.44
1:A:36:ASN:ND2	1:A:132:ARG:HB2	2.33	0.44
1:A:25:LYS:CA	1:A:28:LEU:HG	2.36	0.44
1:B:158:LEU:HA	1:B:161:LYS:HG3	2.00	0.44
1:A:290:LYS:HZ1	1:A:292:ILE:HG22	1.68	0.44
1:B:183:ALA:HB2	1:B:193:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ARG:NE	1:B:8:ILE:HD13	2.31	0.44
1:B:17:LEU:HD11	1:B:60:TYR:HB3	2.00	0.44
1:B:7:ASN:CG	1:B:158:LEU:HD22	2.37	0.44
1:B:146:LYS:HG3	1:B:147:GLU:N	2.32	0.44
1:B:185:HIS:CE1	1:B:189:ASN:ND2	2.86	0.44
1:B:60:TYR:HD2	1:B:98:ILE:HG21	1.80	0.44
1:A:189:ASN:HB3	1:A:191:ARG:HE	1.82	0.44
1:A:223:ASN:ND2	1:A:226:GLU:HB2	2.33	0.44
1:A:67:GLN:HG2	1:A:71:LYS:HD2	2.00	0.44
1:A:31:TYR:O	1:A:32:SER:O	2.36	0.43
1:A:22:VAL:O	1:A:56:PHE:HD2	2.01	0.43
1:B:273:MET:CE	1:B:316:LEU:CD1	2.96	0.43
1:B:153:GLU:CG	1:B:157:MET:HE1	2.49	0.43
1:B:246:LYS:O	1:B:249:GLN:HG3	2.18	0.43
1:A:220:LEU:HD23	1:A:221:PHE:N	2.33	0.43
1:B:118:GLN:HB3	1:B:119:PRO:HD2	2.00	0.43
1:B:41:ALA:HB2	1:B:135:ILE:HG22	1.99	0.43
1:B:314:LYS:HB3	1:B:315:PRO:HD2	2.00	0.43
1:A:102:LYS:HD3	1:A:102:LYS:HA	1.43	0.43
1:A:138:LEU:HD11	2:A:500:89I:C23	2.48	0.43
1:A:60:TYR:O	1:A:102:LYS:HE3	2.18	0.43
1:B:122:THR:O	1:B:136:ALA:HA	2.19	0.43
1:B:146:LYS:HB2	1:B:150:LEU:HB3	2.01	0.43
1:B:223:ASN:ND2	1:B:226:GLU:CG	2.78	0.43
1:B:241:ILE:HG23	1:B:242:LYS:N	2.33	0.43
1:A:284:VAL:HG23	3:A:518:HOH:O	2.17	0.43
1:A:301:ALA:HB2	1:A:330:ILE:CD1	2.49	0.43
1:B:67:GLN:HB2	1:B:86:PHE:CZ	2.54	0.43
1:A:231:ALA:HA	1:A:236:PHE:CD2	2.54	0.43
1:B:28:LEU:HD22	1:B:33:LEU:HD12	2.01	0.43
1:B:57:LYS:O	1:B:58:VAL:HG22	2.18	0.43
1:B:188:GLU:HA	1:B:188:GLU:OE1	2.19	0.43
1:B:7:ASN:HB3	1:B:158:LEU:HD22	2.01	0.43
1:A:328:SER:HB2	1:A:330:ILE:H	1.82	0.43
1:B:12:MET:CE	1:B:144:TYR:CE2	3.01	0.43
1:B:223:ASN:HD22	1:B:226:GLU:H	1.66	0.43
1:A:15:PRO:HG2	1:A:89:CYS:O	2.18	0.42
1:B:278:GLU:HG2	1:B:279:VAL:H	1.84	0.42
1:B:35:PRO:O	1:B:131:ASN:HB3	2.19	0.42
1:A:172:LEU:O	1:A:176:PRO:HD3	2.20	0.42
1:A:285:LEU:CD1	1:A:285:LEU:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASP:C	1:A:287:GLN:NE2	2.73	0.42
2:A:500:89I:H10	2:A:500:89I:H482	1.72	0.42
1:A:55:LYS:C	1:A:56:PHE:CD1	2.93	0.42
1:B:214:MET:N	1:B:215:PRO:CD	2.81	0.42
1:B:249:GLN:HB2	1:B:249:GLN:HE21	1.66	0.42
1:A:56:PHE:N	1:A:56:PHE:CD1	2.87	0.42
1:B:146:LYS:HB3	1:B:178:SER:HB2	2.01	0.42
1:B:273:MET:CE	1:B:316:LEU:HD13	2.49	0.42
2:B:500:89I:H272	2:B:500:89I:H21	1.66	0.42
1:B:324:HIS:HA	1:B:327:ALA:HB3	2.02	0.42
1:B:245:ALA:HB1	1:B:274:ALA:HB2	2.00	0.42
1:B:90:ILE:HG21	1:B:99:LEU:CD1	2.48	0.42
1:B:154:LYS:HG3	1:B:155:ASN:HD22	1.85	0.42
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.77	0.42
1:B:288:ASP:O	1:B:289:GLN:HG3	2.19	0.42
1:A:309:GLN:O	1:A:314:LYS:HG3	2.20	0.42
1:B:288:ASP:O	1:B:289:GLN:NE2	2.37	0.42
1:A:2:THR:HG22	1:A:3:SER:H	1.83	0.41
1:B:106:ALA:O	1:B:107:HIS:HB2	2.20	0.41
1:B:124:ALA:O	1:B:134:LEU:HA	2.19	0.41
1:A:195:LEU:HD22	1:A:217:VAL:HG21	2.03	0.41
1:B:238:THR:HG23	1:B:244:ILE:HG13	2.02	0.41
1:B:306:PHE:HA	1:B:319:CYS:O	2.20	0.41
1:A:7:ASN:ND2	1:A:158:LEU:HD22	2.35	0.41
1:A:25:LYS:C	1:A:27:PHE:N	2.73	0.41
1:A:44:LYS:HB2	1:A:44:LYS:HE3	1.84	0.41
1:A:8:ILE:HG22	1:A:83:ALA:O	2.20	0.41
1:A:213:VAL:HG12	1:A:213:VAL:O	2.21	0.41
1:A:8:ILE:HG21	1:A:311:VAL:HG21	2.02	0.41
1:B:25:LYS:HE2	1:B:29:ASP:OD2	2.20	0.41
1:B:66:THR:HG23	1:B:168:ALA:N	2.27	0.41
1:A:109:ASP:OD1	1:A:111:HIS:CE1	2.73	0.41
1:B:232:ARG:CZ	3:B:610:HOH:O	2.68	0.41
1:A:104:ALA:C	1:A:106:ALA:N	2.71	0.41
1:B:169:GLY:N	1:B:198:SER:OG	2.54	0.41
1:B:223:ASN:HD21	1:B:226:GLU:H	1.67	0.41
1:B:5:ARG:HG2	1:B:5:ARG:H	1.65	0.41
1:A:122:THR:OG1	1:A:122:THR:O	2.36	0.41
1:B:301:ALA:HB1	1:B:326:ALA:O	2.20	0.41
1:B:309:GLN:HB2	1:B:319:CYS:HA	2.02	0.41
1:A:301:ALA:HB1	1:A:330:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.78	0.41
1:A:14:ASN:ND2	1:A:174:VAL:HG21	2.28	0.41
1:A:25:LYS:C	1:A:27:PHE:H	2.23	0.41
1:A:172:LEU:HD21	1:A:179:VAL:HG11	2.02	0.41
1:A:193:PHE:O	1:A:218:ASP:HB2	2.21	0.41
1:B:102:LYS:HA	1:B:102:LYS:HD3	1.52	0.41
1:B:302:PHE:HE1	1:B:324:HIS:CD2	2.38	0.41
1:A:94:LYS:NZ	3:A:578:HOH:O	2.53	0.41
1:B:100:LYS:NZ	1:B:114:GLU:CD	2.74	0.41
1:B:251:LEU:HB3	1:B:252:PRO:HD2	2.03	0.41
1:A:272:ILE:N	1:A:272:ILE:CD1	2.74	0.40
1:B:259:GLN:HG3	1:B:260:ARG:N	2.35	0.40
1:B:305:GLY:HA3	1:B:323:GLY:HA2	2.03	0.40
1:A:270:ASP:HA	1:A:282:PHE:O	2.22	0.40
1:A:79:GLN:HB2	1:A:79:GLN:HE21	1.60	0.40
1:B:153:GLU:CG	1:B:157:MET:CE	2.98	0.40
1:B:95:PHE:HB3	1:B:120:THR:CG2	2.49	0.40
1:A:293:ILE:O	1:A:294:ASP:C	2.60	0.40
1:B:288:ASP:C	1:B:289:GLN:HG3	2.42	0.40
1:B:60:TYR:C	1:B:61:HIS:HD2	2.25	0.40
1:A:144:TYR:O	1:A:145:LYS:HD3	2.22	0.40
1:B:101:ARG:NH2	1:B:102:LYS:HZ1	2.20	0.40
1:A:301:ALA:HB3	1:A:327:ALA:HB2	2.03	0.40
1:B:223:ASN:C	1:B:223:ASN:ND2	2.74	0.40
1:B:94:LYS:C	1:B:98:ILE:HD12	2.41	0.40

All (1) 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:A:117:GLU:OE2	1:B:233:GLU:O[1_445]	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	A	327/345 (95%)	273 (84%)	38 (12%)	16 (5%)	2	1
1	B	324/345 (94%)	246 (76%)	57 (18%)	21 (6%)	1	0
All	All	651/690 (94%)	519 (80%)	95 (15%)	37 (6%)	1	1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	269	ASP
1	A	288	ASP
1	B	117	GLU
1	B	257	LYS
1	B	288	ASP
1	A	25	LYS
1	A	290	LYS
1	A	293	ILE
1	B	55	LYS
1	B	57	LYS
1	B	105	GLU
1	B	269	ASP
1	B	295	THR
1	A	224	GLU
1	A	277	SER
1	A	294	ASP
1	B	32	SER
1	B	102	LYS
1	B	119	PRO
1	B	130	ASP
1	B	149	HIS
1	B	181	LYS
1	B	277	SER
1	B	327	ALA
1	A	295	THR
1	B	58	VAL
1	A	35	PRO
1	A	48	LEU
1	A	254	MET
1	B	22	VAL
1	B	78	GLN
1	A	252	PRO

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Mol	Chain	Res	Type
1	B	190	ASN
1	A	23	VAL
1	B	293	ILE
1	A	77	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/292 (95%)	217 (78%)	60 (22%)	1	1
1	B	274/292 (94%)	221 (81%)	53 (19%)	1	1
All	All	551/584 (94%)	438 (80%)	113 (20%)	1	1

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	VAL
1	A	5	ARG
1	A	19	ILE
1	A	24	ASP
1	A	28	LEU
1	A	36	ASN
1	A	38	GLN
1	A	39	ILE
1	A	40	LEU
1	A	44	LYS
1	A	50	ASP
1	A	52	LEU
1	A	54	LYS
1	A	55	LYS
1	A	65	SER
1	A	70	ILE
1	A	71	LYS
1	A	76	MET

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Mol	Chain	Res	Type
1	A	77	ILE
1	A	78	GLN
1	A	85	THR
1	A	94	LYS
1	A	97	GLU
1	A	100	LYS
1	A	102	LYS
1	A	115	GLN
1	A	127	ILE
1	A	135	ILE
1	A	163	ARG
1	A	178	SER
1	A	187	SER
1	A	191	ARG
1	A	207	LYS
1	A	208	GLU
1	A	220	LEU
1	A	223	ASN
1	A	224	GLU
1	A	238	THR
1	A	239	LYS
1	A	249	GLN
1	A	253	LYS
1	A	260	ARG
1	A	263	ILE
1	A	265	THR
1	A	270	ASP
1	A	272	ILE
1	A	280	THR
1	A	285	LEU
1	A	287	GLN
1	A	290	LYS
1	A	291	GLU
1	A	292	ILE
1	A	293	ILE
1	A	310	LEU
1	A	311	VAL
1	A	312	SER
1	A	320	ILE
1	A	329	ILE
1	A	330	ILE
1	B	9	LEU

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Mol	Chain	Res	Type
1	B	20	SER
1	B	30	LYS
1	B	36	ASN
1	B	55	LYS
1	B	57	LYS
1	B	58	VAL
1	B	66	THR
1	B	70	ILE
1	B	71	LYS
1	B	78	GLN
1	B	85	THR
1	B	94	LYS
1	B	99	LEU
1	B	102	LYS
1	B	111	HIS
1	B	115	GLN
1	B	116	ASN
1	B	117	GLU
1	B	122	THR
1	B	128	THR
1	B	134	LEU
1	B	148	LYS
1	B	153	GLU
1	B	161	LYS
1	B	178	SER
1	B	191	ARG
1	B	194	THR
1	B	207	LYS
1	B	208	GLU
1	B	212	LYS
1	B	220	LEU
1	B	223	ASN
1	B	224	GLU
1	B	239	LYS
1	B	249	GLN
1	B	253	LYS
1	B	254	MET
1	B	256	SER
1	B	258	ARG
1	B	261	ILE
1	B	279	VAL
1	B	280	THR

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Mol	Chain	Res	Type
1	B	285	LEU
1	B	287	GLN
1	B	288	ASP
1	B	289	GLN
1	B	290	LYS
1	B	293	ILE
1	B	307	LEU
1	B	310	LEU
1	B	312	SER
1	B	328	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	14	ASN
1	A	36	ASN
1	A	45	HIS
1	A	61	HIS
1	A	68	ASN
1	A	79	GLN
1	A	111	HIS
1	A	115	GLN
1	A	118	GLN
1	A	137	ASN
1	A	142	ASN
1	A	189	ASN
1	A	223	ASN
1	A	234	GLN
1	A	249	GLN
1	A	259	GLN
1	A	287	GLN
1	A	324	HIS
1	B	7	ASN
1	B	14	ASN
1	B	36	ASN
1	B	45	HIS
1	B	61	HIS
1	B	68	ASN
1	B	78	GLN
1	B	79	GLN
1	B	115	GLN

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Mol	Chain	Res	Type
1	B	118	GLN
1	B	137	ASN
1	B	142	ASN
1	B	155	ASN
1	B	185	HIS
1	B	189	ASN
1	B	190	ASN
1	B	223	ASN
1	B	234	GLN
1	B	249	GLN
1	B	259	GLN
1	B	287	GLN
1	B	324	HIS

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	89I	A	500	-	32,33,33	1.35	7 (21%)	44,45,45	2.77	19 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	89I	B	500	-	32,33,33	1.35	7 (21%)	44,45,45	2.77	19 (43%)

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	89I	A	500	-	-	2/14/25/25	0/4/4/4
2	89I	B	500	-	-	2/14/25/25	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	89I	C31-N32	-2.86	1.42	1.46
2	A	500	89I	C31-N32	-2.86	1.42	1.46
2	A	500	89I	C23-C42	-2.63	1.38	1.44
2	B	500	89I	C23-C42	-2.60	1.38	1.44
2	A	500	89I	C11-N43	2.53	1.43	1.37
2	B	500	89I	C11-N43	2.53	1.43	1.37
2	B	500	89I	C4-C5	-2.33	1.38	1.43
2	A	500	89I	C4-C5	-2.29	1.38	1.43
2	A	500	89I	C4-C8	-2.28	1.45	1.50
2	B	500	89I	C4-C8	-2.25	1.45	1.50
2	A	500	89I	C3-C41	-2.13	1.41	1.43
2	B	500	89I	C18-C23	-2.08	1.36	1.39
2	B	500	89I	C3-C41	-2.06	1.41	1.43
2	A	500	89I	C18-C23	-2.04	1.36	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	89I	C48-N43-C11	-9.82	103.70	120.54
2	B	500	89I	C48-N43-C11	-9.82	103.70	120.54
2	A	500	89I	C31-N32-C27	5.04	122.65	111.52
2	B	500	89I	C31-N32-C27	5.03	122.63	111.52
2	B	500	89I	C4-C5-N6	4.51	122.74	118.71
2	A	500	89I	C4-C5-N6	4.49	122.72	118.71
2	A	500	89I	C12-C11-N43	4.34	127.51	121.63
2	B	500	89I	C12-C11-N43	4.33	127.49	121.63
2	A	500	89I	C13-C8-C4	4.22	127.79	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	89I	C13-C8-C4	4.19	127.75	120.79
2	B	500	89I	C23-C42-C41	-3.72	165.20	176.32
2	A	500	89I	C23-C42-C41	-3.70	165.24	176.32
2	A	500	89I	C30-C31-N32	-3.53	103.51	110.02
2	B	500	89I	C30-C31-N32	-3.53	103.51	110.02
2	B	500	89I	C3-C41-C42	-3.52	167.87	176.51
2	A	500	89I	C3-C41-C42	-3.52	167.88	176.51
2	A	500	89I	C10-C11-N43	-3.40	117.02	121.63
2	B	500	89I	C10-C11-N43	-3.39	117.04	121.63
2	B	500	89I	C21-C20-N32	-3.26	115.84	121.70
2	A	500	89I	C21-C20-N32	-3.25	115.86	121.70
2	A	500	89I	C1-N2-C3	-3.25	113.02	117.75
2	B	500	89I	C3-C4-C5	-3.25	113.35	115.93
2	B	500	89I	C1-N2-C3	-3.25	113.03	117.75
2	A	500	89I	C3-C4-C5	-3.24	113.35	115.93
2	B	500	89I	C9-C8-C4	-3.19	115.50	120.79
2	A	500	89I	C9-C8-C4	-3.18	115.51	120.79
2	B	500	89I	N19-C20-N32	2.63	120.72	116.79
2	A	500	89I	N19-C20-N32	2.59	120.67	116.79
2	B	500	89I	C8-C4-C5	2.50	124.04	120.42
2	B	500	89I	C21-C22-C23	-2.49	117.13	120.35
2	A	500	89I	C21-C22-C23	-2.49	117.13	120.35
2	A	500	89I	C8-C4-C5	2.47	124.01	120.42
2	B	500	89I	O29-C30-C31	-2.17	107.02	111.80
2	A	500	89I	O29-C30-C31	-2.16	107.04	111.80
2	A	500	89I	C44-N43-C11	-2.08	116.98	120.54
2	B	500	89I	C44-N43-C11	-2.07	116.99	120.54
2	A	500	89I	O29-C28-C27	-2.04	107.31	111.80
2	B	500	89I	O29-C28-C27	-2.04	107.31	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

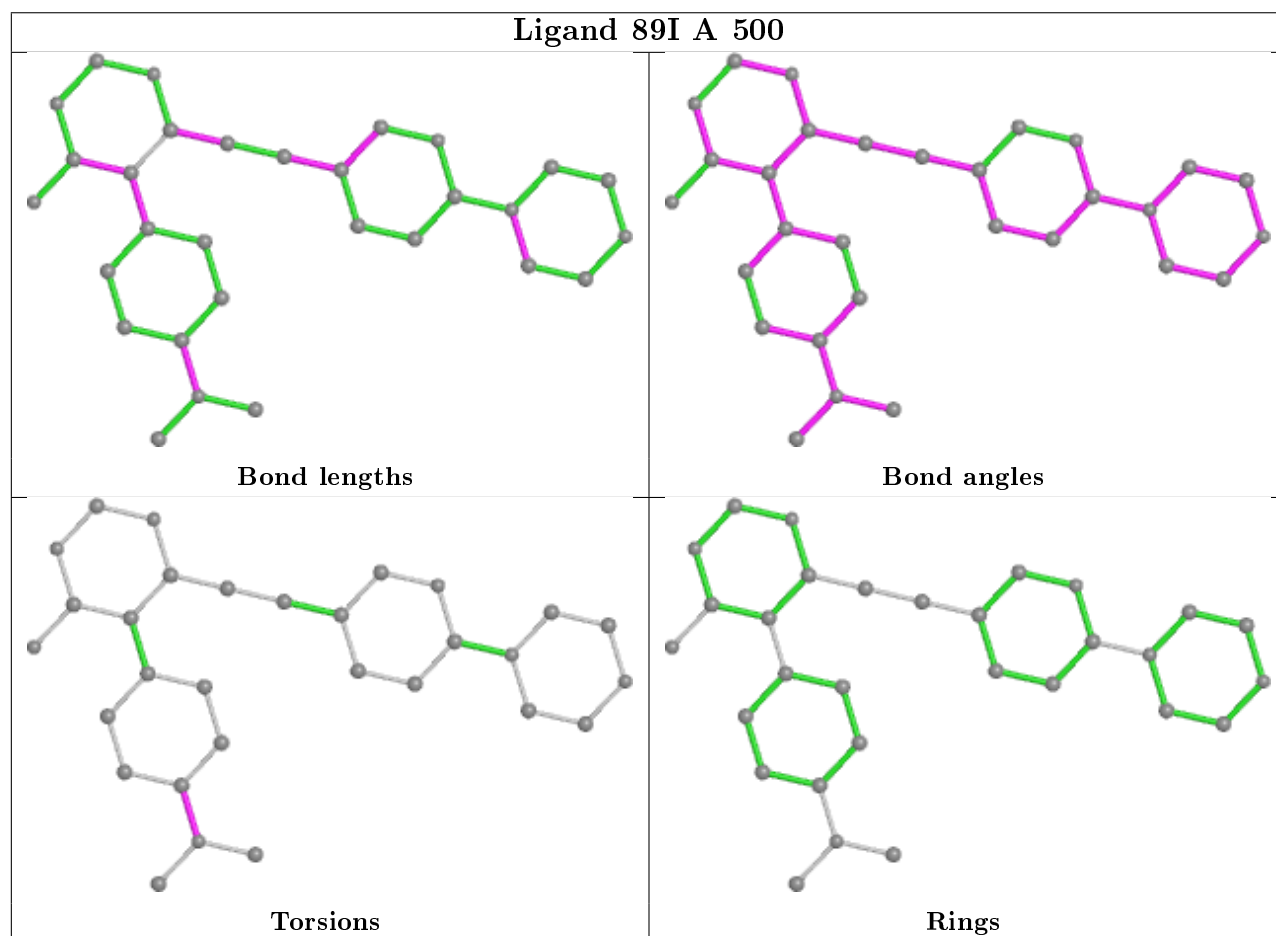
Mol	Chain	Res	Type	Atoms
2	A	500	89I	C12-C11-N43-C48
2	B	500	89I	C12-C11-N43-C48
2	A	500	89I	C10-C11-N43-C48
2	B	500	89I	C10-C11-N43-C48

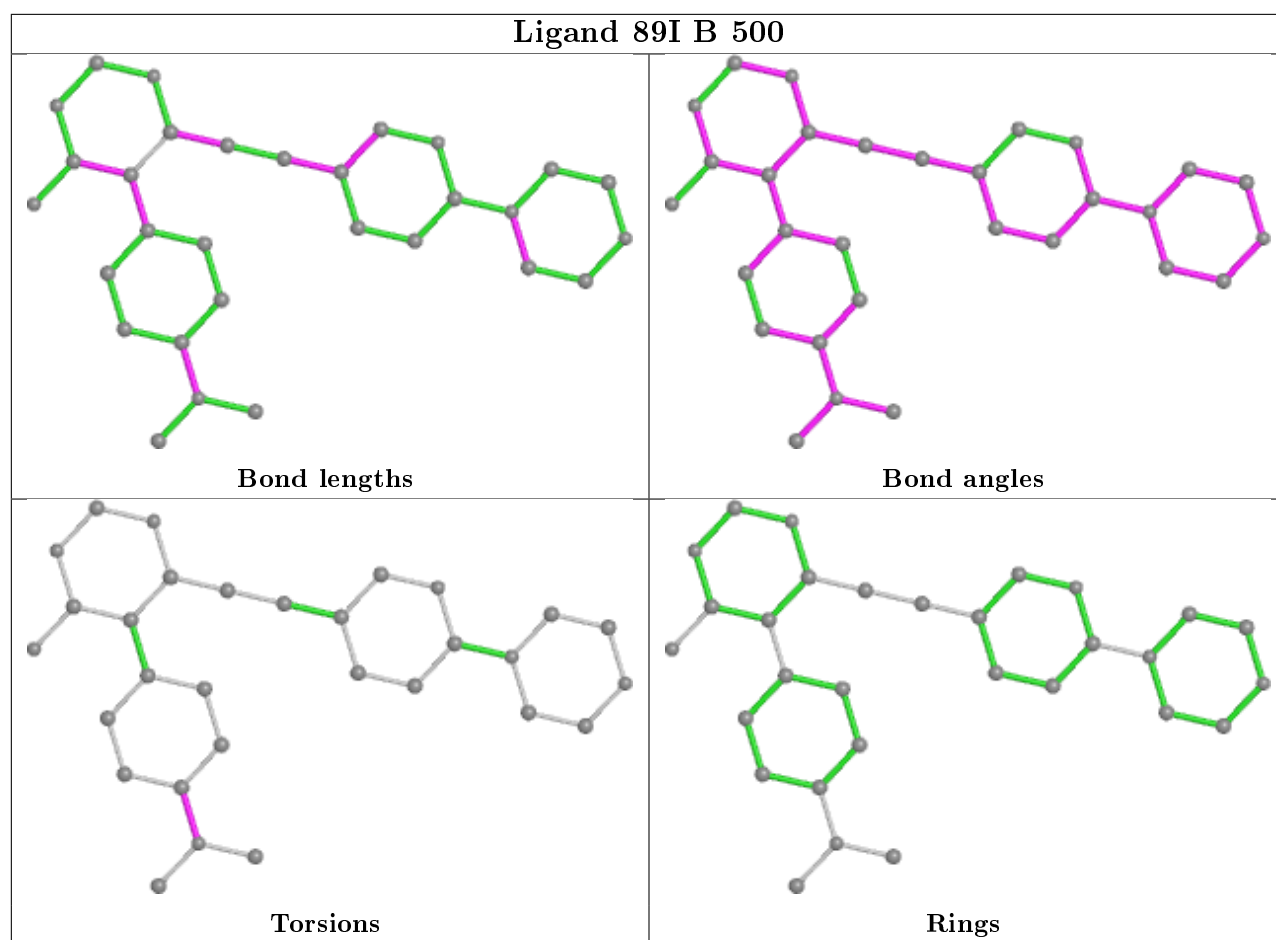
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	89I	5	0
2	B	500	89I	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.