



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:45 PM UTC

PDB ID : 2NMT / pdb\_00002nmt  
Title : MYRISTOYL-COA:PROTEIN N-MYRISTOYLTRANSFERASE BOUND  
TO MYRISTOYL-COA AND PEPTIDE ANALOGS  
Authors : Fuetterer, K.; Bhatnagar, R.S.; Waksman, G.  
Deposited on : 1998-07-14  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

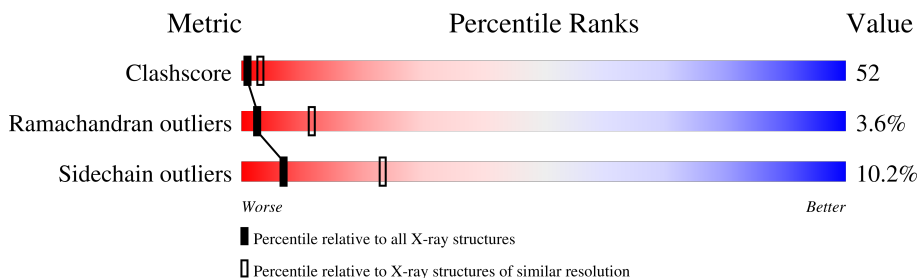
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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  $\geq 3$ , 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	422	 33% 50% 15%

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
4	GOL	A	804	-	-	X	-
4	GOL	A	807	-	-	X	-

## 2 Entry composition [i](#)

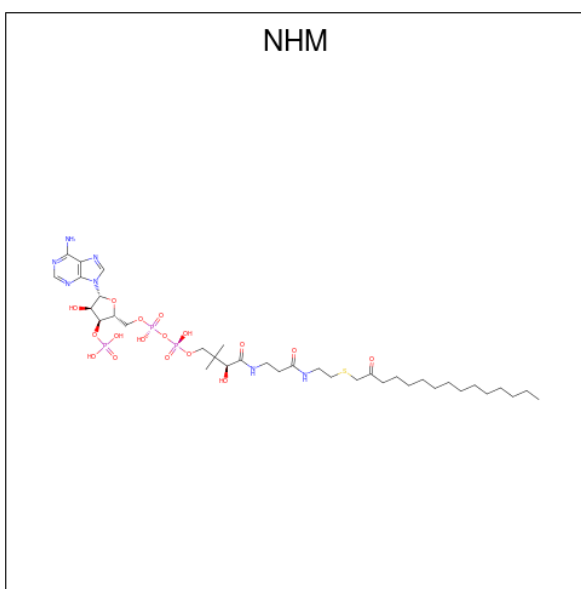
There are 5 unique types of molecules in this entry. The entry contains 3601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MYRISTOYL-COA\;:PROTEIN N-MYRISTOYLTRANSFERASE.

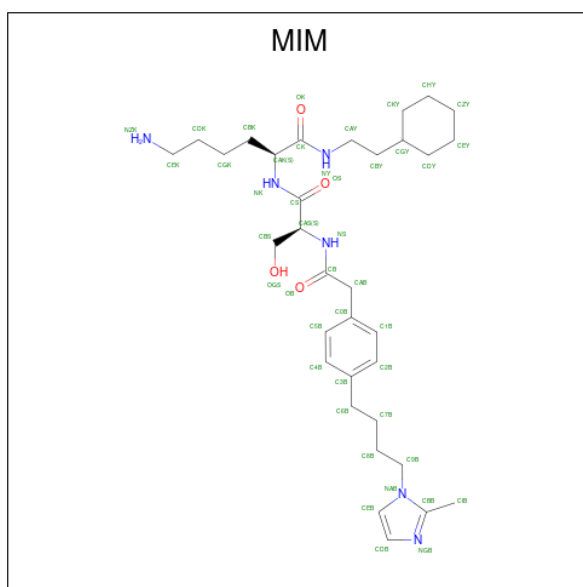
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3388	2190	558	630	10	0	0	0

- Molecule 2 is S-(2-OXO)PENTADECYLCOA (CCD ID: NHM) (formula: C<sub>36</sub>H<sub>64</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	64	36	7	17	3	1	0	0

- Molecule 3 is [CYCLOHEXYLETHYL]-[[[4-[2-METHYL-1-IMIDAZOLYL]-BUTYL]PHENYL]ACETYL]-SERYL]-LYSINY]-AMINE (CCD ID: MIM) (formula: C<sub>33</sub>H<sub>52</sub>N<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	43	33	6	4	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

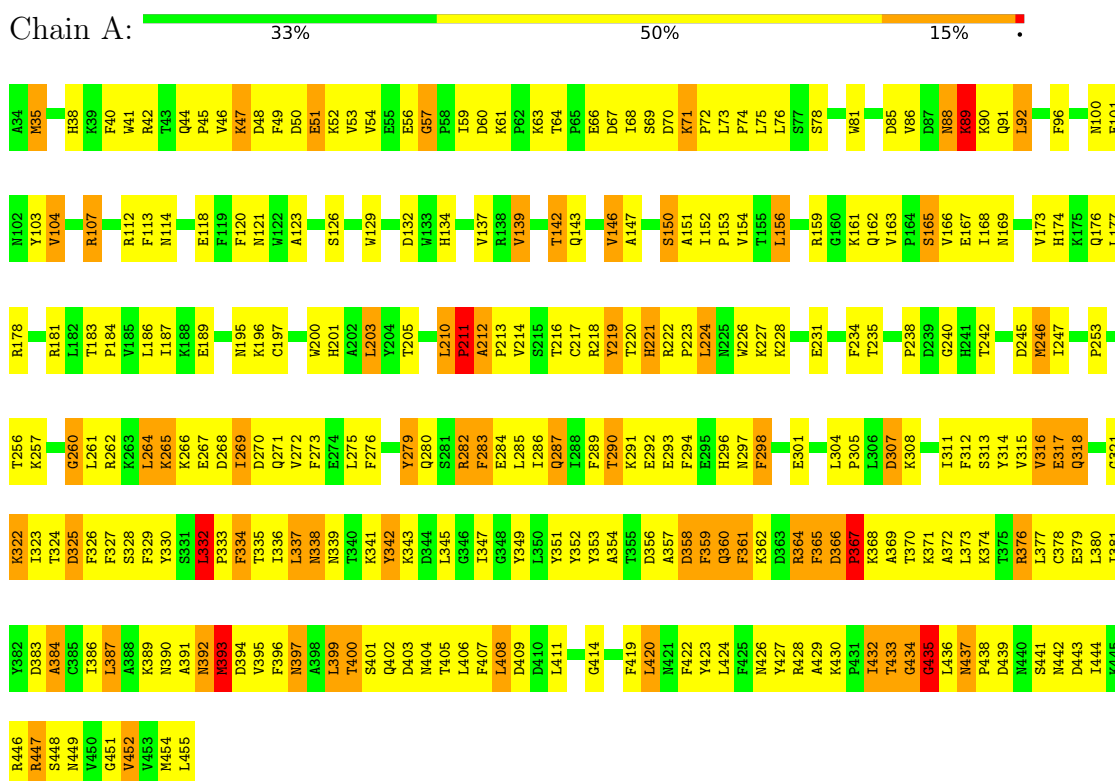
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0

### 3 Residue-property plots

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. 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: MYRISTOYL-COA\;:PROTEIN N-MYRISTOYLTRANSFERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.40Å 105.40Å 106.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	91.7 (30.00-2.90)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.228 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MIM, NHM, GOL

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	0.86	2/3477 (0.1%)	1.42	62/4726 (1.3%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	THR	CA-CB	5.09	1.61	1.53
1	A	433	THR	CA-CB	5.02	1.60	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	LEU	N-CA-C	12.88	129.49	112.88
1	A	358	ASP	N-CA-C	10.03	123.14	111.11
1	A	290	THR	N-CA-C	-9.05	95.67	109.79
1	A	92	LEU	N-CA-C	-8.89	101.55	111.07
1	A	359	PHE	N-CA-C	8.36	120.39	111.28
1	A	335	THR	N-CA-C	-8.16	95.98	108.96
1	A	61	LYS	N-CA-C	-7.65	100.11	109.83
1	A	234	PHE	N-CA-C	-7.60	102.65	112.23
1	A	433	THR	N-CA-C	7.51	120.97	108.73
1	A	338	ASN	CA-C-N	-7.26	110.97	122.73
1	A	338	ASN	C-N-CA	-7.26	110.97	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	GLY	N-CA-C	-7.24	106.07	114.69
1	A	437	ASN	N-CA-C	-7.14	99.91	110.20
1	A	71	LYS	N-CA-C	7.12	119.86	109.04
1	A	436	LEU	N-CA-C	7.06	120.03	108.52
1	A	435	GLY	N-CA-C	6.99	129.74	113.18
1	A	384	ALA	N-CA-C	-6.56	104.21	111.36
1	A	57	GLY	CA-C-N	6.52	126.54	119.89
1	A	57	GLY	C-N-CA	6.52	126.54	119.89
1	A	304	LEU	CA-C-N	6.50	126.68	120.31
1	A	304	LEU	C-N-CA	6.50	126.68	120.31
1	A	316	VAL	N-CA-C	6.32	115.83	106.85
1	A	336	ILE	CB-CA-C	-6.27	105.15	111.80
1	A	52	LYS	N-CA-C	-6.26	100.72	110.42
1	A	150	SER	N-CA-C	6.19	118.82	109.23
1	A	401	SER	N-CA-C	-6.18	101.05	110.14
1	A	134	HIS	N-CA-C	-6.18	100.34	109.11
1	A	298	PHE	N-CA-C	6.15	121.72	113.72
1	A	434	GLY	N-CA-C	-6.12	98.69	113.18
1	A	283	PHE	N-CA-C	6.10	119.76	109.76
1	A	240	GLY	N-CA-C	-6.09	106.92	115.32
1	A	44	GLN	N-CA-C	6.02	118.59	110.29
1	A	211	PRO	N-CA-C	6.01	124.85	112.47
1	A	287	GLN	N-CA-C	-5.99	100.43	109.95
1	A	123	ALA	N-CA-C	5.93	118.70	111.82
1	A	337	LEU	N-CA-C	-5.91	102.73	110.53
1	A	104	VAL	N-CA-C	5.91	117.34	109.37
1	A	210	LEU	CA-C-N	5.89	127.20	119.84
1	A	210	LEU	C-N-CA	5.89	127.20	119.84
1	A	318	GLN	CA-C-N	5.88	127.19	119.84
1	A	318	GLN	C-N-CA	5.88	127.19	119.84
1	A	437	ASN	CA-C-N	5.88	127.20	119.84
1	A	437	ASN	C-N-CA	5.88	127.20	119.84
1	A	439	ASP	N-CA-C	-5.84	105.97	112.57
1	A	221	HIS	N-CA-C	5.75	117.74	107.80
1	A	325	ASP	N-CA-C	5.74	118.83	109.24
1	A	139	VAL	N-CA-C	-5.74	101.32	108.89
1	A	332	LEU	CA-C-N	5.56	126.33	120.11
1	A	332	LEU	C-N-CA	5.56	126.33	120.11
1	A	224	LEU	N-CA-C	-5.53	105.32	112.68
1	A	54	VAL	CB-CA-C	-5.28	105.74	110.91
1	A	282	ARG	N-CA-C	5.27	119.19	112.34
1	A	360	GLN	N-CA-C	-5.26	106.70	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	MET	N-CA-C	-5.25	100.62	109.07
1	A	187	ILE	N-CA-C	-5.22	105.99	110.74
1	A	397	ASN	N-CA-C	5.19	118.47	110.42
1	A	452	VAL	CB-CA-C	-5.19	102.77	111.29
1	A	304	LEU	N-CA-C	5.18	121.27	109.81
1	A	89	LYS	N-CA-C	5.18	119.32	112.89
1	A	219	TYR	N-CA-C	-5.15	102.86	110.48
1	A	212	ALA	CA-C-N	-5.07	113.50	119.84
1	A	212	ALA	C-N-CA	-5.07	113.50	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	TYR	Sidechain
1	A	342	TYR	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	3388	0	3257	365	2
2	A	64	0	60	8	0
3	A	43	0	52	6	0
4	A	72	0	95	15	4
5	A	34	0	0	8	0
All	All	3601	0	3464	368	4

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 (368) 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:383:ASP:O	1:A:387:LEU:HD23	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:HB	1:A:325:ASP:HB2	1.45	0.95
1:A:246:MET:HE3	1:A:246:MET:HA	1.53	0.91
1:A:47:LYS:HB3	1:A:212:ALA:CB	2.02	0.90
1:A:269:ILE:CG2	1:A:291:LYS:HE3	2.02	0.90
1:A:364:ARG:HA	1:A:364:ARG:HH11	1.35	0.89
1:A:159:ARG:NH2	1:A:430:LYS:HB2	1.88	0.89
1:A:432:ILE:HG13	1:A:449:ASN:HB2	1.54	0.89
1:A:405:THR:CG2	1:A:444:ILE:HA	2.03	0.88
1:A:56:GLU:OE1	1:A:159:ARG:HG3	1.72	0.88
1:A:47:LYS:HB3	1:A:212:ALA:HB2	1.53	0.87
1:A:47:LYS:HZ3	1:A:428:ARG:HA	1.44	0.82
1:A:284:GLU:HB2	1:A:432:ILE:HD12	1.61	0.81
1:A:132:ASP:OD1	4:A:809:GOL:O2	2.00	0.80
1:A:367:PRO:O	1:A:370:THR:HG22	1.81	0.80
1:A:269:ILE:HG21	1:A:291:LYS:HE3	1.64	0.79
1:A:88:ASN:HD22	1:A:89:LYS:N	1.81	0.79
1:A:74:PRO:C	1:A:75:LEU:HD12	2.08	0.78
1:A:361:PHE:CE2	1:A:369:ALA:HB2	2.18	0.78
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.21	0.76
1:A:432:ILE:HG13	1:A:449:ASN:CB	2.15	0.76
1:A:359:PHE:HD1	1:A:360:GLN:N	1.84	0.75
1:A:64:THR:HG23	1:A:66:GLU:HG3	1.68	0.75
1:A:269:ILE:HG22	1:A:291:LYS:HE3	1.69	0.75
1:A:85:ASP:H	1:A:91:GLN:NE2	1.85	0.74
1:A:283:PHE:HB3	1:A:449:ASN:O	1.88	0.74
1:A:356:ASP:HA	1:A:359:PHE:CZ	2.22	0.73
1:A:152:ILE:HD12	1:A:152:ILE:O	1.88	0.73
1:A:222:ARG:NH1	1:A:223:PRO:O	2.22	0.73
1:A:268:ASP:O	1:A:272:VAL:HG23	1.89	0.72
1:A:364:ARG:C	1:A:366:ASP:H	1.97	0.72
1:A:432:ILE:HD11	1:A:449:ASN:C	2.13	0.72
1:A:197:CYS:HB3	4:A:803:GOL:H12	1.72	0.72
1:A:364:ARG:HD3	1:A:365:PHE:H	1.55	0.72
1:A:47:LYS:NZ	1:A:428:ARG:HA	2.04	0.71
1:A:405:THR:HG21	1:A:444:ILE:HA	1.70	0.71
1:A:70:ASP:OD1	1:A:196:LYS:NZ	2.22	0.71
1:A:323:ILE:O	1:A:323:ILE:HD12	1.91	0.71
1:A:214:VAL:HG12	1:A:432:ILE:HG23	1.73	0.70
1:A:405:THR:HG22	1:A:444:ILE:HA	1.72	0.70
1:A:114:ASN:HB3	1:A:333:PRO:HG2	1.74	0.70
1:A:364:ARG:HA	1:A:364:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:HG2	1:A:48:ASP:N	2.06	0.69
1:A:296:HIS:CG	4:A:804:GOL:O2	2.45	0.69
1:A:50:ASP:CG	1:A:51:GLU:H	2.01	0.69
1:A:60:ASP:H	1:A:426:ASN:HD21	1.39	0.68
1:A:323:ILE:HD12	1:A:323:ILE:C	2.18	0.68
1:A:266:LYS:O	1:A:269:ILE:HD13	1.92	0.68
1:A:403:ASP:OD2	1:A:447:ARG:HD2	1.92	0.68
1:A:291:LYS:O	1:A:294:PHE:HB3	1.93	0.68
1:A:228:LYS:HE3	1:A:342:TYR:CD2	2.30	0.67
1:A:205:THR:HB	1:A:420:LEU:HD21	1.74	0.67
1:A:220:THR:HG21	1:A:408:LEU:HD13	1.77	0.67
1:A:137:VAL:HB	1:A:147:ALA:HB3	1.77	0.67
1:A:296:HIS:HA	5:A:1043:HOH:O	1.95	0.67
1:A:264:LEU:HD12	1:A:265:LYS:H	1.60	0.66
1:A:286:ILE:HG22	1:A:451:GLY:HA3	1.77	0.66
1:A:358:ASP:O	1:A:361:PHE:HB3	1.95	0.66
1:A:404:ASN:HA	1:A:407:PHE:CZ	2.29	0.66
1:A:96:PHE:C	1:A:96:PHE:CD2	2.74	0.66
1:A:289:PHE:HE2	1:A:297:ASN:ND2	1.93	0.66
1:A:47:LYS:HG2	1:A:48:ASP:H	1.59	0.66
1:A:370:THR:HG23	1:A:371:LYS:N	2.11	0.66
1:A:85:ASP:H	1:A:91:GLN:HE22	1.42	0.65
1:A:391:ALA:O	1:A:392:ASN:HB2	1.94	0.65
1:A:361:PHE:C	1:A:361:PHE:CD2	2.74	0.65
1:A:432:ILE:HG13	1:A:433:THR:H	1.62	0.65
1:A:289:PHE:HE2	1:A:297:ASN:HD22	1.45	0.65
1:A:317:GLU:OE2	1:A:321:GLY:HA2	1.97	0.64
1:A:361:PHE:HD2	1:A:362:LYS:N	1.95	0.64
1:A:377:LEU:HA	1:A:380:LEU:HD12	1.80	0.64
1:A:359:PHE:CD1	1:A:360:GLN:N	2.66	0.64
1:A:364:ARG:HG3	1:A:366:ASP:H	1.63	0.64
1:A:285:LEU:HB3	1:A:432:ILE:HD13	1.79	0.64
1:A:376:ARG:O	1:A:380:LEU:HG	1.97	0.64
1:A:321:GLY:O	1:A:323:ILE:N	2.31	0.64
1:A:59:ILE:CD1	1:A:428:ARG:HG2	2.27	0.63
1:A:101:GLU:HA	1:A:112:ARG:HH21	1.61	0.63
1:A:205:THR:HB	1:A:420:LEU:CD2	2.28	0.63
1:A:367:PRO:HA	1:A:370:THR:HG22	1.80	0.63
1:A:406:LEU:HD11	1:A:447:ARG:HH11	1.64	0.63
1:A:266:LYS:HA	1:A:269:ILE:HD13	1.81	0.63
1:A:290:THR:HG23	1:A:293:GLU:CD	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:CD2	1:A:369:ALA:HB2	2.34	0.63
1:A:260:GLY:O	1:A:316:VAL:HA	1.99	0.63
1:A:268:ASP:HB3	1:A:272:VAL:CG2	2.28	0.63
1:A:56:GLU:OE2	1:A:430:LYS:HG3	1.99	0.62
1:A:261:LEU:HD12	5:A:1060:HOH:O	1.99	0.62
1:A:296:HIS:ND1	4:A:804:GOL:O2	2.32	0.62
1:A:165:SER:HB3	1:A:201:HIS:O	1.99	0.62
1:A:90:LYS:O	1:A:90:LYS:HD3	2.00	0.62
1:A:223:PRO:CG	3:A:700:MIM:HEY1	2.29	0.62
1:A:227:LYS:HD3	1:A:247:ILE:HD11	1.80	0.61
1:A:59:ILE:H	1:A:426:ASN:ND2	1.98	0.61
1:A:381:ILE:HG22	1:A:411:LEU:HD23	1.81	0.61
1:A:56:GLU:CG	1:A:430:LYS:HG3	2.30	0.61
1:A:64:THR:HG23	1:A:66:GLU:CG	2.30	0.61
1:A:203:LEU:HD23	1:A:423:TYR:O	2.00	0.61
1:A:253:PRO:HG2	1:A:257:LYS:HE2	1.81	0.61
1:A:287:GLN:HB3	1:A:289:PHE:CE1	2.36	0.61
1:A:315:VAL:HG23	1:A:325:ASP:O	2.01	0.61
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.66	0.60
1:A:433:THR:H	1:A:449:ASN:HB2	1.65	0.60
1:A:68:ILE:HB	1:A:196:LYS:HE2	1.82	0.60
1:A:435:GLY:H	1:A:448:SER:HB2	1.65	0.60
1:A:56:GLU:CD	1:A:430:LYS:HG3	2.27	0.60
1:A:313:SER:HB2	4:A:805:GOL:O2	2.02	0.60
1:A:316:VAL:HB	1:A:325:ASP:CB	2.25	0.60
1:A:156:LEU:HD22	1:A:165:SER:OG	2.02	0.59
1:A:159:ARG:CZ	1:A:430:LYS:HB2	2.31	0.59
1:A:269:ILE:HG21	1:A:291:LYS:CE	2.32	0.59
1:A:432:ILE:HD11	1:A:449:ASN:O	2.02	0.59
1:A:364:ARG:HG3	1:A:366:ASP:N	2.17	0.59
1:A:224:LEU:HD12	1:A:393:MET:O	2.02	0.59
1:A:356:ASP:HA	1:A:359:PHE:CE2	2.36	0.59
1:A:96:PHE:HA	1:A:120:PHE:HE1	1.68	0.58
1:A:139:VAL:CG1	1:A:142:THR:HG23	2.32	0.58
1:A:142:THR:O	1:A:143:GLN:HB2	2.02	0.58
1:A:296:HIS:HB2	4:A:804:GOL:H32	1.85	0.58
1:A:85:ASP:HB3	1:A:91:GLN:HE22	1.68	0.58
1:A:235:THR:HG22	3:A:700:MIM:HGY	1.84	0.58
1:A:270:ASP:OD1	1:A:291:LYS:NZ	2.34	0.58
1:A:174:HIS:HD2	1:A:176:GLN:H	1.52	0.57
1:A:369:ALA:O	1:A:372:ALA:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:HE3	1:A:454:MET:HA	1.86	0.57
1:A:246:MET:HA	1:A:246:MET:CE	2.31	0.57
1:A:370:THR:CG2	1:A:371:LYS:N	2.67	0.57
1:A:173:VAL:HG23	2:A:500:NHM:H141	1.87	0.56
1:A:227:LYS:HB2	1:A:247:ILE:HD11	1.86	0.56
1:A:265:LYS:HD3	1:A:268:ASP:OD2	2.05	0.56
1:A:432:ILE:HG13	1:A:433:THR:N	2.21	0.56
1:A:88:ASN:HD22	1:A:89:LYS:H	1.51	0.56
1:A:64:THR:HG22	1:A:67:ASP:OD2	2.05	0.56
1:A:317:GLU:OE2	4:A:810:GOL:H12	2.05	0.56
1:A:290:THR:HG23	1:A:293:GLU:HG2	1.88	0.56
1:A:327:PHE:HA	1:A:353:TYR:HA	1.89	0.55
1:A:407:PHE:CE1	1:A:408:LEU:HD23	2.41	0.55
1:A:315:VAL:HA	1:A:325:ASP:O	2.07	0.55
1:A:88:ASN:HD22	1:A:88:ASN:C	2.12	0.55
1:A:326:PHE:O	1:A:354:ALA:N	2.34	0.55
1:A:433:THR:O	1:A:449:ASN:N	2.40	0.55
1:A:63:LYS:HB2	1:A:200:TRP:CZ3	2.41	0.55
1:A:361:PHE:C	1:A:361:PHE:HD2	2.15	0.55
1:A:437:ASN:HB2	1:A:441:SER:OG	2.07	0.55
1:A:126:SER:HA	1:A:296:HIS:NE2	2.21	0.55
1:A:205:THR:O	2:A:500:NHM:HP2	2.07	0.55
1:A:45:PRO:O	1:A:426:ASN:HA	2.07	0.54
1:A:75:LEU:HD11	1:A:81:TRP:CZ2	2.42	0.54
1:A:174:HIS:CD2	1:A:176:GLN:H	2.26	0.54
1:A:314:TYR:CZ	1:A:387:LEU:HD12	2.43	0.54
1:A:377:LEU:C	1:A:379:GLU:N	2.64	0.54
1:A:284:GLU:HB2	1:A:449:ASN:HB3	1.88	0.54
1:A:256:THR:HG23	5:A:1036:HOH:O	2.06	0.54
1:A:64:THR:O	1:A:67:ASP:HB2	2.06	0.54
1:A:75:LEU:HD11	1:A:81:TRP:CE2	2.43	0.54
1:A:126:SER:HA	1:A:296:HIS:CD2	2.43	0.53
1:A:330:TYR:CE1	1:A:349:TYR:HB2	2.43	0.53
1:A:101:GLU:HA	1:A:112:ARG:NH2	2.22	0.53
1:A:284:GLU:CB	1:A:432:ILE:HD12	2.36	0.53
1:A:316:VAL:CB	1:A:325:ASP:HB2	2.30	0.53
1:A:280:GLN:NE2	1:A:286:ILE:HB	2.24	0.53
1:A:337:LEU:O	1:A:338:ASN:HB2	2.08	0.53
1:A:139:VAL:HG13	1:A:142:THR:HG23	1.90	0.53
1:A:201:HIS:CD2	4:A:807:GOL:H12	2.44	0.53
1:A:269:ILE:HG22	1:A:270:ASP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:HG3	1:A:428:ARG:HH11	1.72	0.53
1:A:452:VAL:HA	5:A:1024:HOH:O	2.09	0.52
1:A:159:ARG:NH2	1:A:430:LYS:CB	2.68	0.52
1:A:223:PRO:HG2	3:A:700:MIM:HEY1	1.91	0.52
1:A:411:LEU:N	1:A:411:LEU:HD12	2.23	0.52
1:A:57:GLY:H	1:A:428:ARG:HB2	1.74	0.52
1:A:228:LYS:NZ	1:A:394:ASP:OD1	2.41	0.52
1:A:406:LEU:HD11	1:A:447:ARG:NH1	2.24	0.52
1:A:364:ARG:HD3	1:A:365:PHE:N	2.23	0.52
1:A:433:THR:OG1	1:A:449:ASN:N	2.43	0.52
1:A:402:GLN:N	1:A:448:SER:HB3	2.25	0.52
1:A:113:PHE:CE2	1:A:332:LEU:HD13	2.45	0.52
1:A:367:PRO:HA	1:A:370:THR:CG2	2.40	0.51
1:A:223:PRO:HG3	3:A:700:MIM:HEY1	1.91	0.51
1:A:205:THR:HG22	1:A:422:PHE:HA	1.93	0.51
1:A:201:HIS:NE2	4:A:807:GOL:H31	2.25	0.51
1:A:347:ILE:HG23	1:A:395:VAL:HG13	1.92	0.51
1:A:74:PRO:O	1:A:75:LEU:HD12	2.11	0.51
1:A:370:THR:CG2	1:A:371:LYS:H	2.24	0.51
1:A:434:GLY:HA2	1:A:448:SER:OG	2.11	0.51
1:A:311:ILE:O	4:A:805:GOL:H12	2.10	0.51
1:A:316:VAL:HG12	1:A:316:VAL:O	2.11	0.51
1:A:152:ILE:HD12	1:A:152:ILE:C	2.36	0.51
2:A:500:NHM:H2A	2:A:500:NHM:H5M2	1.93	0.51
1:A:217:CYS:HB3	1:A:399:LEU:O	2.11	0.50
1:A:290:THR:HG23	1:A:293:GLU:CG	2.41	0.50
1:A:267:GLU:CD	1:A:267:GLU:H	2.19	0.50
1:A:356:ASP:CA	1:A:359:PHE:CZ	2.94	0.50
1:A:432:ILE:CD1	1:A:449:ASN:HB3	2.41	0.50
1:A:222:ARG:NH1	1:A:222:ARG:HG3	2.26	0.50
1:A:279:TYR:CD1	1:A:279:TYR:C	2.89	0.50
1:A:318:GLN:O	1:A:321:GLY:N	2.39	0.50
1:A:59:ILE:HG12	1:A:427:TYR:N	2.26	0.50
1:A:113:PHE:HE2	1:A:332:LEU:HD13	1.76	0.50
1:A:126:SER:O	1:A:129:TRP:HD1	1.95	0.49
1:A:70:ASP:OD1	1:A:196:LYS:CE	2.60	0.49
1:A:268:ASP:HB3	1:A:272:VAL:HG21	1.93	0.49
1:A:48:ASP:OD2	1:A:50:ASP:OD1	2.31	0.49
1:A:183:THR:HB	1:A:184:PRO:HD3	1.93	0.49
1:A:269:ILE:O	1:A:273:PHE:N	2.30	0.49
1:A:324:THR:OG1	1:A:356:ASP:OD2	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CG	1:A:104:VAL:N	2.79	0.49
1:A:47:LYS:CG	1:A:48:ASP:H	2.25	0.49
1:A:151:ALA:HB2	1:A:168:ILE:CD1	2.42	0.49
1:A:432:ILE:CG1	1:A:433:THR:N	2.75	0.49
1:A:88:ASN:C	1:A:88:ASN:ND2	2.71	0.49
1:A:161:LYS:O	1:A:163:VAL:HG23	2.12	0.49
1:A:201:HIS:NE2	4:A:807:GOL:H12	2.28	0.49
1:A:289:PHE:C	1:A:290:THR:O	2.51	0.49
1:A:386:ILE:O	1:A:390:ASN:ND2	2.46	0.49
1:A:40:PHE:CD1	1:A:184:PRO:HB3	2.47	0.49
1:A:47:LYS:HB3	1:A:212:ALA:HB1	1.90	0.49
1:A:264:LEU:HD12	1:A:265:LYS:N	2.28	0.49
1:A:381:ILE:N	1:A:381:ILE:HD12	2.28	0.49
1:A:214:VAL:CG1	1:A:432:ILE:HG23	2.40	0.48
1:A:377:LEU:C	1:A:379:GLU:H	2.20	0.48
1:A:405:THR:HG21	1:A:443:ASP:C	2.38	0.48
1:A:183:THR:HA	1:A:186:LEU:HD12	1.95	0.48
1:A:406:LEU:HG	1:A:447:ARG:HD3	1.95	0.48
1:A:316:VAL:HG11	1:A:325:ASP:OD2	2.12	0.48
1:A:152:ILE:HD11	1:A:167:GLU:HB3	1.95	0.48
1:A:293:GLU:O	1:A:293:GLU:HG3	2.13	0.48
1:A:282:ARG:HD2	1:A:283:PHE:CZ	2.48	0.48
1:A:405:THR:HG21	1:A:443:ASP:O	2.14	0.48
1:A:408:LEU:HD12	1:A:442:ASN:OD1	2.14	0.48
1:A:48:ASP:CG	1:A:49:PHE:H	2.22	0.47
1:A:56:GLU:HA	1:A:428:ARG:O	2.13	0.47
1:A:70:ASP:OD1	1:A:196:LYS:HE3	2.14	0.47
1:A:292:GLU:C	1:A:294:PHE:H	2.20	0.47
1:A:339:ASN:OD1	1:A:341:LYS:N	2.46	0.47
1:A:285:LEU:HD12	1:A:286:ILE:N	2.29	0.47
1:A:317:GLU:HB2	1:A:323:ILE:HG22	1.97	0.47
1:A:359:PHE:C	1:A:361:PHE:H	2.22	0.47
1:A:56:GLU:CD	1:A:159:ARG:HG3	2.39	0.47
1:A:96:PHE:O	1:A:100:ASN:HB2	2.14	0.47
1:A:408:LEU:O	1:A:409:ASP:C	2.58	0.47
2:A:500:NHM:S1	3:A:700:MIM:H9B2	2.54	0.47
1:A:118:GLU:H	1:A:118:GLU:CD	2.21	0.47
1:A:47:LYS:NZ	1:A:429:ALA:H	2.13	0.47
1:A:47:LYS:CG	1:A:48:ASP:N	2.74	0.47
1:A:151:ALA:HB1	1:A:166:VAL:CG2	2.45	0.47
1:A:201:HIS:NE2	4:A:807:GOL:C3	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:O	1:A:379:GLU:N	2.48	0.47
1:A:219:TYR:HA	1:A:399:LEU:HD23	1.97	0.47
1:A:311:ILE:HD12	1:A:329:PHE:O	2.15	0.47
1:A:454:MET:HE3	1:A:454:MET:CA	2.45	0.47
1:A:296:HIS:HB2	4:A:804:GOL:O2	2.15	0.46
1:A:317:GLU:HA	1:A:323:ILE:HA	1.97	0.46
1:A:68:ILE:HG13	1:A:195:ASN:HB3	1.97	0.46
1:A:227:LYS:HD3	1:A:247:ILE:CD1	2.44	0.46
1:A:283:PHE:CE2	1:A:402:GLN:HA	2.50	0.46
1:A:290:THR:H	1:A:293:GLU:CG	2.29	0.46
1:A:53:VAL:HG21	1:A:428:ARG:HD3	1.97	0.46
1:A:85:ASP:N	1:A:91:GLN:NE2	2.58	0.46
1:A:146:VAL:HG22	1:A:177:LEU:HD23	1.97	0.46
1:A:205:THR:HG21	1:A:454:MET:HG3	1.97	0.46
1:A:397:ASN:N	1:A:397:ASN:HD22	2.14	0.46
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.81	0.46
1:A:361:PHE:CD2	1:A:362:LYS:N	2.81	0.46
1:A:220:THR:HA	1:A:414:GLY:O	2.15	0.46
1:A:298:PHE:CE2	1:A:352:TYR:HB2	2.51	0.46
1:A:88:ASN:ND2	1:A:89:LYS:N	2.56	0.46
1:A:181:ARG:NH2	2:A:500:NHM:O7A	2.49	0.46
1:A:265:LYS:HD3	1:A:268:ASP:CG	2.41	0.46
1:A:334:PHE:HB2	1:A:345:LEU:HB3	1.97	0.46
1:A:433:THR:O	1:A:448:SER:OG	2.19	0.45
1:A:383:ASP:O	1:A:387:LEU:CD2	2.50	0.45
1:A:428:ARG:HH11	1:A:428:ARG:CG	2.29	0.45
1:A:38:HIS:HB3	2:A:500:NHM:O9A	2.16	0.45
1:A:81:TRP:CZ2	1:A:189:GLU:HG2	2.52	0.45
1:A:216:THR:HG22	1:A:217:CYS:N	2.31	0.45
1:A:231:GLU:OE1	1:A:231:GLU:HA	2.17	0.45
1:A:315:VAL:CG2	1:A:325:ASP:O	2.65	0.45
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.78	0.45
1:A:73:LEU:HA	1:A:73:LEU:HD23	1.80	0.44
1:A:85:ASP:HB3	1:A:91:GLN:NE2	2.31	0.44
1:A:361:PHE:HZ	1:A:368:LYS:CB	2.30	0.44
1:A:361:PHE:HD2	1:A:362:LYS:CB	2.31	0.44
1:A:174:HIS:HB3	1:A:177:LEU:HD23	1.98	0.44
1:A:266:LYS:CA	1:A:269:ILE:HD13	2.47	0.44
1:A:381:ILE:O	1:A:384:ALA:HB3	2.17	0.44
1:A:262:ARG:HD2	1:A:265:LYS:HE3	1.99	0.44
1:A:454:MET:HE2	5:A:1015:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:NH1	5:A:1041:HOH:O	2.43	0.44
1:A:268:ASP:C	1:A:272:VAL:HG23	2.43	0.44
1:A:285:LEU:HD12	1:A:285:LEU:C	2.43	0.44
1:A:351:TYR:CZ	1:A:455:LEU:HD21	2.52	0.44
1:A:210:LEU:HB3	1:A:211:PRO:HD2	1.99	0.44
1:A:411:LEU:N	1:A:411:LEU:CD1	2.81	0.44
1:A:422:PHE:N	1:A:422:PHE:CD1	2.85	0.44
1:A:266:LYS:HA	1:A:269:ILE:CD1	2.47	0.43
1:A:268:ASP:O	1:A:269:ILE:C	2.61	0.43
1:A:81:TRP:CH2	1:A:189:GLU:HG2	2.53	0.43
1:A:242:THR:O	1:A:245:ASP:HB2	2.18	0.43
1:A:50:ASP:CG	1:A:51:GLU:N	2.74	0.43
1:A:224:LEU:HD13	1:A:389:LYS:HA	2.00	0.43
1:A:165:SER:HB3	1:A:201:HIS:C	2.44	0.43
1:A:71:LYS:HA	1:A:72:PRO:HD2	1.88	0.43
1:A:85:ASP:HB2	4:A:812:GOL:H12	2.00	0.43
1:A:154:VAL:HG23	1:A:156:LEU:CD1	2.49	0.43
1:A:176:GLN:HE21	1:A:176:GLN:HB2	1.61	0.43
1:A:212:ALA:O	1:A:213:PRO:C	2.61	0.43
1:A:59:ILE:HD11	1:A:428:ARG:N	2.32	0.43
1:A:296:HIS:HB2	4:A:804:GOL:C3	2.48	0.43
1:A:151:ALA:HB1	1:A:166:VAL:HG21	2.00	0.43
1:A:152:ILE:CD1	1:A:167:GLU:HB3	2.48	0.43
1:A:396:PHE:C	1:A:397:ASN:HD22	2.27	0.43
1:A:96:PHE:O	1:A:100:ASN:CB	2.67	0.43
1:A:235:THR:CG2	3:A:700:MIM:HG Y	2.49	0.43
1:A:381:ILE:N	1:A:381:ILE:CD1	2.82	0.43
1:A:181:ARG:NH1	1:A:181:ARG:HB3	2.33	0.43
1:A:427:TYR:OH	5:A:1071:HOH:O	2.21	0.43
1:A:214:VAL:CG1	1:A:432:ILE:CG2	2.97	0.42
1:A:271:GLN:OE1	1:A:322:LYS:HA	2.17	0.42
1:A:292:GLU:C	1:A:294:PHE:N	2.77	0.42
1:A:205:THR:CG2	1:A:454:MET:HG3	2.50	0.42
1:A:238:PRO:HG3	1:A:246:MET:SD	2.59	0.42
1:A:266:LYS:C	1:A:269:ILE:HD13	2.45	0.42
1:A:381:ILE:CD1	1:A:381:ILE:H	2.31	0.42
1:A:446:ARG:HG2	5:A:1054:HOH:O	2.20	0.42
1:A:307:ASP:OD1	1:A:308:LYS:HG2	2.19	0.42
1:A:59:ILE:HG12	1:A:426:ASN:C	2.45	0.42
1:A:85:ASP:N	1:A:91:GLN:HE22	2.15	0.42
1:A:276:PHE:CD2	1:A:294:PHE:HE1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:C	1:A:361:PHE:N	2.75	0.42
1:A:89:LYS:HA	1:A:89:LYS:HZ3	1.85	0.42
1:A:218:ARG:HD2	1:A:419:PHE:CE1	2.54	0.42
1:A:279:TYR:HE1	1:A:283:PHE:CZ	2.38	0.42
1:A:312:PHE:O	1:A:328:SER:HA	2.19	0.42
1:A:226:TRP:CE3	1:A:247:ILE:HG13	2.55	0.42
1:A:428:ARG:CG	1:A:428:ARG:NH1	2.82	0.42
1:A:285:LEU:HB3	1:A:432:ILE:CD1	2.49	0.42
1:A:73:LEU:HB3	1:A:74:PRO:CD	2.49	0.42
1:A:146:VAL:HG22	1:A:174:HIS:CB	2.50	0.42
1:A:53:VAL:O	1:A:430:LYS:NZ	2.51	0.41
1:A:88:ASN:HB3	1:A:91:GLN:HE21	1.84	0.41
1:A:361:PHE:CZ	1:A:368:LYS:C	2.98	0.41
1:A:159:ARG:NH1	1:A:284:GLU:OE1	2.53	0.41
1:A:285:LEU:C	1:A:286:ILE:HG23	2.44	0.41
1:A:38:HIS:HB3	1:A:41:TRP:HB2	2.02	0.41
1:A:46:VAL:O	1:A:47:LYS:O	2.38	0.41
1:A:216:THR:O	1:A:434:GLY:HA3	2.21	0.41
1:A:262:ARG:CZ	1:A:265:LYS:HE3	2.51	0.41
1:A:356:ASP:C	1:A:356:ASP:OD1	2.61	0.41
1:A:150:SER:O	1:A:168:ILE:HG23	2.20	0.41
1:A:178:ARG:HD2	2:A:500:NHM:O10	2.20	0.41
1:A:181:ARG:HB3	1:A:181:ARG:HH11	1.86	0.41
1:A:262:ARG:NE	1:A:265:LYS:HE3	2.36	0.41
1:A:214:VAL:HG21	1:A:424:LEU:CD1	2.51	0.41
1:A:221:HIS:O	1:A:223:PRO:HD3	2.21	0.41
1:A:285:LEU:CB	1:A:432:ILE:HD13	2.48	0.41
1:A:367:PRO:C	1:A:369:ALA:N	2.78	0.41
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.86	0.41
2:A:500:NHM:H5M2	2:A:500:NHM:C2A	2.51	0.41
1:A:35:MET:HE2	1:A:42:ARG:HA	2.03	0.40
1:A:38:HIS:O	1:A:42:ARG:HG2	2.21	0.40
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.80	0.40
1:A:365:PHE:CD1	1:A:365:PHE:C	2.99	0.40
1:A:68:ILE:HG22	1:A:69:SER:N	2.37	0.40
1:A:75:LEU:O	1:A:76:LEU:C	2.63	0.40
1:A:168:ILE:HG22	1:A:169:ASN:N	2.36	0.40
1:A:272:VAL:O	1:A:275:LEU:HB3	2.22	0.40
1:A:88:ASN:HB3	1:A:91:GLN:HB2	2.03	0.40

All (4) 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)
4:A:811:GOL:O1	4:A:811:GOL:O1[5_556]	1.32	0.88
4:A:811:GOL:O3	4:A:811:GOL:O3[5_556]	1.99	0.21
1:A:245:ASP:OD2	4:A:809:GOL:O2[6_666]	2.04	0.16
1:A:70:ASP:OD2	4:A:811:GOL:O1[5_556]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	420/422 (100%)	348 (83%)	57 (14%)	15 (4%)	<b>2</b> <b>11</b>

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	211	PRO
1	A	264	LEU
1	A	269	ILE
1	A	322	LYS
1	A	357	ALA
1	A	408	LEU
1	A	435	GLY
1	A	447	ARG
1	A	51	GLU
1	A	392	ASN
1	A	367	PRO
1	A	374	LYS
1	A	35	MET
1	A	378	CYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	362/381 (95%)	325 (90%)	37 (10%)	<b>7</b> <b>23</b>

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	SER
1	A	86	VAL
1	A	88	ASN
1	A	89	LYS
1	A	92	LEU
1	A	107	ARG
1	A	121	ASN
1	A	142	THR
1	A	146	VAL
1	A	153	PRO
1	A	156	LEU
1	A	162	GLN
1	A	165	SER
1	A	203	LEU
1	A	211	PRO
1	A	246	MET
1	A	265	LYS
1	A	301	GLU
1	A	305	PRO
1	A	307	ASP
1	A	317	GLU
1	A	332	LEU
1	A	334	PHE
1	A	343	LYS
1	A	361	PHE
1	A	364	ARG
1	A	365	PHE
1	A	366	ASP
1	A	367	PRO
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	376	ARG
1	A	387	LEU
1	A	393	MET
1	A	400	THR
1	A	420	LEU
1	A	432	ILE
1	A	438	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	91	GLN
1	A	100	ASN
1	A	102	ASN
1	A	114	ASN
1	A	121	ASN
1	A	162	GLN
1	A	174	HIS
1	A	176	GLN
1	A	195	ASN
1	A	225	ASN
1	A	297	ASN
1	A	338	ASN
1	A	390	ASN
1	A	397	ASN
1	A	402	GLN
1	A	404	ASN
1	A	421	ASN
1	A	426	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](#)

14 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
4	GOL	A	806	-	5,5,5	0.89	0	5,5,5	0.62	0
4	GOL	A	810	-	5,5,5	1.15	0	5,5,5	0.64	0
4	GOL	A	805	-	5,5,5	0.87	0	5,5,5	0.50	0
4	GOL	A	811	-	5,5,5	0.99	1 (20%)	5,5,5	0.38	0
4	GOL	A	812	-	5,5,5	0.95	1 (20%)	5,5,5	0.54	0
2	NHM	A	500	-	64,66,66	1.54	10 (15%)	87,92,92	1.64	10 (11%)
3	MIM	A	700	-	45,45,45	1.80	15 (33%)	54,57,57	1.58	8 (14%)
4	GOL	A	809	-	5,5,5	0.98	0	5,5,5	0.93	0
4	GOL	A	801	-	5,5,5	0.85	0	5,5,5	0.54	0
4	GOL	A	808	-	5,5,5	1.14	1 (20%)	5,5,5	0.55	0
4	GOL	A	802	-	5,5,5	1.32	1 (20%)	5,5,5	0.69	0
4	GOL	A	804	-	5,5,5	1.97	1 (20%)	5,5,5	0.66	0
4	GOL	A	803	-	5,5,5	1.10	0	5,5,5	0.59	0
4	GOL	A	807	-	5,5,5	0.86	0	5,5,5	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	806	-	-	0/4/4/4	-
4	GOL	A	810	-	-	2/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	811	-	-	2/4/4/4	-
4	GOL	A	812	-	-	2/4/4/4	-
2	NHM	A	500	-	-	17/65/81/81	0/3/3/3
3	MIM	A	700	-	-	17/40/48/48	0/3/3/3
4	GOL	A	809	-	-	1/4/4/4	-
4	GOL	A	801	-	-	0/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	A	802	-	-	2/4/4/4	-
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	A	803	-	-	2/4/4/4	-
4	GOL	A	807	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NHM	C4A-N3A	5.94	1.45	1.34
4	A	804	GOL	O2-C2	-4.28	1.30	1.43
2	A	500	NHM	C5A-C4A	3.76	1.45	1.39
3	A	700	MIM	CBB-NAB	3.53	1.43	1.36
3	A	700	MIM	CBB-NGB	3.48	1.39	1.32
2	A	500	NHM	C8A-N7A	3.34	1.38	1.31
2	A	500	NHM	P1A-O2A	3.30	1.62	1.50
3	A	700	MIM	CIB-CBB	3.18	1.54	1.49
2	A	500	NHM	C6A-N6A	3.10	1.42	1.34
3	A	700	MIM	C5B-C0B	3.08	1.45	1.38
3	A	700	MIM	CEB-CDB	3.06	1.42	1.35
3	A	700	MIM	CB-NS	-2.95	1.27	1.34
3	A	700	MIM	C4B-C3B	2.92	1.44	1.38
2	A	500	NHM	P3X-O7A	2.76	1.65	1.54
2	A	500	NHM	P3X-O9A	2.70	1.58	1.50
3	A	700	MIM	C4B-C5B	2.68	1.43	1.38
3	A	700	MIM	CAB-CB	-2.38	1.47	1.52
3	A	700	MIM	CAS-CS	-2.37	1.46	1.52
3	A	700	MIM	C1B-C0B	2.36	1.43	1.38
2	A	500	NHM	P2A-O4A	2.34	1.58	1.50
2	A	500	NHM	P3X-O8A	2.31	1.63	1.54
3	A	700	MIM	CAB-C0B	2.30	1.55	1.51
3	A	700	MIM	OK-CK	2.23	1.27	1.23
4	A	802	GOL	O2-C2	-2.22	1.36	1.43
2	A	500	NHM	C5A-C6A	2.13	1.46	1.41
4	A	811	GOL	O2-C2	-2.12	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	MIM	CBS-CAS	2.07	1.59	1.53
4	A	808	GOL	C1-C2	2.06	1.59	1.51
4	A	812	GOL	O2-C2	-2.04	1.37	1.43
3	A	700	MIM	CS-NK	-2.00	1.29	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	NHM	C5A-C4A-N3A	-6.52	117.74	126.72
2	A	500	NHM	N9A-C8A-N7A	5.52	121.77	113.94
2	A	500	NHM	O4X-C1X-N9A	5.34	118.35	108.09
2	A	500	NHM	C4A-N9A-C8A	-5.08	100.40	105.74
3	A	700	MIM	CBY-CAY-NY	-4.76	98.83	111.88
2	A	500	NHM	N3A-C4A-N9A	4.04	134.04	127.17
2	A	500	NHM	C5A-N7A-C8A	-3.83	97.43	103.45
3	A	700	MIM	C1B-CBB-NAB	3.72	127.33	123.50
3	A	700	MIM	CAB-CB-NS	3.25	120.94	115.88
2	A	500	NHM	C2-C3-N4	-3.04	106.08	112.41
2	A	500	NHM	CP-C1M-C2M	2.83	121.55	115.55
3	A	700	MIM	C6B-C3B-C2B	-2.53	114.71	121.18
3	A	700	MIM	C8B-C7B-C6B	-2.52	103.21	113.74
3	A	700	MIM	CAK-CK-NY	-2.43	111.32	116.54
3	A	700	MIM	C0B-CAB-CB	-2.30	105.47	112.33
2	A	500	NHM	C5A-C4A-N9A	2.22	108.23	105.81
3	A	700	MIM	CAB-C0B-C1B	-2.21	117.63	120.89
2	A	500	NHM	C7-C6-C5	2.08	115.86	112.39

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	MIM	CAY-CBY-CGY-CKY
4	A	803	GOL	C1-C2-C3-O3
4	A	805	GOL	C1-C2-C3-O3
4	A	807	GOL	C1-C2-C3-O3
4	A	810	GOL	C1-C2-C3-O3
3	A	700	MIM	C7B-C8B-C9B-NAB
3	A	700	MIM	CK-CAK-NK-CS
2	A	500	NHM	C1M-C2M-C3M-C4M
4	A	802	GOL	C1-C2-C3-O3
4	A	811	GOL	C1-C2-C3-O3
4	A	812	GOL	C1-C2-C3-O3

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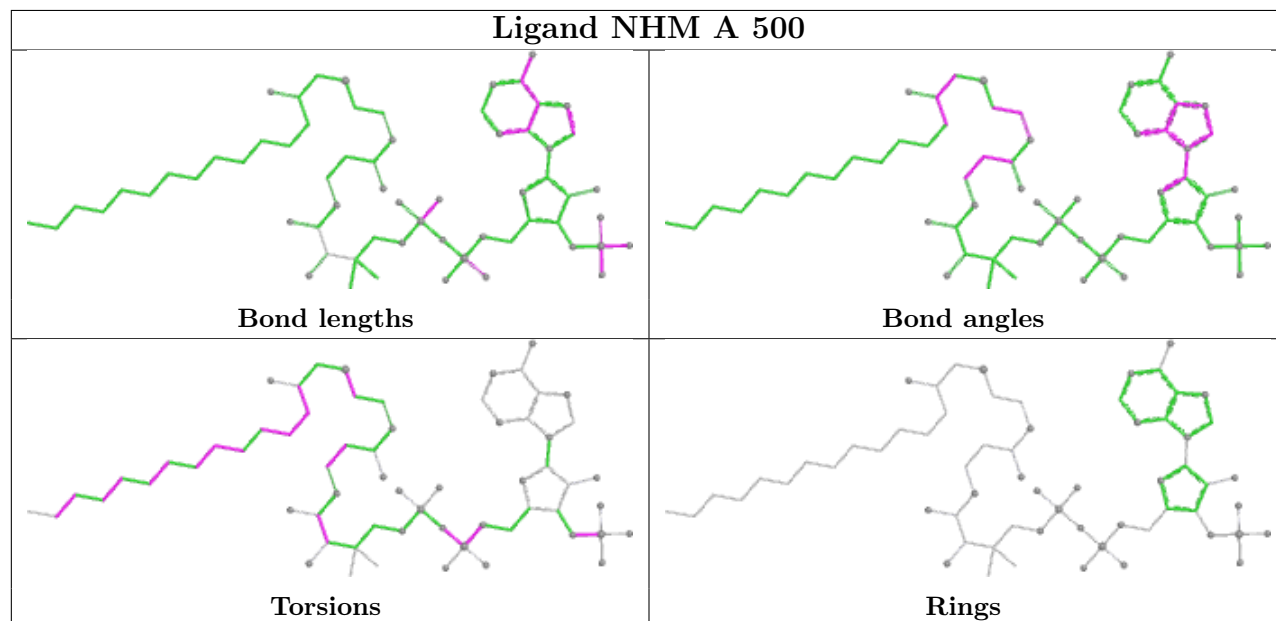
Mol	Chain	Res	Type	Atoms
2	A	500	NHM	C2M-C3M-C4M-C5M
4	A	803	GOL	O2-C2-C3-O3
4	A	805	GOL	O2-C2-C3-O3
4	A	807	GOL	O2-C2-C3-O3
4	A	810	GOL	O2-C2-C3-O3
2	A	500	NHM	C5M-C6M-C7M-C8M
2	A	500	NHM	C5-C6-C7-N8
4	A	812	GOL	O2-C2-C3-O3
2	A	500	NHM	C9M-CAM-CBM-CCM
3	A	700	MIM	NK-CAK-CK-OK
2	A	500	NHM	CBM-CCM-CDM-CEM
3	A	700	MIM	CS-CAS-NS-CB
3	A	700	MIM	NS-CAS-CS-OS
4	A	802	GOL	O2-C2-C3-O3
3	A	700	MIM	NK-CAK-CK-NY
3	A	700	MIM	CBK-CAK-CK-OK
2	A	500	NHM	C4M-C5M-C6M-C7M
3	A	700	MIM	CBK-CAK-NK-CS
3	A	700	MIM	C8B-C9B-NAB-CEB
4	A	811	GOL	O2-C2-C3-O3
2	A	500	NHM	O10-C10-C9-O9
3	A	700	MIM	C8B-C9B-NAB-CBB
3	A	700	MIM	CAK-CBK-CGK-CDK
2	A	500	NHM	C5X-O5X-P1A-O2A
3	A	700	MIM	NS-CAS-CS-NK
2	A	500	NHM	O1M-C1M-C2M-C3M
2	A	500	NHM	CP-C1M-C2M-C3M
2	A	500	NHM	C3X-O3X-P3X-O7A
3	A	700	MIM	CBK-CAK-CK-NY
4	A	809	GOL	O2-C2-C3-O3
3	A	700	MIM	CAY-CBY-CGY-CDY
2	A	500	NHM	C3-C2-S1-CP
2	A	500	NHM	P2A-O3A-P1A-O1A
2	A	500	NHM	C7M-C8M-C9M-CAM
3	A	700	MIM	C2B-C3B-C6B-C7B
3	A	700	MIM	C3B-C6B-C7B-C8B
2	A	500	NHM	P2A-O3A-P1A-O2A
2	A	500	NHM	O10-C10-C9-N8

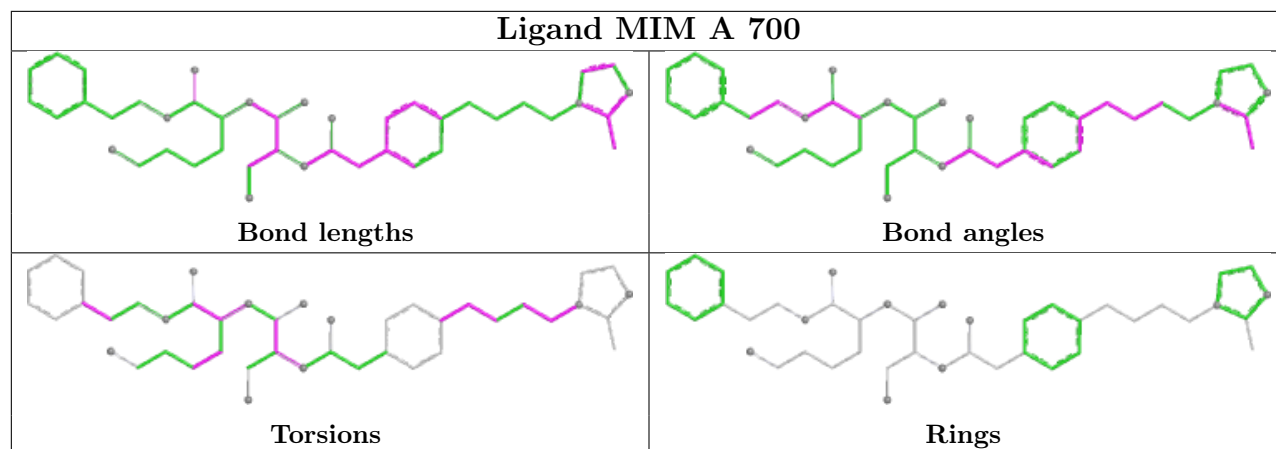
There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	810	GOL	1	0
4	A	805	GOL	2	0
4	A	811	GOL	0	3
4	A	812	GOL	1	0
2	A	500	NHM	8	0
3	A	700	MIM	6	0
4	A	809	GOL	1	1
4	A	804	GOL	5	0
4	A	803	GOL	1	0
4	A	807	GOL	4	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.