



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:22 AM UTC

PDB ID : 1MND / pdb_00001mnd
Title : TRUNCATED HEAD OF MYOSIN FROM DICTYOSTELIUM DIS-
COIDEUM COMPLEXED WITH MGADP-ALF4
Authors : Smith, C.A.; Rayment, I.
Deposited on : 1995-04-15
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)	:	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

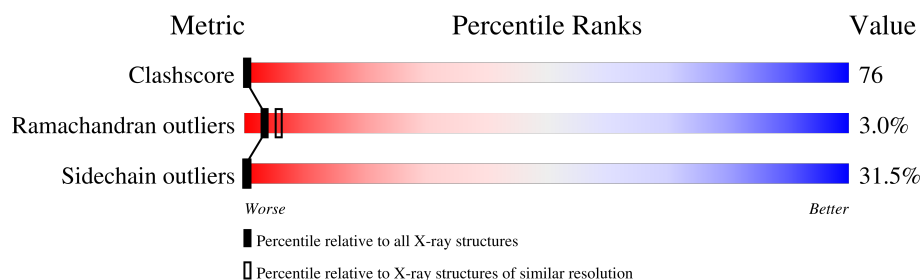
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5141 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5005	3181	856	953	15			

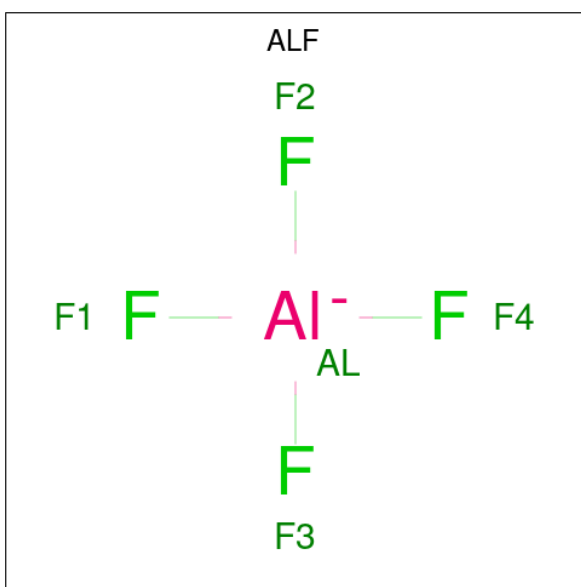
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	LYS	conflict	UNP P08799
A	312	CYS	TYR	conflict	UNP P08799
A	321	GLU	SER	conflict	UNP P08799
A	322	ASP	GLU	conflict	UNP P08799
A	443	SER	GLN	conflict	UNP P08799
A	446	ALA	LYS	conflict	UNP P08799
A	489	VAL	LEU	conflict	UNP P08799

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



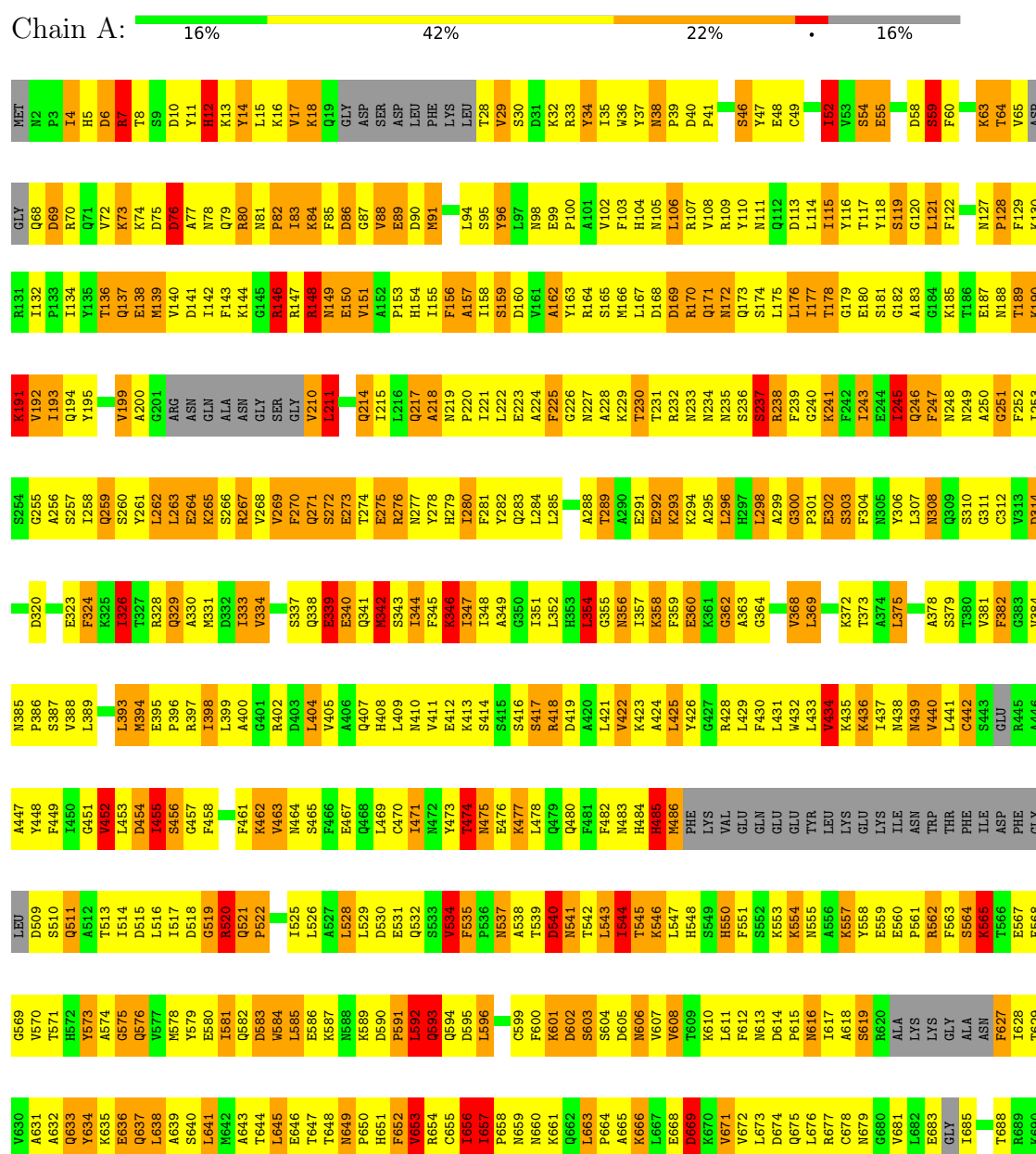
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	0	0

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: MYOSIN



LEU	ALA	ARG	ILE	GLU	GLU	ALA	ARG	GLU	GLU	LEU	PRO	ASN	LYS	VAL	PHE	ASP	ALA	TYR	ILE	ARG	ASN	PRO	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.90Å 149.00Å 153.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5141	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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: ALF, MG, ADP

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	1.22	14/5096 (0.3%)	1.75	93/6889 (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	3	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	MET	CA-C	-10.50	1.30	1.52
1	A	592	LEU	CA-C	-7.86	1.42	1.52
1	A	593	GLN	CA-C	7.37	1.61	1.52
1	A	485	HIS	CA-C	6.90	1.61	1.52
1	A	565	LYS	CA-C	6.75	1.61	1.52
1	A	521	GLN	CA-C	-6.44	1.44	1.52
1	A	342	MET	SD-CE	6.26	1.95	1.79
1	A	653	VAL	N-CA	-5.57	1.40	1.46
1	A	593	GLN	N-CA	5.57	1.53	1.46
1	A	584	TRP	NE1-CE2	-5.47	1.31	1.37
1	A	565	LYS	N-CA	5.47	1.52	1.46
1	A	442	CYS	CA-CB	-5.45	1.44	1.53
1	A	547	LEU	N-CA	-5.24	1.40	1.46
1	A	530	ASP	CA-C	5.21	1.59	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	CYS	CA-CB-SG	13.77	146.06	114.40
1	A	592	LEU	CA-C-N	-11.45	103.70	121.56
1	A	592	LEU	C-N-CA	-11.45	103.70	121.56
1	A	657	ILE	CB-CA-C	11.20	122.70	110.71
1	A	442	CYS	N-CA-C	9.92	124.56	108.99
1	A	169	ASP	CA-CB-CG	-9.82	102.78	112.60
1	A	12	HIS	CA-CB-CG	-9.30	104.50	113.80
1	A	613	ASN	CB-CA-C	8.90	125.44	111.02
1	A	541	ASN	N-CA-CB	8.78	122.74	110.01
1	A	575	GLY	CA-C-N	8.69	133.16	120.90
1	A	575	GLY	C-N-CA	8.69	133.16	120.90
1	A	52	ILE	N-CA-CB	8.21	119.93	110.82
1	A	237	SER	O-C-N	7.98	133.42	122.41
1	A	657	ILE	N-CA-C	7.96	115.80	107.76
1	A	522	PRO	N-CA-C	-7.62	101.40	110.70
1	A	82	PRO	O-C-N	7.47	131.60	123.01
1	A	452	VAL	N-CA-C	7.36	117.30	106.85
1	A	225	PHE	CA-CB-CG	7.19	120.99	113.80
1	A	14	TYR	N-CA-C	7.18	121.27	112.23
1	A	528	LEU	N-CA-C	-7.17	103.51	111.82
1	A	537	ASN	N-CA-C	-7.14	103.83	112.54
1	A	656	ILE	N-CA-C	7.12	118.99	108.45
1	A	603	SER	N-CA-CB	7.11	122.22	110.63
1	A	564	SER	CA-C-N	-7.02	110.89	120.44
1	A	564	SER	C-N-CA	-7.02	110.89	120.44
1	A	591	PRO	O-C-N	6.91	131.97	122.64
1	A	191	LYS	N-CA-C	-6.74	105.59	113.88
1	A	550	HIS	CA-CB-CG	-6.73	107.07	113.80
1	A	434	VAL	N-CA-C	6.64	117.40	110.62
1	A	454	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	583	ASP	CB-CA-C	-6.59	100.62	111.36
1	A	308	ASN	CB-CA-C	-6.44	103.23	111.22
1	A	590	ASP	O-C-N	-6.37	113.99	121.32
1	A	59	SER	N-CA-C	6.35	118.82	109.24
1	A	358	LYS	N-CA-C	6.30	119.14	107.99
1	A	474	THR	N-CA-CB	6.27	119.07	109.91
1	A	190	LYS	CB-CA-C	6.26	122.01	110.11
1	A	634	TYR	O-C-N	6.24	128.75	122.08
1	A	76	ASP	CB-CA-C	6.23	121.25	110.72
1	A	34	TYR	N-CA-C	6.21	119.34	109.65
1	A	324	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	247	PHE	CA-CB-CG	-6.14	107.66	113.80
1	A	540	ASP	CA-CB-CG	6.10	118.70	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	ASN	N-CA-CB	6.10	119.34	110.32
1	A	345	PHE	CB-CA-C	6.06	120.39	110.88
1	A	245	ILE	N-CA-CB	6.06	117.90	111.00
1	A	115	ILE	N-CA-C	5.96	116.74	110.72
1	A	634	TYR	N-CA-CB	5.87	118.75	109.82
1	A	455	ILE	CA-CB-CG2	5.83	120.41	110.50
1	A	570	VAL	N-CA-C	5.78	116.19	107.75
1	A	619	SER	N-CA-C	5.76	116.98	108.86
1	A	88	VAL	CA-C-N	5.75	132.03	122.54
1	A	88	VAL	C-N-CA	5.75	132.03	122.54
1	A	238	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	346	LYS	N-CA-CB	5.65	118.92	110.22
1	A	246	GLN	N-CA-C	5.63	117.89	107.99
1	A	522	PRO	CA-N-CD	5.59	119.83	112.00
1	A	485	HIS	O-C-N	5.59	127.84	122.03
1	A	70	ARG	N-CA-C	5.57	118.57	110.17
1	A	603	SER	N-CA-C	5.54	119.09	110.17
1	A	339	GLU	N-CA-CB	5.54	118.64	110.33
1	A	601	LYS	N-CA-CB	5.54	120.17	110.42
1	A	676	LEU	N-CA-C	-5.50	105.28	111.28
1	A	80	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	A	211	LEU	N-CA-C	-5.40	104.63	111.11
1	A	146	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	563	PHE	O-C-N	5.37	129.73	122.59
1	A	562	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	96	TYR	CA-C-N	-5.35	115.56	123.05
1	A	96	TYR	C-N-CA	-5.35	115.56	123.05
1	A	534	VAL	N-CA-C	5.34	120.45	109.34
1	A	162	ALA	N-CA-C	-5.34	105.46	111.28
1	A	148	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	147	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	356	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	652	PHE	N-CA-C	5.30	118.12	107.41
1	A	276	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	520	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	156	PHE	CA-CB-CG	5.25	119.06	113.80
1	A	169	ASP	CB-CA-C	5.18	118.31	109.24
1	A	128	PRO	N-CA-CB	5.16	108.66	103.25
1	A	656	ILE	CA-C-N	-5.15	118.88	122.59
1	A	656	ILE	C-N-CA	-5.15	118.88	122.59
1	A	76	ASP	N-CA-CB	5.14	118.69	110.73
1	A	364	GLY	O-C-N	5.13	129.37	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLU	O-C-N	5.13	128.75	122.34
1	A	38	ASN	CA-C-O	5.12	123.66	119.36
1	A	576	GLN	N-CA-CB	-5.05	101.66	109.69
1	A	575	GLY	O-C-N	5.04	129.25	122.70
1	A	534	VAL	N-CA-CB	5.03	119.53	111.23
1	A	289	THR	N-CA-CB	5.01	117.41	110.04
1	A	522	PRO	CB-CA-C	5.01	117.04	110.92
1	A	7	ARG	NE-CZ-NH2	5.00	123.70	119.20

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	169	ASP	CA
1	A	534	VAL	CA
1	A	613	ASN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ILE	Mainchain
1	A	354	LEU	Mainchain
1	A	540	ASP	Mainchain
1	A	544	ILE	Mainchain
1	A	596	LEU	Mainchain

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	A	5005	0	4841	751	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
4	A	27	0	12	5	0
5	A	103	0	0	21	0
All	All	5141	0	4853	752	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 76.

All (752) 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:614:ASP:HB3	1:A:617:ILE:CB	1.72	1.19
1:A:279:HIS:CE1	5:A:1002:HOH:O	1.98	1.16
1:A:285:LEU:HD21	1:A:298:LEU:HG	1.26	1.15
1:A:561:PRO:HG3	1:A:567:GLU:O	1.47	1.13
1:A:268:VAL:HA	1:A:277:ASN:HD21	1.14	1.12
1:A:211:LEU:HD11	1:A:255:GLY:HA2	1.16	1.10
1:A:561:PRO:CG	1:A:567:GLU:O	2.01	1.06
1:A:224:ALA:HB1	1:A:280:ILE:HG23	1.25	1.06
1:A:343:SER:HA	1:A:346:LYS:HG3	1.40	1.04
1:A:614:ASP:O	1:A:618:ALA:N	1.91	1.02
1:A:273:GLU:O	1:A:310:SER:O	1.77	1.02
1:A:210:VAL:HG12	1:A:211:LEU:H	1.23	1.01
1:A:396:PRO:HB3	1:A:593:GLN:HG2	1.40	1.00
1:A:614:ASP:CB	1:A:617:ILE:CB	2.40	0.99
1:A:521:GLN:CB	1:A:522:PRO:CD	2.40	0.99
1:A:657:ILE:HG12	1:A:658:PRO:HD2	1.42	0.99
1:A:485:HIS:HD2	1:A:650:PRO:HG2	1.25	0.98
1:A:217:GLN:HB3	1:A:330:ALA:HB1	1.48	0.96
1:A:521:GLN:CB	1:A:522:PRO:HD3	1.96	0.95
1:A:628:ILE:CB	1:A:628:ILE:CD1	2.45	0.94
1:A:592:LEU:O	1:A:593:GLN:C	2.06	0.94
1:A:59:SER:HA	1:A:74:LYS:HG3	1.50	0.93
1:A:160:ASP:HB2	1:A:195:TYR:CE2	2.05	0.91
1:A:243:ILE:HD13	1:A:258:ILE:HG23	1.52	0.91
1:A:614:ASP:CG	1:A:617:ILE:CB	2.43	0.90
1:A:396:PRO:HB3	1:A:593:GLN:CG	2.00	0.90
1:A:276:ARG:HB3	1:A:282:TYR:CE2	2.05	0.90
1:A:331:MET:HB3	1:A:341:GLN:NE2	1.86	0.90
1:A:359:PHE:HB2	1:A:411:VAL:HG23	1.51	0.90
1:A:264:GLU:OE2	1:A:267:ARG:NE	2.05	0.88
1:A:535:PHE:CD2	1:A:537:ASN:HB3	2.08	0.88
1:A:359:PHE:CB	1:A:411:VAL:HG23	2.03	0.87
1:A:272:SER:HB2	1:A:275:GLU:OE1	1.74	0.87
1:A:559:GLU:HG3	1:A:562:ARG:HH21	1.40	0.87
1:A:614:ASP:OD1	1:A:617:ILE:N	2.08	0.87
1:A:300:GLY:O	1:A:303:SER:OG	1.93	0.86
1:A:395:GLU:HG2	1:A:408:HIS:CD2	2.11	0.86
1:A:285:LEU:CD2	1:A:298:LEU:HG	2.06	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:HG13	1:A:195:TYR:HD1	1.41	0.85
1:A:396:PRO:CB	1:A:593:GLN:HG2	2.06	0.85
1:A:516:LEU:HD11	1:A:558:TYR:HB2	1.58	0.84
1:A:569:GLY:HA3	1:A:578:MET:HE2	1.56	0.84
1:A:343:SER:HA	1:A:346:LYS:CG	2.06	0.84
1:A:239:PHE:CZ	1:A:430:PHE:HZ	1.95	0.84
1:A:224:ALA:CB	1:A:280:ILE:HG23	2.08	0.84
1:A:139:MET:HA	1:A:142:ILE:HG13	1.59	0.84
1:A:89:GLU:HB3	1:A:153:PRO:CG	2.07	0.83
1:A:657:ILE:CG1	1:A:658:PRO:HD2	2.08	0.83
1:A:39:PRO:HG3	1:A:48:GLU:HB2	1.59	0.82
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.13	0.82
1:A:268:VAL:HA	1:A:277:ASN:ND2	1.94	0.82
1:A:103:PHE:CE2	1:A:669:ASP:HB3	2.14	0.82
1:A:398:ILE:HD12	1:A:399:LEU:H	1.45	0.82
1:A:351:ILE:CD1	1:A:426:TYR:HB2	2.10	0.81
1:A:217:GLN:HB3	1:A:330:ALA:CB	2.11	0.81
1:A:211:LEU:HD11	1:A:255:GLY:CA	2.05	0.80
1:A:304:PHE:CE1	1:A:352:LEU:HD23	2.17	0.79
1:A:217:GLN:HB2	1:A:333:ILE:HD11	1.62	0.79
1:A:329:GLN:O	1:A:333:ILE:HG23	1.83	0.79
1:A:334:VAL:HG11	1:A:437:ILE:HD13	1.64	0.79
1:A:89:GLU:HB3	1:A:153:PRO:HG3	1.63	0.79
1:A:182:GLY:HA2	1:A:233:ASN:HD22	1.46	0.79
1:A:140:VAL:HG13	1:A:195:TYR:CD1	2.17	0.78
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.17	0.78
1:A:279:HIS:HE1	5:A:1002:HOH:O	1.49	0.78
1:A:243:ILE:HD13	1:A:258:ILE:HG12	1.64	0.78
1:A:278:TYR:HB2	1:A:281:PHE:CD2	2.19	0.78
1:A:643:ALA:O	1:A:646:GLU:HG2	1.83	0.78
1:A:99:GLU:N	1:A:100:PRO:HD2	1.99	0.77
1:A:177:ILE:HG23	1:A:653:VAL:CG2	2.14	0.77
1:A:337:SER:O	1:A:341:GLN:HB2	1.84	0.77
1:A:405:VAL:HG23	1:A:405:VAL:O	1.83	0.77
1:A:91:MET:HE3	1:A:102:VAL:CG1	2.14	0.77
1:A:593:GLN:O	1:A:596:LEU:HB2	1.84	0.77
1:A:605:ASP:CG	1:A:608:VAL:HG23	2.10	0.76
1:A:673:LEU:O	1:A:677:ARG:HB2	1.85	0.76
1:A:63:LYS:HG3	1:A:69:ASP:OD2	1.86	0.76
1:A:614:ASP:OD1	1:A:617:ILE:CB	2.34	0.76
1:A:268:VAL:CA	1:A:277:ASN:HD21	1.97	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:TYR:CE2	1:A:48:GLU:HB3	2.20	0.75
1:A:37:TYR:CZ	1:A:48:GLU:HB3	2.20	0.75
1:A:63:LYS:HA	1:A:69:ASP:OD2	1.86	0.75
1:A:17:VAL:HG23	1:A:114:LEU:HD12	1.69	0.75
1:A:347:ILE:CG1	1:A:429:LEU:HD22	2.16	0.75
1:A:64:THR:HB	1:A:68:GLN:C	2.12	0.74
1:A:153:PRO:HG2	5:A:1040:HOH:O	1.87	0.74
1:A:467:GLU:O	1:A:471:ILE:HD13	1.88	0.74
1:A:589:LYS:HG3	1:A:591:PRO:HD3	1.70	0.74
1:A:81:ASN:ND2	1:A:94:LEU:HB3	2.03	0.74
1:A:121:LEU:HD23	1:A:121:LEU:N	2.02	0.74
1:A:551:PHE:HB2	1:A:558:TYR:CD2	2.23	0.74
1:A:485:HIS:CD2	1:A:650:PRO:HG2	2.16	0.74
1:A:389:LEU:HG	1:A:393:LEU:HD22	1.70	0.73
1:A:160:ASP:HB2	1:A:195:TYR:HE2	1.52	0.73
1:A:354:LEU:HD23	1:A:422:VAL:HG23	1.70	0.72
1:A:59:SER:CA	1:A:74:LYS:HG3	2.19	0.72
1:A:73:LYS:HG3	1:A:76:ASP:H	1.53	0.72
1:A:474:THR:HG22	1:A:638:LEU:HD13	1.71	0.72
1:A:561:PRO:HG3	1:A:567:GLU:C	2.14	0.72
1:A:398:ILE:CD1	1:A:399:LEU:H	2.02	0.71
1:A:91:MET:HG3	1:A:94:LEU:HD11	1.71	0.71
1:A:172:ASN:HB3	1:A:648:THR:HG22	1.70	0.71
1:A:343:SER:HB2	1:A:607:VAL:HG21	1.70	0.71
1:A:580:GLU:HB3	5:A:1011:HOH:O	1.88	0.71
1:A:120:GLY:O	1:A:148:ARG:NH2	2.22	0.71
1:A:605:ASP:HB3	1:A:608:VAL:HG23	1.69	0.71
1:A:605:ASP:OD1	1:A:608:VAL:HG23	1.90	0.71
1:A:528:LEU:HD11	1:A:550:HIS:ND1	2.06	0.71
1:A:283:GLN:HE21	1:A:324:PHE:HA	1.56	0.71
1:A:453:LEU:HD23	1:A:478:LEU:HD13	1.73	0.70
1:A:517:ILE:O	1:A:526:LEU:HD12	1.92	0.70
1:A:539:THR:N	1:A:542:THR:OG1	2.25	0.70
1:A:343:SER:CB	1:A:607:VAL:HG21	2.22	0.70
1:A:238:ARG:NH1	1:A:264:GLU:OE2	2.23	0.69
1:A:385:ASN:ND2	1:A:386:PRO:HD2	2.07	0.69
1:A:643:ALA:HB2	5:A:1015:HOH:O	1.93	0.69
1:A:453:LEU:HD21	1:A:455:ILE:HD13	1.74	0.69
1:A:342:MET:O	1:A:346:LYS:HG2	1.92	0.69
1:A:15:LEU:HD21	1:A:134:ILE:CG2	2.23	0.69
1:A:344:ILE:HD13	1:A:433:LEU:HD21	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ASP:CB	1:A:608:VAL:HG23	2.22	0.68
1:A:160:ASP:HB2	1:A:195:TYR:CZ	2.28	0.68
1:A:259:GLN:O	1:A:259:GLN:HG3	1.91	0.68
1:A:440:VAL:HG12	1:A:441:LEU:HD12	1.74	0.68
1:A:91:MET:HE3	1:A:102:VAL:HG13	1.76	0.68
1:A:105:ASN:O	1:A:109:ARG:HG3	1.94	0.68
1:A:73:LYS:HD2	1:A:75:ASP:N	2.09	0.68
1:A:347:ILE:HD11	1:A:429:LEU:CD2	2.24	0.68
1:A:629:THR:O	1:A:632:ALA:HB3	1.94	0.68
1:A:234:ASN:ND2	5:A:1079:HOH:O	2.27	0.68
1:A:394:MET:C	1:A:396:PRO:HD3	2.19	0.68
1:A:516:LEU:HD23	1:A:516:LEU:O	1.94	0.68
1:A:663:LEU:HD13	1:A:666:LYS:HD3	1.75	0.68
1:A:144:LYS:HE3	1:A:164:ARG:HH22	1.59	0.67
1:A:224:ALA:HB1	1:A:280:ILE:CG2	2.15	0.67
1:A:655:CYS:O	1:A:656:ILE:HG12	1.93	0.67
1:A:262:LEU:HD21	1:A:634:TYR:CE2	2.30	0.67
1:A:263:LEU:HD11	1:A:278:TYR:OH	1.94	0.67
1:A:17:VAL:HG23	1:A:114:LEU:CD1	2.25	0.67
1:A:217:GLN:OE1	1:A:329:GLN:NE2	2.28	0.67
1:A:337:SER:OG	1:A:340:GLU:N	2.25	0.67
1:A:593:GLN:HA	1:A:593:GLN:OE1	1.94	0.67
1:A:435:LYS:HG3	1:A:436:LYS:H	1.58	0.67
1:A:229:LYS:O	1:A:275:GLU:HG2	1.95	0.67
1:A:243:ILE:HD13	1:A:258:ILE:CG2	2.25	0.67
1:A:192:VAL:HG12	1:A:193:ILE:N	2.10	0.67
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.67
1:A:561:PRO:HB2	1:A:564:SER:HB3	1.76	0.67
1:A:664:PRO:O	1:A:666:LYS:N	2.25	0.66
1:A:146:ARG:NH1	1:A:150:GLU:OE1	2.28	0.66
1:A:233:ASN:OD1	1:A:235:ASN:N	2.25	0.66
1:A:163:TYR:CD2	1:A:199:VAL:HG21	2.31	0.66
1:A:534:VAL:HG13	5:A:1043:HOH:O	1.94	0.66
1:A:636:GLU:O	1:A:638:LEU:N	2.29	0.66
1:A:226:GLY:HA3	1:A:239:PHE:CD2	2.30	0.66
1:A:227:ASN:OD1	1:A:237:SER:HA	1.94	0.66
1:A:347:ILE:HG12	1:A:429:LEU:HD22	1.77	0.65
1:A:531:GLU:O	1:A:534:VAL:N	2.28	0.65
1:A:476:GLU:O	1:A:514:ILE:HD11	1.96	0.65
1:A:10:ASP:O	1:A:14:TYR:N	2.27	0.65
1:A:149:ASN:N	1:A:149:ASN:OD1	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:GLN:NE2	1:A:538:ALA:HB1	2.11	0.65
1:A:262:LEU:CD2	1:A:634:TYR:CD2	2.80	0.65
1:A:72:VAL:HG22	1:A:73:LYS:O	1.98	0.64
1:A:405:VAL:O	1:A:405:VAL:CG2	2.45	0.64
1:A:683:GLU:O	1:A:685:ILE:N	2.31	0.64
1:A:178:THR:O	1:A:655:CYS:HB2	1.96	0.64
1:A:227:ASN:HA	1:A:236:SER:O	1.98	0.64
1:A:239:PHE:CE1	1:A:430:PHE:HZ	2.14	0.64
1:A:257:SER:HB2	1:A:438:ASN:ND2	2.12	0.64
1:A:269:VAL:CG2	1:A:423:LYS:HD3	2.28	0.64
1:A:245:ILE:O	1:A:449:PHE:HA	1.97	0.64
1:A:262:LEU:HD21	1:A:634:TYR:CZ	2.33	0.64
1:A:138:GLU:O	1:A:142:ILE:HG12	1.98	0.63
1:A:210:VAL:HG12	1:A:211:LEU:N	2.05	0.63
1:A:221:ILE:HD12	1:A:334:VAL:HG21	1.78	0.63
1:A:245:ILE:HG22	1:A:253:ILE:CD1	2.29	0.63
1:A:516:LEU:CD2	1:A:525:ILE:HG13	2.28	0.63
1:A:243:ILE:CD1	1:A:258:ILE:HG23	2.28	0.63
1:A:245:ILE:HG22	1:A:253:ILE:HD12	1.80	0.63
1:A:262:LEU:HD21	1:A:634:TYR:CD2	2.33	0.63
1:A:396:PRO:CB	1:A:593:GLN:CG	2.70	0.63
1:A:49:CYS:SG	1:A:80:ARG:HD2	2.39	0.63
1:A:269:VAL:HG21	1:A:423:LYS:HD3	1.81	0.63
1:A:475:ASN:H	1:A:475:ASN:HD22	1.46	0.63
1:A:226:GLY:HA3	1:A:239:PHE:HE2	1.63	0.63
1:A:279:HIS:ND1	5:A:1002:HOH:O	2.17	0.63
1:A:73:LYS:HD2	1:A:75:ASP:H	1.63	0.63
1:A:291:GLU:O	1:A:294:LYS:HB3	1.99	0.63
1:A:109:ARG:NH2	5:A:1040:HOH:O	2.25	0.63
1:A:582:GLN:HG2	1:A:583:ASP:OD1	1.99	0.63
1:A:296:LEU:HB3	1:A:298:LEU:HD22	1.81	0.62
1:A:400:ALA:HB2	1:A:405:VAL:HG11	1.80	0.62
1:A:52:ILE:HD12	1:A:60:PHE:HD2	1.64	0.62
1:A:219:ASN:N	1:A:220:PRO:HD2	2.14	0.62
1:A:641:LEU:HG	1:A:645:LEU:HD22	1.80	0.62
1:A:592:LEU:HD12	1:A:593:GLN:N	2.14	0.62
1:A:357:ILE:HB	1:A:418:ARG:HH21	1.65	0.62
1:A:464:ASN:HB2	1:A:580:GLU:OE1	2.00	0.62
1:A:146:ARG:HB2	1:A:151:VAL:CG1	2.29	0.62
1:A:160:ASP:HB2	1:A:195:TYR:OH	2.00	0.62
1:A:592:LEU:HD12	1:A:592:LEU:C	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HD2	1:A:75:ASP:HB2	1.82	0.62
1:A:453:LEU:HD21	1:A:455:ILE:CD1	2.29	0.62
1:A:528:LEU:HD21	1:A:550:HIS:CE1	2.35	0.62
1:A:347:ILE:HD11	1:A:429:LEU:HD22	1.81	0.62
1:A:384:VAL:HG11	1:A:600:PHE:CE2	2.35	0.62
1:A:241:LYS:HE2	1:A:454:ASP:OD1	2.00	0.62
1:A:543:LEU:O	1:A:543:LEU:HD12	2.00	0.62
1:A:559:GLU:HG3	1:A:562:ARG:NH2	2.15	0.61
1:A:103:PHE:HE2	1:A:669:ASP:HB3	1.61	0.61
1:A:351:ILE:HD11	1:A:426:TYR:HB2	1.82	0.61
1:A:15:LEU:HD21	1:A:134:ILE:HG21	1.81	0.61
1:A:81:ASN:HD21	1:A:94:LEU:HB3	1.64	0.61
1:A:239:PHE:CE2	1:A:430:PHE:HZ	2.18	0.61
1:A:289:THR:OG1	1:A:292:GLU:HG2	2.00	0.61
1:A:163:TYR:CE2	1:A:199:VAL:HG23	2.35	0.61
1:A:354:LEU:C	1:A:418:ARG:HE	2.07	0.61
1:A:146:ARG:HB2	1:A:151:VAL:HG11	1.81	0.61
1:A:178:THR:HG21	1:A:654:ARG:NH1	2.15	0.61
1:A:453:LEU:HD23	1:A:478:LEU:CD1	2.30	0.61
1:A:605:ASP:HB3	1:A:608:VAL:CG2	2.31	0.61
1:A:217:GLN:HG3	1:A:333:ILE:CD1	2.31	0.61
1:A:247:PHE:CE2	1:A:253:ILE:HG12	2.35	0.61
1:A:304:PHE:CD1	1:A:352:LEU:HD23	2.35	0.61
1:A:58:ASP:OD1	1:A:58:ASP:C	2.43	0.61
1:A:277:ASN:OD1	1:A:281:PHE:CE2	2.53	0.61
1:A:458:PHE:N	1:A:475:ASN:OD1	2.34	0.61
1:A:79:GLN:HG2	5:A:1059:HOH:O	2.00	0.61
1:A:338:GLN:O	1:A:342:MET:HB2	2.00	0.61
1:A:657:ILE:O	1:A:675:GLN:NE2	2.34	0.60
1:A:398:ILE:HD12	1:A:399:LEU:N	2.14	0.60
1:A:638:LEU:HG	1:A:639:ALA:N	1.93	0.60
1:A:217:GLN:CB	1:A:333:ILE:HD11	2.32	0.60
1:A:516:LEU:HD23	1:A:525:ILE:HG13	1.84	0.60
1:A:248:ASN:OD1	1:A:250:ALA:HB3	2.01	0.60
1:A:38:ASN:ND2	1:A:46:SER:O	2.34	0.60
1:A:435:LYS:HG3	1:A:436:LYS:N	2.17	0.60
1:A:569:GLY:CA	1:A:578:MET:HE2	2.28	0.60
1:A:73:LYS:HD2	1:A:75:ASP:CB	2.32	0.60
1:A:359:PHE:CZ	1:A:414:SER:HB3	2.37	0.60
1:A:418:ARG:NH1	1:A:418:ARG:HG2	2.15	0.60
1:A:600:PHE:C	1:A:602:ASP:H	2.10	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:PHE:O	1:A:434:VAL:HG23	2.02	0.60
1:A:480:GLN:O	1:A:484:HIS:N	2.34	0.60
1:A:639:ALA:O	5:A:1015:HOH:O	2.16	0.60
1:A:324:PHE:HE2	1:A:328:ARG:HH21	1.50	0.60
1:A:627:PHE:N	1:A:627:PHE:CD1	2.70	0.60
1:A:243:ILE:CD1	1:A:258:ILE:HG12	2.30	0.59
1:A:288:ALA:HB3	1:A:293:LYS:HG3	1.84	0.59
1:A:330:ALA:O	1:A:334:VAL:HG23	2.02	0.59
1:A:344:ILE:O	1:A:348:ILE:HG12	2.02	0.59
1:A:115:ILE:HG13	1:A:116:TYR:N	2.16	0.59
1:A:347:ILE:CD1	1:A:429:LEU:HD22	2.32	0.59
1:A:307:LEU:O	5:A:1047:HOH:O	2.16	0.59
1:A:11:TYR:CE1	1:A:16:LYS:HD3	2.37	0.59
1:A:221:ILE:CD1	1:A:334:VAL:HG21	2.32	0.59
1:A:248:ASN:HD21	1:A:252:PHE:HB2	1.68	0.59
1:A:276:ARG:NH1	1:A:320:ASP:OD1	2.25	0.59
1:A:573:TYR:C	1:A:575:GLY:H	2.10	0.59
1:A:239:PHE:CE2	1:A:430:PHE:CZ	2.90	0.59
1:A:334:VAL:HG11	1:A:437:ILE:CD1	2.33	0.59
1:A:359:PHE:HB3	1:A:411:VAL:HG23	1.83	0.59
1:A:139:MET:O	1:A:142:ILE:HB	2.02	0.59
1:A:636:GLU:C	1:A:638:LEU:N	2.60	0.59
1:A:520:ARG:NH1	1:A:521:GLN:HA	2.17	0.59
1:A:535:PHE:CD1	1:A:535:PHE:N	2.71	0.59
1:A:257:SER:HA	1:A:438:ASN:ND2	2.17	0.59
1:A:511:GLN:O	1:A:515:ASP:N	2.28	0.59
1:A:529:LEU:HD12	1:A:529:LEU:O	2.03	0.59
1:A:210:VAL:O	1:A:214:GLN:HG2	2.03	0.59
1:A:532:GLN:HE22	1:A:542:THR:HB	1.68	0.59
1:A:248:ASN:C	1:A:447:ALA:HB3	2.27	0.58
1:A:39:PRO:CG	1:A:48:GLU:HB2	2.33	0.58
1:A:99:GLU:N	1:A:100:PRO:CD	2.66	0.58
1:A:222:LEU:N	1:A:222:LEU:HD12	2.16	0.58
1:A:636:GLU:C	1:A:638:LEU:H	2.09	0.58
1:A:224:ALA:O	1:A:280:ILE:HG13	2.03	0.58
1:A:243:ILE:HB	1:A:452:VAL:HG22	1.85	0.58
1:A:278:TYR:HB2	1:A:281:PHE:CE2	2.38	0.58
1:A:106:LEU:HD12	5:A:1073:HOH:O	2.03	0.58
1:A:217:GLN:OE1	1:A:330:ALA:HB2	2.04	0.58
1:A:474:THR:HG21	1:A:634:TYR:OH	2.02	0.58
1:A:580:GLU:O	5:A:1038:HOH:O	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:CD2	1:A:634:TYR:CG	2.87	0.58
1:A:304:PHE:O	1:A:308:ASN:ND2	2.36	0.58
1:A:217:GLN:HG3	1:A:333:ILE:HD11	1.86	0.58
1:A:369:LEU:HD13	1:A:394:MET:CE	2.34	0.58
1:A:467:GLU:H	1:A:467:GLU:CD	2.08	0.58
1:A:398:ILE:CG1	1:A:399:LEU:H	2.16	0.57
1:A:410:ASN:OD1	1:A:413:LYS:N	2.35	0.57
1:A:509:ASP:OD2	1:A:511:GLN:HG3	2.05	0.57
1:A:628:ILE:CD1	1:A:628:ILE:HA	2.34	0.57
1:A:179:GLY:O	1:A:185:LYS:HE3	2.05	0.57
1:A:233:ASN:ND2	4:A:998:ADP:H5'1	2.19	0.57
1:A:296:LEU:CB	1:A:298:LEU:HD22	2.34	0.57
1:A:382:PHE:CZ	1:A:425:LEU:HD21	2.39	0.57
1:A:258:ILE:N	1:A:438:ASN:HD21	2.01	0.57
1:A:343:SER:CA	1:A:346:LYS:HG3	2.26	0.57
1:A:627:PHE:N	1:A:627:PHE:HD1	2.03	0.57
1:A:453:LEU:CD2	1:A:478:LEU:HD13	2.34	0.57
1:A:509:ASP:OD2	1:A:511:GLN:CG	2.52	0.57
1:A:629:THR:O	1:A:633:GLN:HG3	2.03	0.57
1:A:262:LEU:HD21	1:A:634:TYR:CE1	2.40	0.57
1:A:343:SER:O	1:A:347:ILE:N	2.32	0.57
1:A:535:PHE:N	1:A:535:PHE:HD1	2.03	0.57
1:A:596:LEU:O	1:A:599:CYS:HB3	2.04	0.57
1:A:239:PHE:CZ	1:A:430:PHE:CZ	2.86	0.56
1:A:262:LEU:HD21	1:A:634:TYR:CG	2.39	0.56
1:A:337:SER:HG	1:A:340:GLU:H	1.48	0.56
1:A:122:PHE:HB2	1:A:652:PHE:O	2.04	0.56
1:A:146:ARG:CB	1:A:151:VAL:HG11	2.34	0.56
1:A:453:LEU:CD2	1:A:455:ILE:HD13	2.35	0.56
1:A:516:LEU:HD23	1:A:516:LEU:C	2.30	0.56
1:A:640:SER:O	1:A:643:ALA:N	2.38	0.56
1:A:119:SER:HB3	1:A:685:ILE:HD11	1.87	0.56
1:A:237:SER:O	1:A:456:SER:OG	2.22	0.56
1:A:586:GLU:OE2	1:A:589:LYS:HD2	2.05	0.56
1:A:629:THR:OG1	1:A:632:ALA:HB2	2.05	0.56
1:A:339:GLU:OE2	1:A:342:MET:HE3	2.06	0.56
1:A:40:ASP:OD2	1:A:41:PRO:HD2	2.06	0.56
1:A:360:GLU:C	1:A:362:GLY:H	2.12	0.56
1:A:10:ASP:O	1:A:13:LYS:HB3	2.05	0.56
1:A:455:ILE:HB	5:A:1081:HOH:O	2.06	0.55
1:A:576:GLN:CD	1:A:576:GLN:H	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLY:O	1:A:88:VAL:C	2.49	0.55
1:A:146:ARG:NH1	1:A:150:GLU:OE2	2.39	0.55
1:A:146:ARG:CB	1:A:151:VAL:CG1	2.83	0.55
1:A:535:PHE:CD2	1:A:537:ASN:CB	2.87	0.55
1:A:655:CYS:C	1:A:656:ILE:HG12	2.31	0.55
1:A:103:PHE:CZ	1:A:669:ASP:HA	2.41	0.55
1:A:128:PRO:O	1:A:129:PHE:HB2	2.07	0.55
1:A:155:ILE:O	1:A:158:ILE:HG22	2.05	0.55
1:A:349:ALA:O	1:A:352:LEU:HB2	2.07	0.55
1:A:603:SER:C	1:A:605:ASP:H	2.13	0.55
1:A:58:ASP:C	1:A:74:LYS:HD2	2.30	0.55
1:A:91:MET:O	1:A:94:LEU:HG	2.06	0.55
1:A:247:PHE:CZ	1:A:253:ILE:HD11	2.42	0.55
1:A:561:PRO:HG2	1:A:567:GLU:O	2.03	0.55
1:A:12:HIS:HA	1:A:16:LYS:HG3	1.88	0.55
1:A:579:TYR:HA	1:A:580:GLU:OE1	2.06	0.55
1:A:263:LEU:O	1:A:265:LYS:HG2	2.07	0.55
1:A:82:PRO:O	1:A:85:PHE:HB2	2.07	0.55
1:A:108:VAL:HG12	1:A:109:ARG:N	2.22	0.55
1:A:176:LEU:HD12	1:A:453:LEU:HB3	1.89	0.55
1:A:267:ARG:O	1:A:277:ASN:ND2	2.40	0.55
1:A:409:LEU:HB3	1:A:413:LYS:HB2	1.88	0.55
1:A:118:TYR:CD1	1:A:148:ARG:NH1	2.75	0.55
1:A:144:LYS:CE	1:A:164:ARG:HH22	2.20	0.55
1:A:659:ASN:HB2	1:A:668:GLU:CD	2.32	0.55
1:A:73:LYS:HG3	1:A:73:LYS:O	1.97	0.54
1:A:187:GLU:OE2	1:A:191:LYS:NZ	2.36	0.54
1:A:432:TRP:O	1:A:436:LYS:HB2	2.06	0.54
1:A:225:PHE:CD2	1:A:280:ILE:HG12	2.41	0.54
1:A:354:LEU:HD23	1:A:422:VAL:CG2	2.36	0.54
1:A:521:GLN:CB	1:A:522:PRO:HD2	2.33	0.54
1:A:109:ARG:HD3	1:A:117:THR:OG1	2.07	0.54
1:A:548:HIS:NE2	1:A:561:PRO:HD2	2.22	0.54
1:A:580:GLU:OE1	1:A:580:GLU:N	2.40	0.54
1:A:4:ILE:HG22	1:A:5:HIS:ND1	2.23	0.54
1:A:471:ILE:N	1:A:471:ILE:CD1	2.70	0.54
1:A:233:ASN:HD21	4:A:998:ADP:H5'2	1.72	0.54
1:A:258:ILE:H	1:A:438:ASN:HD21	1.56	0.54
1:A:6:ASP:C	1:A:8:THR:H	2.14	0.54
1:A:163:TYR:HD2	1:A:199:VAL:HG21	1.69	0.54
1:A:225:PHE:CE2	1:A:280:ILE:HG21	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD12	1:A:324:PHE:CZ	2.43	0.54
1:A:304:PHE:C	1:A:308:ASN:ND2	2.66	0.54
1:A:674:ASP:HA	1:A:677:ARG:HH12	1.72	0.54
1:A:233:ASN:OD1	1:A:234:ASN:N	2.40	0.54
1:A:349:ALA:O	1:A:352:LEU:N	2.41	0.54
1:A:457:GLY:HA2	1:A:475:ASN:OD1	2.08	0.54
1:A:29:VAL:HG12	1:A:29:VAL:O	2.08	0.53
1:A:638:LEU:CG	1:A:639:ALA:N	2.65	0.53
1:A:4:ILE:HG22	1:A:5:HIS:CE1	2.43	0.53
1:A:163:TYR:CD2	1:A:164:ARG:NH1	2.75	0.53
1:A:257:SER:CA	1:A:438:ASN:ND2	2.72	0.53
1:A:581:ILE:O	1:A:582:GLN:C	2.48	0.53
1:A:154:HIS:ND1	1:A:155:ILE:N	2.56	0.53
1:A:166:MET:CE	1:A:167:LEU:HD23	2.38	0.53
1:A:177:ILE:HG23	1:A:653:VAL:HG22	1.88	0.53
1:A:614:ASP:OD1	1:A:616:ASN:OD1	2.26	0.53
1:A:195:TYR:O	1:A:199:VAL:HG13	2.08	0.53
1:A:382:PHE:CZ	1:A:425:LEU:CD2	2.92	0.53
1:A:421:LEU:HB2	1:A:596:LEU:HD13	1.89	0.53
1:A:517:ILE:HG22	1:A:526:LEU:CD1	2.38	0.53
1:A:10:ASP:HA	1:A:13:LYS:HB3	1.89	0.53
1:A:12:HIS:HA	1:A:16:LYS:CG	2.39	0.53
1:A:86:ASP:OD1	1:A:104:HIS:CE1	2.62	0.53
1:A:513:THR:OG1	1:A:557:LYS:HG3	2.09	0.53
1:A:529:LEU:HD12	1:A:529:LEU:C	2.34	0.53
1:A:233:ASN:HD21	4:A:998:ADP:C5'	2.22	0.53
1:A:283:GLN:HE21	1:A:324:PHE:CA	2.21	0.53
1:A:314:ASP:O	5:A:1078:HOH:O	2.18	0.53
1:A:568:PHE:HZ	1:A:584:TRP:CH2	2.27	0.53
1:A:474:THR:CG2	1:A:638:LEU:HD13	2.36	0.53
1:A:538:ALA:C	1:A:539:THR:HG23	2.34	0.53
1:A:569:GLY:HA3	1:A:578:MET:CE	2.33	0.53
1:A:248:ASN:ND2	1:A:252:PHE:HB2	2.24	0.53
1:A:13:LYS:HG2	1:A:14:TYR:CE1	2.44	0.53
1:A:474:THR:O	1:A:477:LYS:N	2.32	0.52
1:A:561:PRO:CD	1:A:567:GLU:O	2.56	0.52
1:A:174:SER:OG	1:A:650:PRO:HA	2.09	0.52
1:A:171:GLN:HE21	1:A:173:GLN:HE22	1.57	0.52
1:A:269:VAL:HG12	1:A:306:TYR:CE2	2.44	0.52
1:A:339:GLU:OE1	1:A:339:GLU:O	2.27	0.52
1:A:461:PHE:HB2	1:A:463:VAL:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:C	1:A:333:ILE:HD12	2.34	0.52
1:A:396:PRO:HB3	1:A:593:GLN:HG3	1.87	0.52
1:A:526:LEU:O	1:A:529:LEU:HB3	2.09	0.52
1:A:11:TYR:CD2	1:A:15:LEU:HD12	2.44	0.52
1:A:238:ARG:HH11	1:A:264:GLU:CD	2.17	0.52
1:A:347:ILE:HD11	1:A:429:LEU:HD23	1.90	0.52
1:A:163:TYR:OH	1:A:251:GLY:O	2.27	0.52
1:A:276:ARG:HB3	1:A:282:TYR:CZ	2.45	0.52
1:A:368:VAL:HG23	1:A:369:LEU:N	2.25	0.52
1:A:385:ASN:CG	1:A:386:PRO:HD2	2.35	0.52
1:A:467:GLU:OE1	1:A:467:GLU:N	2.27	0.52
1:A:663:LEU:CD1	1:A:666:LYS:HD3	2.40	0.52
1:A:174:SER:HA	1:A:451:GLY:O	2.10	0.52
1:A:228:ALA:HA	1:A:279:HIS:CE1	2.45	0.52
1:A:304:PHE:HD2	1:A:356:ASN:HD21	1.57	0.51
1:A:304:PHE:HD2	1:A:356:ASN:ND2	2.08	0.51
1:A:326:ILE:O	1:A:329:GLN:NE2	2.44	0.51
1:A:351:ILE:HD13	1:A:426:TYR:HB2	1.91	0.51
1:A:674:ASP:HA	1:A:677:ARG:NH1	2.24	0.51
1:A:54:SER:OG	1:A:55:GLU:N	2.44	0.51
1:A:146:ARG:NH1	1:A:150:GLU:CD	2.69	0.51
1:A:10:ASP:O	1:A:13:LYS:N	2.44	0.51
1:A:90:ASP:HA	1:A:118:TYR:O	2.10	0.51
1:A:267:ARG:HA	1:A:270:PHE:O	2.11	0.51
1:A:400:ALA:CB	1:A:405:VAL:HG11	2.41	0.51
1:A:429:LEU:O	1:A:432:TRP:HB3	2.11	0.51
1:A:113:ASP:OD1	1:A:130:LYS:NZ	2.36	0.51
1:A:368:VAL:CG2	1:A:369:LEU:N	2.73	0.51
1:A:12:HIS:O	1:A:16:LYS:HB2	2.10	0.51
1:A:268:VAL:HG13	1:A:281:PHE:CZ	2.46	0.51
1:A:306:TYR:CZ	1:A:355:GLY:HA3	2.45	0.51
1:A:144:LYS:CE	1:A:164:ARG:NH2	2.74	0.51
1:A:640:SER:O	1:A:643:ALA:HB3	2.10	0.51
1:A:641:LEU:O	1:A:645:LEU:N	2.35	0.51
1:A:177:ILE:HG23	1:A:653:VAL:HG21	1.90	0.51
1:A:539:THR:H	1:A:542:THR:HG1	1.57	0.50
1:A:58:ASP:OD1	1:A:59:SER:HB3	2.10	0.50
1:A:236:SER:O	1:A:238:ARG:HG2	2.12	0.50
1:A:347:ILE:HD12	1:A:347:ILE:C	2.36	0.50
1:A:525:ILE:HD13	1:A:568:PHE:CE1	2.46	0.50
1:A:218:ALA:C	1:A:220:PRO:HD2	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG13	1:A:72:VAL:O	2.11	0.50
1:A:163:TYR:CD2	1:A:199:VAL:CG2	2.95	0.50
1:A:222:LEU:HB3	1:A:239:PHE:HZ	1.75	0.50
1:A:654:ARG:NH2	1:A:679:ASN:O	2.43	0.50
1:A:98:ASN:OD1	1:A:100:PRO:HG2	2.12	0.50
1:A:104:HIS:O	1:A:107:ARG:HB3	2.11	0.50
1:A:109:ARG:NH2	1:A:114:LEU:HD13	2.26	0.50
1:A:177:ILE:HD13	1:A:653:VAL:HG22	1.93	0.50
1:A:628:ILE:CD1	1:A:628:ILE:CA	2.89	0.50
1:A:177:ILE:HD13	1:A:653:VAL:CG2	2.42	0.50
1:A:28:THR:O	1:A:30:SER:N	2.45	0.50
1:A:17:VAL:HG12	1:A:17:VAL:O	2.11	0.50
1:A:171:GLN:NE2	5:A:1055:HOH:O	2.44	0.50
1:A:233:ASN:ND2	4:A:998:ADP:C5'	2.75	0.50
1:A:474:THR:HG22	1:A:638:LEU:CD1	2.40	0.50
1:A:29:VAL:O	1:A:29:VAL:CG1	2.60	0.49
1:A:330:ALA:HA	1:A:333:ILE:HG13	1.94	0.49
1:A:509:ASP:C	1:A:511:GLN:H	2.20	0.49
1:A:36:TRP:CD1	1:A:80:ARG:HA	2.47	0.49
1:A:359:PHE:CE1	1:A:414:SER:HB3	2.47	0.49
1:A:440:VAL:C	1:A:442:CYS:N	2.71	0.49
1:A:378:ALA:O	1:A:382:PHE:HB2	2.12	0.49
1:A:36:TRP:NE1	1:A:80:ARG:HA	2.27	0.49
1:A:357:ILE:HB	1:A:418:ARG:NH2	2.26	0.49
1:A:418:ARG:CG	1:A:418:ARG:HH11	2.25	0.49
1:A:39:PRO:HD2	1:A:46:SER:O	2.13	0.49
1:A:633:GLN:O	1:A:636:GLU:N	2.45	0.49
1:A:259:GLN:HG3	1:A:261:TYR:CE2	2.48	0.49
1:A:375:LEU:HD12	1:A:389:LEU:HD23	1.95	0.49
1:A:7:ARG:O	1:A:7:ARG:HG3	2.12	0.49
1:A:482:PHE:CD1	1:A:482:PHE:C	2.89	0.49
1:A:74:LYS:O	1:A:76:ASP:N	2.46	0.49
1:A:162:ALA:HB2	1:A:651:HIS:CD2	2.47	0.49
1:A:180:GLU:HG3	1:A:181:SER:N	2.27	0.49
1:A:230:THR:C	1:A:232:ARG:H	2.21	0.49
1:A:223:GLU:O	1:A:227:ASN:HB2	2.13	0.49
1:A:398:ILE:CG1	1:A:399:LEU:N	2.75	0.49
1:A:540:ASP:O	1:A:543:LEU:HB3	2.12	0.49
1:A:140:VAL:O	1:A:143:PHE:N	2.42	0.48
1:A:612:PHE:C	1:A:618:ALA:CB	2.86	0.48
1:A:136:THR:HG22	1:A:137:GLN:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ILE:HG22	1:A:438:ASN:N	2.26	0.48
1:A:247:PHE:CE2	1:A:253:ILE:CD1	2.96	0.48
1:A:163:TYR:CE2	1:A:199:VAL:CG2	2.96	0.48
1:A:173:GLN:OE1	1:A:649:ASN:HB3	2.13	0.48
1:A:247:PHE:CE2	1:A:253:ILE:HD11	2.48	0.48
1:A:262:LEU:HD23	1:A:634:TYR:CG	2.48	0.48
1:A:33:ARG:C	1:A:34:TYR:CD2	2.92	0.48
1:A:91:MET:HB3	1:A:685:ILE:HD13	1.94	0.48
1:A:175:LEU:HD23	1:A:651:HIS:HB2	1.95	0.48
1:A:276:ARG:HA	1:A:282:TYR:OH	2.13	0.48
1:A:532:GLN:HE22	1:A:542:THR:CB	2.25	0.48
1:A:359:PHE:HB2	1:A:411:VAL:CG2	2.34	0.48
1:A:573:TYR:HD1	1:A:573:TYR:HA	1.59	0.48
1:A:418:ARG:HG2	1:A:418:ARG:HH11	1.78	0.48
1:A:565:LYS:HA	1:A:565:LYS:HD3	1.46	0.48
1:A:612:PHE:C	1:A:618:ALA:HB2	2.39	0.48
1:A:4:ILE:HG22	1:A:5:HIS:CG	2.48	0.48
1:A:168:ASP:O	1:A:169:ASP:HB3	2.13	0.48
1:A:395:GLU:HA	1:A:407:GLN:O	2.14	0.48
1:A:532:GLN:HE21	1:A:538:ALA:HB1	1.79	0.48
1:A:177:ILE:HA	1:A:653:VAL:HG22	1.96	0.47
1:A:471:ILE:HD13	1:A:471:ILE:H	1.79	0.47
1:A:660:ASN:OD1	1:A:671:VAL:HG11	2.14	0.47
1:A:72:VAL:HG22	1:A:73:LYS:N	2.29	0.47
1:A:81:ASN:OD1	1:A:96:TYR:HB2	2.15	0.47
1:A:269:VAL:HG12	1:A:306:TYR:OH	2.13	0.47
1:A:289:THR:N	1:A:292:GLU:HG3	2.28	0.47
1:A:518:ASP:O	1:A:519:GLY:C	2.57	0.47
1:A:681:VAL:HG12	1:A:681:VAL:O	2.13	0.47
1:A:532:GLN:NE2	1:A:542:THR:OG1	2.46	0.47
1:A:671:VAL:O	1:A:675:GLN:HG2	2.14	0.47
1:A:121:LEU:HD21	1:A:688:THR:HG23	1.95	0.47
1:A:156:PHE:O	1:A:159:SER:HB2	2.13	0.47
1:A:248:ASN:OD1	1:A:250:ALA:N	2.46	0.47
1:A:278:TYR:HB2	1:A:281:PHE:HD2	1.75	0.47
1:A:217:GLN:CG	1:A:333:ILE:HD11	2.45	0.47
1:A:421:LEU:HD11	1:A:600:PHE:CE1	2.50	0.47
1:A:15:LEU:CD2	1:A:134:ILE:HG21	2.44	0.47
1:A:37:TYR:O	1:A:47:TYR:HA	2.15	0.47
1:A:99:GLU:CG	1:A:673:LEU:HD22	2.45	0.47
1:A:84:LYS:HG2	1:A:85:PHE:N	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:HB3	1:A:241:LYS:HZ1	1.79	0.47
1:A:240:GLY:O	1:A:241:LYS:HB3	2.14	0.47
1:A:263:LEU:CD1	1:A:278:TYR:OH	2.62	0.47
1:A:440:VAL:C	1:A:442:CYS:H	2.23	0.47
1:A:274:THR:HG23	1:A:274:THR:O	2.15	0.47
1:A:410:ASN:OD1	1:A:412:GLU:HB3	2.15	0.47
1:A:538:ALA:O	1:A:539:THR:HG23	2.15	0.47
1:A:139:MET:O	1:A:143:PHE:HD1	1.98	0.47
1:A:535:PHE:O	1:A:538:ALA:HB3	2.15	0.47
1:A:122:PHE:HB3	1:A:652:PHE:HB2	1.96	0.47
1:A:275:GLU:H	1:A:310:SER:HB2	1.79	0.47
1:A:341:GLN:HA	1:A:344:ILE:HG13	1.96	0.47
1:A:228:ALA:N	1:A:236:SER:O	2.47	0.46
1:A:359:PHE:CE1	1:A:414:SER:CB	2.98	0.46
1:A:160:ASP:OD2	1:A:195:TYR:OH	2.28	0.46
1:A:258:ILE:H	1:A:438:ASN:ND2	2.14	0.46
1:A:518:ASP:O	1:A:635:LYS:NZ	2.46	0.46
1:A:654:ARG:HA	1:A:654:ARG:HD2	1.83	0.46
1:A:138:GLU:OE1	1:A:142:ILE:HD11	2.15	0.46
1:A:657:ILE:HD13	1:A:657:ILE:HG21	1.55	0.46
1:A:13:LYS:HG2	1:A:14:TYR:CD1	2.49	0.46
1:A:18:LYS:HD3	1:A:18:LYS:HA	1.44	0.46
1:A:137:GLN:NE2	1:A:141:ASP:OD2	2.42	0.46
1:A:225:PHE:O	1:A:278:TYR:CE1	2.68	0.46
1:A:74:LYS:O	1:A:77:ALA:N	2.28	0.46
1:A:280:ILE:HD13	1:A:348:ILE:HD12	1.97	0.46
1:A:399:LEU:CD2	1:A:404:LEU:HD22	2.45	0.46
1:A:674:ASP:O	1:A:678:CYS:N	2.38	0.46
1:A:109:ARG:NH2	5:A:1058:HOH:O	2.49	0.46
1:A:119:SER:CB	1:A:685:ILE:HD11	2.45	0.46
1:A:146:ARG:HH12	1:A:150:GLU:CD	2.23	0.46
1:A:262:LEU:HD21	1:A:634:TYR:CD1	2.49	0.46
1:A:301:PRO:HA	1:A:307:LEU:HD12	1.97	0.46
1:A:139:MET:HA	1:A:142:ILE:CG1	2.40	0.46
1:A:144:LYS:HE2	1:A:164:ARG:NH2	2.30	0.46
1:A:311:GLY:N	5:A:1045:HOH:O	2.23	0.46
1:A:417:SER:C	1:A:419:ASP:N	2.73	0.46
1:A:669:ASP:OD1	1:A:669:ASP:N	2.45	0.46
1:A:259:GLN:O	1:A:261:TYR:CE2	2.68	0.46
1:A:230:THR:HA	1:A:275:GLU:HG2	1.98	0.46
1:A:557:LYS:HD3	1:A:557:LYS:HA	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ASN:O	1:A:610:LYS:HB2	2.16	0.46
1:A:106:LEU:O	1:A:110:TYR:HB2	2.16	0.46
1:A:247:PHE:HE2	1:A:253:ILE:HG12	1.81	0.46
1:A:330:ALA:O	1:A:334:VAL:N	2.45	0.46
1:A:643:ALA:HA	1:A:646:GLU:HG2	1.98	0.46
1:A:661:LYS:HB2	1:A:663:LEU:CD1	2.46	0.46
1:A:425:LEU:CD1	1:A:612:PHE:CE1	2.99	0.45
1:A:600:PHE:C	1:A:602:ASP:N	2.74	0.45
1:A:396:PRO:CG	1:A:593:GLN:HG2	2.46	0.45
1:A:438:ASN:O	1:A:439:ASN:C	2.56	0.45
1:A:257:SER:CA	1:A:438:ASN:HD21	2.29	0.45
1:A:283:GLN:NE2	1:A:324:PHE:HA	2.26	0.45
1:A:632:ALA:O	1:A:636:GLU:OE1	2.35	0.45
1:A:6:ASP:C	1:A:8:THR:N	2.75	0.45
1:A:292:GLU:HG2	1:A:292:GLU:H	1.55	0.45
1:A:462:LYS:HD2	1:A:462:LYS:HA	1.68	0.45
1:A:518:ASP:HB2	1:A:635:LYS:HE3	1.99	0.45
1:A:219:ASN:N	1:A:220:PRO:CD	2.79	0.45
1:A:257:SER:CB	1:A:438:ASN:ND2	2.78	0.45
1:A:485:HIS:ND1	1:A:485:HIS:C	2.75	0.45
1:A:544:ILE:CG2	1:A:545:THR:N	2.79	0.45
1:A:464:ASN:H	1:A:580:GLU:CD	2.25	0.45
1:A:526:LEU:HD22	1:A:631:ALA:HB1	1.98	0.45
1:A:64:THR:CG2	1:A:65:VAL:N	2.78	0.45
1:A:331:MET:HB3	1:A:341:GLN:HE21	1.72	0.45
1:A:641:LEU:O	1:A:644:THR:HB	2.17	0.45
1:A:36:TRP:NE1	1:A:80:ARG:HG3	2.32	0.45
1:A:517:ILE:HG22	1:A:526:LEU:HD12	1.98	0.45
1:A:163:TYR:CD1	1:A:163:TYR:C	2.92	0.45
1:A:177:ILE:HD13	1:A:653:VAL:CG1	2.47	0.45
1:A:280:ILE:HG13	1:A:280:ILE:H	1.69	0.44
1:A:606:ASN:HD22	1:A:606:ASN:HA	1.64	0.44
1:A:64:THR:HB	1:A:68:GLN:O	2.16	0.44
1:A:330:ALA:O	1:A:334:VAL:CG2	2.66	0.44
1:A:561:PRO:HD3	1:A:568:PHE:HA	1.99	0.44
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.80	0.44
1:A:265:LYS:O	1:A:268:VAL:HG23	2.18	0.44
1:A:539:THR:OG1	1:A:542:THR:HG23	2.16	0.44
1:A:11:TYR:O	1:A:16:LYS:HG2	2.18	0.44
1:A:247:PHE:CE2	1:A:253:ILE:CG1	3.00	0.44
1:A:471:ILE:HD13	1:A:471:ILE:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:HD22	1:A:585:LEU:HD11	2.00	0.44
1:A:272:SER:CB	1:A:275:GLU:OE1	2.56	0.44
1:A:299:ALA:O	1:A:300:GLY:C	2.59	0.44
1:A:304:PHE:CD2	1:A:356:ASN:ND2	2.83	0.44
1:A:388:VAL:HG12	1:A:599:CYS:SG	2.58	0.44
1:A:99:GLU:HB2	1:A:100:PRO:HD3	1.99	0.44
1:A:127:ASN:O	1:A:658:PRO:HG3	2.18	0.44
1:A:171:GLN:HE21	1:A:171:GLN:HB3	1.50	0.44
1:A:276:ARG:HG2	1:A:312:CYS:O	2.18	0.44
1:A:424:ALA:O	1:A:428:ARG:HG2	2.18	0.44
1:A:531:GLU:O	1:A:534:VAL:HA	2.17	0.44
1:A:543:LEU:HD12	1:A:543:LEU:C	2.42	0.44
3:A:999:ALF:F4	4:A:998:ADP:PB	2.65	0.44
1:A:4:ILE:CG2	1:A:5:HIS:CE1	3.00	0.44
1:A:107:ARG:O	1:A:111:ASN:N	2.47	0.44
1:A:157:ALA:O	1:A:160:ASP:N	2.51	0.44
1:A:268:VAL:HG13	1:A:281:PHE:HZ	1.82	0.44
1:A:381:VAL:HG22	1:A:381:VAL:O	2.17	0.44
1:A:394:MET:O	1:A:396:PRO:HD3	2.17	0.44
1:A:592:LEU:O	1:A:594:GLN:N	2.49	0.44
1:A:292:GLU:O	1:A:295:ALA:N	2.51	0.44
1:A:645:LEU:C	1:A:647:THR:H	2.25	0.44
1:A:72:VAL:CG2	1:A:73:LYS:N	2.80	0.44
1:A:91:MET:CG	1:A:94:LEU:HD11	2.44	0.44
1:A:634:TYR:O	1:A:638:LEU:HB3	2.17	0.44
1:A:666:LYS:NZ	1:A:668:GLU:OE2	2.42	0.44
1:A:509:ASP:O	1:A:511:GLN:N	2.51	0.43
1:A:179:GLY:O	1:A:185:LYS:CE	2.66	0.43
1:A:237:SER:C	1:A:239:PHE:H	2.26	0.43
1:A:355:GLY:HA2	1:A:418:ARG:NE	2.33	0.43
1:A:645:LEU:C	1:A:647:THR:N	2.76	0.43
1:A:200:ALA:HB1	1:A:251:GLY:O	2.18	0.43
1:A:535:PHE:C	1:A:537:ASN:H	2.25	0.43
1:A:91:MET:HG2	1:A:102:VAL:HG13	2.00	0.43
1:A:109:ARG:NH1	1:A:116:TYR:O	2.51	0.43
1:A:121:LEU:HD23	1:A:121:LEU:H	1.81	0.43
1:A:162:ALA:CB	1:A:651:HIS:NE2	2.81	0.43
1:A:348:ILE:HD12	1:A:348:ILE:HG23	1.56	0.43
1:A:154:HIS:CE1	1:A:155:ILE:HG22	2.54	0.43
1:A:160:ASP:O	1:A:163:TYR:HB3	2.19	0.43
1:A:210:VAL:CG1	1:A:211:LEU:H	2.05	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:GLN:OE1	1:A:546:LYS:HD3	2.17	0.43
1:A:679:ASN:HB2	1:A:681:VAL:HG23	2.01	0.43
1:A:174:SER:N	1:A:649:ASN:O	2.48	0.43
1:A:543:LEU:HD22	1:A:585:LEU:CD1	2.49	0.43
1:A:418:ARG:O	1:A:418:ARG:HD3	2.19	0.43
1:A:456:SER:HB2	5:A:1029:HOH:O	2.19	0.43
1:A:571:THR:HA	1:A:576:GLN:HA	1.99	0.43
1:A:127:ASN:HB3	1:A:658:PRO:HD3	2.01	0.43
1:A:127:ASN:HB2	1:A:183:ALA:O	2.18	0.43
1:A:270:PHE:C	1:A:271:GLN:NE2	2.77	0.43
1:A:138:GLU:OE1	1:A:142:ILE:HG12	2.19	0.43
1:A:163:TYR:CD1	1:A:163:TYR:O	2.72	0.43
1:A:219:ASN:C	1:A:221:ILE:H	2.27	0.43
1:A:226:GLY:O	1:A:238:ARG:HB2	2.19	0.43
1:A:375:LEU:O	1:A:379:SER:N	2.42	0.43
1:A:449:PHE:C	1:A:449:PHE:CD2	2.96	0.43
1:A:672:VAL:O	1:A:675:GLN:HG3	2.19	0.43
1:A:146:ARG:HA	1:A:146:ARG:HH11	1.84	0.42
1:A:657:ILE:HG12	1:A:658:PRO:CD	2.31	0.42
1:A:4:ILE:HD11	1:A:151:VAL:HG12	2.01	0.42
1:A:187:GLU:OE2	1:A:187:GLU:HA	2.18	0.42
1:A:359:PHE:CD1	1:A:414:SER:HB2	2.54	0.42
1:A:560:GLU:O	1:A:561:PRO:C	2.60	0.42
1:A:99:GLU:HG2	1:A:673:LEU:HD22	2.02	0.42
1:A:140:VAL:C	1:A:142:ILE:N	2.74	0.42
1:A:237:SER:HB3	1:A:241:LYS:NZ	2.33	0.42
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.67	0.42
1:A:58:ASP:OD1	1:A:59:SER:CB	2.67	0.42
1:A:115:ILE:HG13	1:A:116:TYR:H	1.83	0.42
1:A:132:ILE:HD13	1:A:132:ILE:HG21	1.82	0.42
1:A:163:TYR:CZ	1:A:200:ALA:HB2	2.54	0.42
1:A:171:GLN:NE2	1:A:173:GLN:HE22	2.17	0.42
1:A:256:ALA:O	1:A:441:LEU:HB3	2.19	0.42
1:A:299:ALA:O	1:A:300:GLY:O	2.38	0.42
1:A:400:ALA:HB2	1:A:405:VAL:CG1	2.47	0.42
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.83	0.42
1:A:469:LEU:O	1:A:473:TYR:HB2	2.19	0.42
1:A:517:ILE:HG22	1:A:526:LEU:HD11	2.01	0.42
1:A:146:ARG:CZ	1:A:150:GLU:OE2	2.68	0.42
1:A:153:PRO:HD2	5:A:1040:HOH:O	2.19	0.42
1:A:222:LEU:N	1:A:222:LEU:CD1	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:CG	1:A:281:PHE:CE2	2.98	0.42
1:A:289:THR:N	1:A:292:GLU:CG	2.82	0.42
1:A:551:PHE:C	1:A:554:LYS:HB2	2.45	0.42
1:A:132:ILE:HG22	1:A:134:ILE:HG12	2.01	0.42
1:A:482:PHE:HE1	1:A:486:MET:SD	2.43	0.42
1:A:98:ASN:C	1:A:100:PRO:HD2	2.44	0.42
1:A:103:PHE:CE1	1:A:672:VAL:HG11	2.55	0.42
1:A:138:GLU:OE1	1:A:142:ILE:CD1	2.67	0.42
1:A:219:ASN:C	1:A:221:ILE:N	2.78	0.42
1:A:531:GLU:O	1:A:534:VAL:HG22	2.19	0.42
1:A:330:ALA:O	1:A:333:ILE:HG13	2.20	0.41
1:A:354:LEU:HB3	1:A:422:VAL:CG2	2.50	0.41
1:A:247:PHE:N	1:A:448:TYR:O	2.53	0.41
1:A:302:GLU:H	1:A:302:GLU:HG2	1.51	0.41
1:A:354:LEU:O	1:A:357:ILE:HB	2.20	0.41
1:A:611:LEU:CD1	1:A:611:LEU:N	2.83	0.41
1:A:418:ARG:HG3	1:A:419:ASP:N	2.34	0.41
1:A:633:GLN:O	1:A:636:GLU:HB2	2.21	0.41
1:A:636:GLU:N	1:A:636:GLU:CD	2.78	0.41
1:A:185:LYS:O	1:A:189:THR:HB	2.21	0.41
1:A:258:ILE:HG22	1:A:259:GLN:N	2.35	0.41
1:A:562:ARG:HD3	1:A:562:ARG:HA	1.80	0.41
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.21	0.41
1:A:177:ILE:HD13	1:A:653:VAL:HG13	2.03	0.41
1:A:645:LEU:HD12	1:A:645:LEU:HA	1.74	0.41
1:A:253:ILE:HD12	1:A:253:ILE:HG23	1.69	0.41
1:A:385:ASN:HA	1:A:386:PRO:HD3	1.75	0.41
1:A:509:ASP:C	1:A:511:GLN:N	2.79	0.41
1:A:581:ILE:O	1:A:581:ILE:HG23	2.19	0.41
1:A:34:TYR:CD1	1:A:49:CYS:SG	3.14	0.41
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.56	0.41
1:A:64:THR:CG2	1:A:68:GLN:CB	2.98	0.41
1:A:102:VAL:O	1:A:106:LEU:HD22	2.21	0.41
1:A:262:LEU:CD2	1:A:634:TYR:CE2	2.99	0.41
1:A:270:PHE:C	1:A:270:PHE:CD1	2.96	0.41
1:A:458:PHE:CE1	1:A:574:ALA:HB3	2.56	0.41
1:A:146:ARG:HB2	1:A:151:VAL:HG13	2.01	0.41
1:A:167:LEU:HD21	1:A:251:GLY:HA3	2.03	0.41
1:A:239:PHE:CE1	1:A:430:PHE:CZ	3.01	0.41
1:A:540:ASP:O	1:A:543:LEU:N	2.54	0.41
1:A:304:PHE:HA	1:A:356:ASN:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD13	1:A:394:MET:HE2	2.03	0.40
1:A:551:PHE:HB2	1:A:558:TYR:CG	2.56	0.40
1:A:615:PRO:O	1:A:619:SER:CB	2.69	0.40
1:A:681:VAL:O	1:A:681:VAL:CG1	2.69	0.40
1:A:99:GLU:CG	1:A:673:LEU:CD2	2.99	0.40
1:A:284:LEU:O	1:A:288:ALA:HB2	2.21	0.40
1:A:289:THR:OG1	1:A:292:GLU:OE1	2.27	0.40
1:A:375:LEU:O	1:A:378:ALA:HB3	2.21	0.40
1:A:480:GLN:HA	1:A:483:ASN:HD22	1.85	0.40
1:A:548:HIS:CD2	1:A:558:TYR:OH	2.74	0.40
1:A:116:TYR:OH	1:A:188:ASN:ND2	2.54	0.40
1:A:585:LEU:C	1:A:587:LYS:N	2.79	0.40
1:A:10:ASP:HB3	1:A:14:TYR:CD2	2.56	0.40
1:A:146:ARG:N	1:A:146:ARG:HD2	2.36	0.40
1:A:166:MET:O	1:A:170:ARG:N	2.48	0.40
1:A:246:GLN:N	1:A:255:GLY:O	2.51	0.40
1:A:470:CYS:O	1:A:473:TYR:HB3	2.21	0.40

There are no symmetry-related clashes.

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	625/762 (82%)	510 (82%)	96 (15%)	19 (3%)	3 6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
1	A	669	ASP
1	A	86	ASP
1	A	300	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	362	GLY
1	A	510	SER
1	A	534	VAL
1	A	665	ALA
1	A	83	ILE
1	A	218	ALA
1	A	251	GLY
1	A	272	SER
1	A	363	ALA
1	A	637	GLN
1	A	157	ALA
1	A	231	THR
1	A	264	GLU
1	A	519	GLY
1	A	604	SER

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	530/665 (80%)	363 (68%)	167 (32%)	0 0

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	ASP
1	A	7	ARG
1	A	12	HIS
1	A	17	VAL
1	A	18	LYS
1	A	29	VAL
1	A	35	ILE
1	A	46	SER
1	A	52	ILE
1	A	54	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	GLU
1	A	59	SER
1	A	63	LYS
1	A	64	THR
1	A	69	ASP
1	A	73	LYS
1	A	76	ASP
1	A	78	ASN
1	A	83	ILE
1	A	84	LYS
1	A	91	MET
1	A	95	SER
1	A	106	LEU
1	A	119	SER
1	A	121	LEU
1	A	136	THR
1	A	137	GLN
1	A	138	GLU
1	A	139	MET
1	A	146	ARG
1	A	148	ARG
1	A	149	ASN
1	A	150	GLU
1	A	151	VAL
1	A	159	SER
1	A	165	SER
1	A	170	ARG
1	A	171	GLN
1	A	172	ASN
1	A	176	LEU
1	A	177	ILE
1	A	178	THR
1	A	189	THR
1	A	190	LYS
1	A	191	LYS
1	A	192	VAL
1	A	193	ILE
1	A	194	GLN
1	A	199	VAL
1	A	210	VAL
1	A	211	LEU
1	A	214	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	215	ILE
1	A	217	GLN
1	A	230	THR
1	A	237	SER
1	A	241	LYS
1	A	243	ILE
1	A	245	ILE
1	A	249	ASN
1	A	259	GLN
1	A	260	SER
1	A	262	LEU
1	A	263	LEU
1	A	265	LYS
1	A	266	SER
1	A	267	ARG
1	A	269	VAL
1	A	270	PHE
1	A	271	GLN
1	A	273	GLU
1	A	275	GLU
1	A	280	ILE
1	A	292	GLU
1	A	293	LYS
1	A	296	LEU
1	A	298	LEU
1	A	302	GLU
1	A	303	SER
1	A	314	ASP
1	A	323	GLU
1	A	326	ILE
1	A	329	GLN
1	A	333	ILE
1	A	334	VAL
1	A	339	GLU
1	A	340	GLU
1	A	342	MET
1	A	344	ILE
1	A	346	LYS
1	A	347	ILE
1	A	354	LEU
1	A	358	LYS
1	A	360	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	368	VAL
1	A	369	LEU
1	A	372	LYS
1	A	373	THR
1	A	375	LEU
1	A	382	PHE
1	A	387	SER
1	A	393	LEU
1	A	394	MET
1	A	397	ARG
1	A	398	ILE
1	A	404	LEU
1	A	416	SER
1	A	417	SER
1	A	418	ARG
1	A	422	VAL
1	A	425	LEU
1	A	431	LEU
1	A	434	VAL
1	A	436	LYS
1	A	439	ASN
1	A	440	VAL
1	A	452	VAL
1	A	455	ILE
1	A	456	SER
1	A	462	LYS
1	A	463	VAL
1	A	465	SER
1	A	471	ILE
1	A	474	THR
1	A	475	ASN
1	A	477	LYS
1	A	485	HIS
1	A	511	GLN
1	A	520	ARG
1	A	534	VAL
1	A	535	PHE
1	A	541	ASN
1	A	543	LEU
1	A	544	ILE
1	A	545	THR
1	A	546	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	553	LYS
1	A	554	LYS
1	A	555	ASN
1	A	557	LYS
1	A	565	LYS
1	A	573	TYR
1	A	581	ILE
1	A	585	LEU
1	A	592	LEU
1	A	593	GLN
1	A	595	ASP
1	A	601	LYS
1	A	602	ASP
1	A	606	ASN
1	A	608	VAL
1	A	616	ASN
1	A	627	PHE
1	A	633	GLN
1	A	636	GLU
1	A	637	GLN
1	A	638	LEU
1	A	641	LEU
1	A	645	LEU
1	A	653	VAL
1	A	656	ILE
1	A	657	ILE
1	A	663	LEU
1	A	666	LYS
1	A	669	ASP
1	A	671	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	A	71	GLN
1	A	104	HIS
1	A	171	GLN
1	A	172	ASN
1	A	188	ASN
1	A	194	GLN
1	A	214	GLN
1	A	246	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	271	GLN
1	A	277	ASN
1	A	279	HIS
1	A	283	GLN
1	A	329	GLN
1	A	338	GLN
1	A	341	GLN
1	A	376	ASN
1	A	385	ASN
1	A	408	HIS
1	A	438	ASN
1	A	439	ASN
1	A	485	HIS
1	A	541	ASN
1	A	548	HIS
1	A	606	ASN
1	A	616	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ALF	A	999	2,5,4	4,4,4	1.47	0	-		
4	ADP	A	998	2,3	28,29,29	0.91	0	43,45,45	0.87	2 (4%)

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	ADP	A	998	2,3	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	ADP	O3'-C3'-C2'	2.46	119.71	111.82
4	A	998	ADP	O2B-PB-O3A	2.24	112.16	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	998	ADP	C5'-O5'-PA-O1A
4	A	998	ADP	C5'-O5'-PA-O2A
4	A	998	ADP	C5'-O5'-PA-O3A
4	A	998	ADP	O4'-C4'-C5'-O5'
4	A	998	ADP	C3'-C4'-C5'-O5'

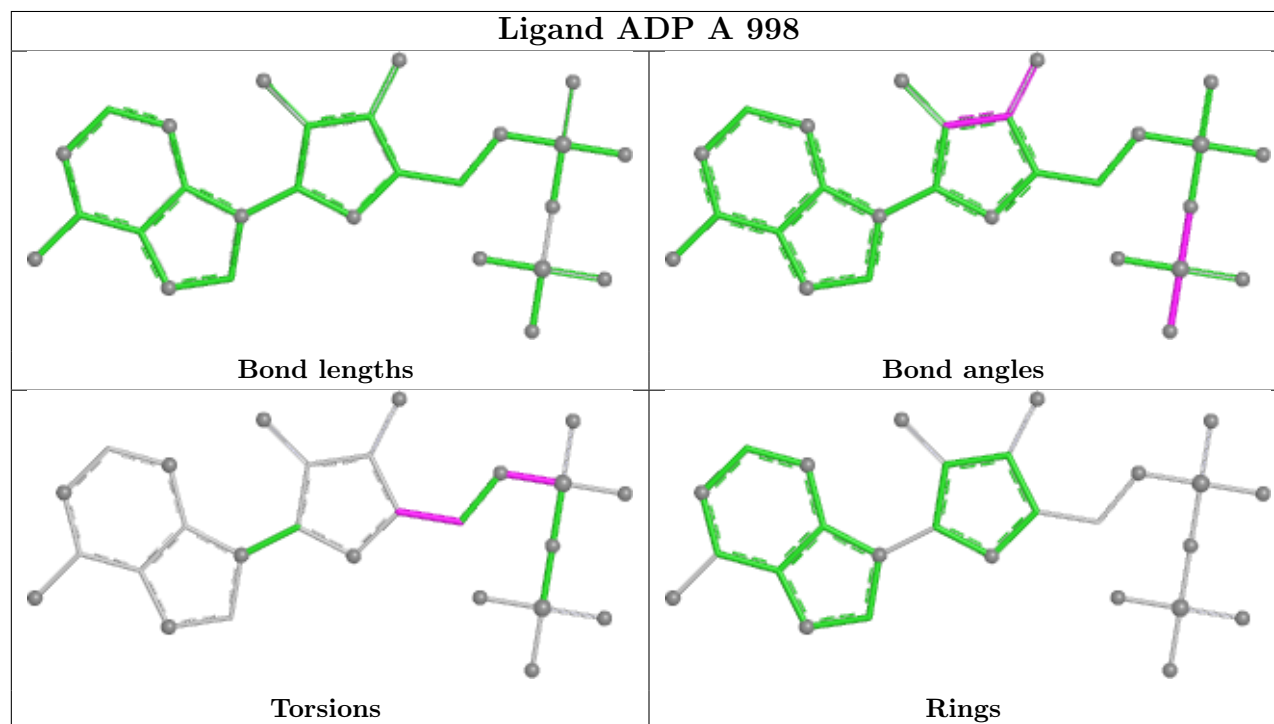
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ALF	1	0
4	A	998	ADP	5	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.