



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2023 – 02:46 AM EDT

PDB ID : 1MMA
Title : X-RAY STRUCTURES OF THE MGADP, MGATPGAMMAS, AND MGAMPPNP COMPLEXES OF THE DICTYOSTELIUM DISCOIDEUM MYOSIN MOTOR DOMAIN
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Rayment, I.
Deposited on : 1997-07-18
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

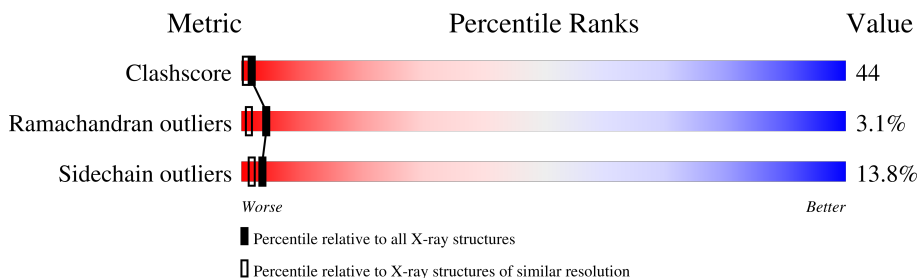
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	 42% 36% 15% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6139 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
			Total	C	N	O	S			
1	A	719	5687	3601	981	1089	16	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	SER	VAL	conflict	UNP P08799
A	312	CYS	TYR	conflict	UNP P08799
A	737	PHE	TYR	conflict	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

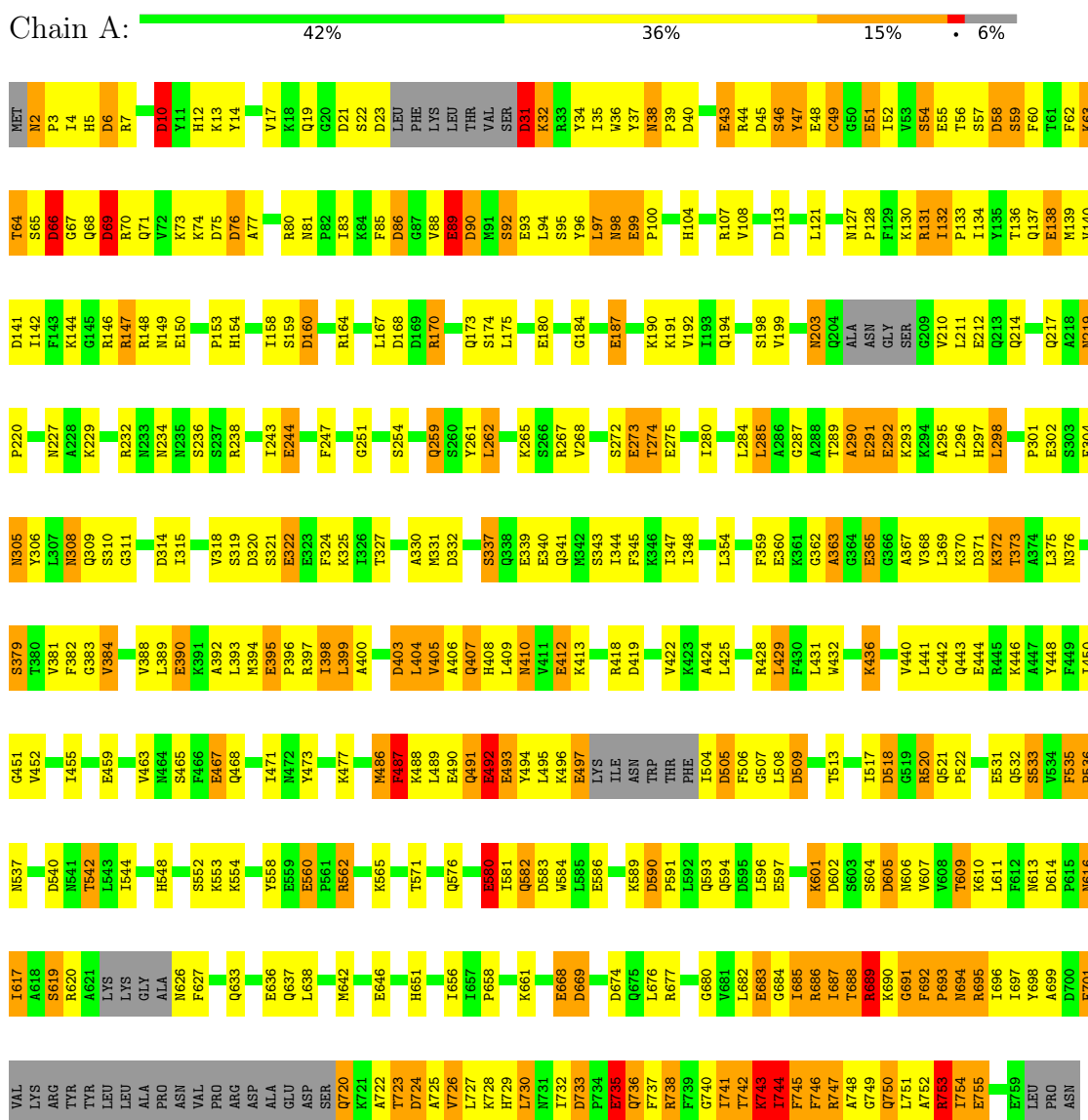
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

3 Residue-property plots i

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.60Å 179.00Å 53.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	96.2 (20.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6139	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: 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	1.13	42/5791 (0.7%)	1.50	85/7818 (1.1%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	695	ARG	C-O	-9.90	1.04	1.23
1	A	735	GLU	CD-OE2	9.05	1.35	1.25
1	A	755	GLU	CD-OE2	8.74	1.35	1.25
1	A	493	GLU	CD-OE2	8.45	1.34	1.25
1	A	668	GLU	CD-OE2	7.77	1.34	1.25
1	A	467	GLU	CD-OE2	7.60	1.34	1.25
1	A	365	GLU	CD-OE1	7.42	1.33	1.25
1	A	586	GLU	CD-OE1	7.38	1.33	1.25
1	A	459	GLU	CD-OE1	7.34	1.33	1.25
1	A	244	GLU	CD-OE1	7.33	1.33	1.25
1	A	412	GLU	CD-OE2	7.27	1.33	1.25
1	A	89	GLU	CD-OE2	7.09	1.33	1.25
1	A	43	GLU	CD-OE1	6.85	1.33	1.25
1	A	755	GLU	CD-OE1	-6.83	1.18	1.25
1	A	492	GLU	CD-OE2	6.78	1.33	1.25
1	A	187	GLU	CD-OE1	6.67	1.32	1.25
1	A	531	GLU	CD-OE2	6.65	1.32	1.25
1	A	302	GLU	CD-OE2	6.33	1.32	1.25
1	A	55	GLU	CD-OE1	6.28	1.32	1.25
1	A	273	GLU	CD-OE1	6.18	1.32	1.25
1	A	497	GLU	CD-OE1	6.11	1.32	1.25
1	A	138	GLU	CD-OE1	6.08	1.32	1.25
1	A	636	GLU	CD-OE1	6.00	1.32	1.25
1	A	322	GLU	CD-OE2	6.00	1.32	1.25
1	A	99	GLU	CD-OE2	5.99	1.32	1.25
1	A	291	GLU	CD-OE2	5.94	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	GLU	CD-OE2	5.93	1.32	1.25
1	A	275	GLU	CD-OE2	5.88	1.32	1.25
1	A	93	GLU	CD-OE1	5.87	1.32	1.25
1	A	395	GLU	CD-OE1	5.87	1.32	1.25
1	A	683	GLU	CD-OE2	5.85	1.32	1.25
1	A	580	GLU	CD-OE1	5.84	1.32	1.25
1	A	292	GLU	CD-OE1	5.76	1.31	1.25
1	A	180	GLU	CD-OE1	5.75	1.31	1.25
1	A	390	GLU	CD-OE1	5.75	1.31	1.25
1	A	646	GLU	CD-OE2	5.54	1.31	1.25
1	A	560	GLU	CD-OE2	5.28	1.31	1.25
1	A	51	GLU	CD-OE2	5.27	1.31	1.25
1	A	212	GLU	CD-OE1	5.27	1.31	1.25
1	A	339	GLU	CD-OE2	5.17	1.31	1.25
1	A	736	GLN	N-CA	-5.16	1.36	1.46
1	A	360	GLU	CD-OE1	5.02	1.31	1.25

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	A	107	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	747	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	753	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	518	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	75	ASP	CB-CG-OD2	8.60	126.04	118.30
1	A	31	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	A	745	PHE	CB-CA-C	8.06	126.52	110.40
1	A	267	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	238	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	160	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	113	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	A	509	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	A	742	THR	N-CA-CB	7.77	125.06	110.30
1	A	164	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	520	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	107	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	735	GLU	CG-CD-OE1	7.56	133.41	118.30
1	A	86	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	518	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	A	620	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	90	ASP	CB-CG-OD1	7.18	124.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	A	314	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	A	54	SER	N-CA-CB	6.92	120.88	110.50
1	A	444	GLU	N-CA-CB	6.88	122.99	110.60
1	A	669	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	267	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	10	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	113	ASP	CB-CG-OD2	6.76	124.39	118.30
1	A	147	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	10	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	66	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	A	562	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	738	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	605	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	23	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	86	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	A	674	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	A	332	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	76	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	23	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	419	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	148	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	509	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	58	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	168	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	58	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	A	590	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	45	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	A	669	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	403	ASP	CB-CG-OD1	-6.09	112.81	118.30
1	A	735	GLU	CG-CD-OE2	-6.09	106.13	118.30
1	A	689	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	733	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	44	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	6	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	571	THR	CA-CB-CG2	-5.99	104.01	112.40
1	A	419	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	583	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	170	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	590	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	76	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	80	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	CB-CA-C	-5.71	99.36	110.20
1	A	747	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	90	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	602	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	A	17	VAL	CB-CA-C	-5.55	100.86	111.40
1	A	132	ILE	CA-CB-CG1	-5.55	100.45	111.00
1	A	320	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	736	GLN	N-CA-CB	5.54	120.57	110.60
1	A	320	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	A	558	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	A	80	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	31	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	487	PHE	CB-CG-CD1	-5.39	117.03	120.80
1	A	254	SER	C-N-CA	-5.35	111.07	122.30
1	A	232	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	131	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	724	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	141	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	332	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	619	SER	CB-CA-C	-5.06	100.48	110.10
1	A	605	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5687	0	5544	498	0
2	A	1	0	0	0	0
3	A	27	0	12	6	0
4	A	424	0	0	22	0
All	All	6139	0	5556	499	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 44.

All (499) 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:730:LEU:HB3	1:A:732:ILE:HD11	1.19	1.14
1:A:397:ARG:HD2	1:A:404:LEU:HD21	1.29	1.13
1:A:98:ASN:HD22	1:A:100:PRO:HD2	1.10	1.08
1:A:736:GLN:O	1:A:747:ARG:HD2	1.57	1.04
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.35	1.03
1:A:362:GLY:HA3	1:A:368:VAL:HG11	1.42	1.01
1:A:736:GLN:CD	1:A:747:ARG:HD3	1.81	1.00
1:A:689:ARG:HH11	1:A:689:ARG:HB2	1.27	0.98
1:A:432:TRP:CZ2	1:A:436:LYS:HD2	1.99	0.98
1:A:744:ILE:HD11	1:A:746:PHE:HB2	1.45	0.96
1:A:34:TYR:CE1	1:A:51:GLU:HG2	2.01	0.94
1:A:98:ASN:HD22	1:A:100:PRO:CD	1.80	0.93
1:A:685:ILE:HG22	1:A:686:ARG:HD3	1.51	0.93
1:A:322:GLU:HA	1:A:325:LYS:HE2	1.50	0.92
1:A:695:ARG:HH21	1:A:748:ALA:HA	1.34	0.91
1:A:308:ASN:ND2	1:A:309:GLN:HG2	1.86	0.91
1:A:736:GLN:HB3	1:A:747:ARG:HG2	1.56	0.88
1:A:730:LEU:HB3	1:A:732:ILE:CD1	2.02	0.88
1:A:535:PHE:HE1	1:A:537:ASN:HB3	1.38	0.87
1:A:273:GLU:O	1:A:274:THR:HG23	1.76	0.86
1:A:504:ILE:HG23	1:A:506:PHE:CZ	2.11	0.86
1:A:695:ARG:O	1:A:745:PHE:HA	1.75	0.85
1:A:158:ILE:HD12	1:A:159:SER:N	1.92	0.85
1:A:687:ILE:HD13	1:A:691:GLY:H	1.41	0.84
1:A:701:PHE:HD1	1:A:701:PHE:H	1.25	0.84
1:A:686:ARG:HA	1:A:689:ARG:HD3	1.60	0.83
1:A:397:ARG:HD2	1:A:404:LEU:CD2	2.07	0.83
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.59	0.83
1:A:465:SER:H	1:A:468:GLN:HE21	1.23	0.82
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.10	0.82
1:A:744:ILE:HG13	1:A:745:PHE:N	1.94	0.82
1:A:34:TYR:HE1	1:A:51:GLU:HG2	1.44	0.81
1:A:432:TRP:CE2	1:A:436:LYS:HD2	2.16	0.80
1:A:98:ASN:ND2	1:A:100:PRO:HD2	1.93	0.79
1:A:695:ARG:NH2	1:A:748:ALA:HA	1.97	0.79
1:A:735:GLU:HA	1:A:735:GLU:OE1	1.83	0.78
1:A:548:HIS:CE1	1:A:560:GLU:HG3	2.19	0.77
1:A:99:GLU:HG3	1:A:686:ARG:NH2	2.00	0.77
1:A:504:ILE:HG23	1:A:506:PHE:CE1	2.20	0.77
1:A:95:SER:HA	1:A:695:ARG:NH2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:CD	1:A:404:LEU:HD21	2.12	0.77
1:A:63:LYS:HG2	1:A:67:GLY:HA2	1.68	0.76
1:A:467:GLU:O	1:A:471:ILE:HD12	1.85	0.76
1:A:147:ARG:HB2	1:A:149:ASN:OD1	1.85	0.76
1:A:32:LYS:NZ	1:A:51:GLU:HB3	2.01	0.75
1:A:372:LYS:CD	1:A:376:ASN:HD21	2.00	0.75
1:A:737:PHE:HB3	1:A:746:PHE:CE1	2.21	0.74
1:A:340:GLU:O	1:A:344:ILE:HG13	1.88	0.74
1:A:691:GLY:O	1:A:693:PRO:HD3	1.87	0.74
1:A:746:PHE:CD2	1:A:751:LEU:HD11	2.22	0.74
1:A:505:ASP:HB2	1:A:508:LEU:CG	2.18	0.74
1:A:582:GLN:N	1:A:582:GLN:OE1	2.20	0.73
1:A:580:GLU:HB2	1:A:582:GLN:HE22	1.53	0.73
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.15	0.72
1:A:746:PHE:CD2	1:A:751:LEU:HD21	2.25	0.72
1:A:372:LYS:HD2	1:A:376:ASN:HD21	1.54	0.72
1:A:133:PRO:HA	4:A:8275:HOH:O	1.91	0.71
1:A:397:ARG:HA	1:A:406:ALA:HA	1.72	0.71
1:A:505:ASP:HB2	1:A:508:LEU:HG	1.71	0.71
1:A:696:ILE:HA	1:A:744:ILE:CG1	2.20	0.71
1:A:487:PHE:HB2	1:A:506:PHE:CE2	2.25	0.71
1:A:287:GLY:HA3	1:A:324:PHE:CD2	2.26	0.71
1:A:138:GLU:O	1:A:142:ILE:HG13	1.90	0.70
1:A:593:GLN:O	1:A:596:LEU:HB2	1.91	0.70
1:A:81:ASN:ND2	1:A:94:LEU:HB3	2.06	0.70
1:A:362:GLY:HA3	1:A:368:VAL:CG1	2.19	0.70
1:A:368:VAL:HG23	1:A:370:LYS:HG3	1.72	0.70
1:A:701:PHE:CD1	1:A:701:PHE:N	2.60	0.70
1:A:81:ASN:HD21	1:A:94:LEU:HB3	1.57	0.70
1:A:368:VAL:HG21	1:A:370:LYS:HE2	1.73	0.70
1:A:382:PHE:HB2	1:A:384:VAL:HG22	1.74	0.70
1:A:203:ASN:N	1:A:203:ASN:OD1	2.24	0.69
1:A:147:ARG:HG3	1:A:150:GLU:CD	2.12	0.69
1:A:343:SER:O	1:A:347:ILE:HG13	1.92	0.69
1:A:99:GLU:HG2	1:A:682:LEU:CD1	2.21	0.69
1:A:508:LEU:N	1:A:508:LEU:HD23	2.07	0.69
1:A:131:ARG:NH1	4:A:8127:HOH:O	2.26	0.69
1:A:455:ILE:O	1:A:455:ILE:HG13	1.91	0.69
1:A:292:GLU:O	1:A:295:ALA:HB3	1.93	0.69
1:A:397:ARG:CB	1:A:404:LEU:HD21	2.23	0.69
1:A:273:GLU:C	1:A:274:THR:HG23	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PHE:CB	1:A:384:VAL:HG22	2.23	0.68
1:A:750:GLN:HE21	1:A:754:ILE:HG13	1.58	0.68
1:A:491:GLN:HE21	1:A:491:GLN:HA	1.59	0.68
1:A:695:ARG:O	1:A:745:PHE:CA	2.42	0.68
1:A:687:ILE:HD13	1:A:691:GLY:N	2.10	0.67
1:A:732:ILE:HD12	1:A:732:ILE:N	2.09	0.67
1:A:736:GLN:C	1:A:747:ARG:HD2	2.13	0.67
1:A:397:ARG:HB2	1:A:404:LEU:HD11	1.76	0.67
1:A:689:ARG:HB2	1:A:689:ARG:NH1	2.04	0.67
1:A:99:GLU:HG2	1:A:682:LEU:HD11	1.77	0.67
1:A:701:PHE:HE2	1:A:754:ILE:HG22	1.59	0.67
1:A:372:LYS:HG3	1:A:376:ASN:HD21	1.58	0.67
1:A:554:LYS:NZ	4:A:8105:HOH:O	2.28	0.67
1:A:746:PHE:CD1	1:A:747:ARG:N	2.60	0.67
1:A:127:ASN:HD21	3:A:999:ADP:C1'	2.08	0.67
1:A:308:ASN:HD22	1:A:309:GLN:N	1.93	0.66
1:A:327:THR:HG22	1:A:331:MET:CE	2.25	0.66
1:A:99:GLU:OE2	1:A:686:ARG:NH2	2.28	0.66
1:A:305:ASN:HA	1:A:308:ASN:OD1	1.95	0.66
1:A:581:ILE:N	1:A:582:GLN:OE1	2.28	0.66
1:A:696:ILE:CA	1:A:744:ILE:HG23	2.26	0.66
1:A:697:ILE:H	1:A:744:ILE:HG12	1.59	0.66
1:A:701:PHE:HD1	1:A:701:PHE:N	1.92	0.66
1:A:751:LEU:HD23	1:A:754:ILE:HG21	1.77	0.66
1:A:750:GLN:NE2	1:A:754:ILE:HG13	2.11	0.66
1:A:397:ARG:HB3	1:A:404:LEU:HD21	1.77	0.65
1:A:43:GLU:HB2	4:A:8300:HOH:O	1.96	0.65
1:A:693:PRO:CG	1:A:694:ASN:H	2.08	0.65
1:A:496:LYS:HG2	1:A:497:GLU:H	1.62	0.65
1:A:693:PRO:CD	1:A:694:ASN:H	2.10	0.65
1:A:308:ASN:HD22	1:A:309:GLN:HG2	1.61	0.65
1:A:35:ILE:O	1:A:49:CYS:HA	1.95	0.65
1:A:327:THR:HG22	1:A:331:MET:HE3	1.77	0.65
1:A:687:ILE:CD1	1:A:691:GLY:HA3	2.27	0.65
1:A:83:ILE:HD12	1:A:83:ILE:N	2.11	0.65
1:A:750:GLN:HB3	1:A:754:ILE:CD1	2.27	0.65
1:A:321:SER:OG	1:A:322:GLU:N	2.29	0.64
1:A:372:LYS:CG	1:A:376:ASN:HD21	2.10	0.64
1:A:365:GLU:OE1	1:A:365:GLU:HA	1.98	0.64
1:A:685:ILE:HG22	1:A:686:ARG:CD	2.26	0.64
1:A:319:SER:OG	1:A:322:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ALA:O	1:A:725:ALA:HB3	1.99	0.63
1:A:292:GLU:O	1:A:296:LEU:N	2.31	0.63
1:A:285:LEU:CD1	1:A:298:LEU:HD13	2.29	0.63
1:A:747:ARG:HA	1:A:747:ARG:NE	2.12	0.63
1:A:7:ARG:HH22	1:A:21:ASP:HB2	1.63	0.63
1:A:98:ASN:ND2	1:A:100:PRO:HG2	2.13	0.63
1:A:685:ILE:O	1:A:688:THR:N	2.33	0.62
1:A:37:TYR:OH	1:A:65:SER:N	2.33	0.62
1:A:696:ILE:HA	1:A:744:ILE:HG23	1.80	0.62
1:A:684:GLY:O	1:A:687:ILE:HG22	1.99	0.62
1:A:582:GLN:CD	1:A:582:GLN:H	2.01	0.61
1:A:685:ILE:HG22	1:A:686:ARG:N	2.15	0.61
1:A:83:ILE:HD12	1:A:83:ILE:H	1.65	0.61
1:A:477:LYS:NZ	4:A:8025:HOH:O	2.33	0.61
1:A:746:PHE:HB3	1:A:751:LEU:HD11	1.82	0.61
1:A:308:ASN:HD21	1:A:309:GLN:HG2	1.64	0.61
1:A:319:SER:HG	1:A:321:SER:HG	1.49	0.61
1:A:158:ILE:HD13	1:A:175:LEU:CD2	2.30	0.61
1:A:695:ARG:HH21	1:A:748:ALA:CA	2.10	0.61
1:A:686:ARG:O	1:A:689:ARG:NH1	2.34	0.60
1:A:736:GLN:HB3	1:A:747:ARG:CG	2.31	0.60
1:A:372:LYS:HG3	1:A:376:ASN:ND2	2.15	0.60
1:A:722:ALA:HA	1:A:725:ALA:HB2	1.84	0.60
1:A:89:GLU:HG3	4:A:8063:HOH:O	1.99	0.60
1:A:265:LYS:O	1:A:268:VAL:HG23	2.01	0.60
1:A:305:ASN:O	1:A:308:ASN:ND2	2.34	0.60
1:A:535:PHE:CE1	1:A:537:ASN:HB3	2.30	0.60
1:A:37:TYR:O	1:A:48:GLU:N	2.33	0.60
1:A:130:LYS:HE2	4:A:8044:HOH:O	2.01	0.60
1:A:680:GLY:HA2	4:A:8198:HOH:O	2.01	0.60
1:A:337:SER:O	1:A:341:GLN:HG3	2.02	0.60
1:A:372:LYS:HD2	1:A:376:ASN:ND2	2.16	0.60
1:A:720:GLN:OE1	1:A:742:THR:HA	2.01	0.60
1:A:2:ASN:O	1:A:6:ASP:N	2.35	0.59
1:A:158:ILE:HD13	1:A:175:LEU:HD23	1.83	0.59
1:A:35:ILE:HG22	1:A:36:TRP:N	2.18	0.59
1:A:132:ILE:HG22	1:A:134:ILE:HG23	1.85	0.59
1:A:210:VAL:O	1:A:214:GLN:HG3	2.03	0.59
1:A:399:LEU:HD23	1:A:400:ALA:N	2.18	0.59
1:A:344:ILE:HD11	1:A:432:TRP:HZ3	1.67	0.59
1:A:690:LYS:O	1:A:692:PHE:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLY:HA2	4:A:8221:HOH:O	2.01	0.59
1:A:412:GLU:HG2	1:A:413:LYS:N	2.18	0.59
1:A:687:ILE:O	1:A:689:ARG:N	2.36	0.59
1:A:63:LYS:CG	1:A:67:GLY:HA2	2.33	0.58
1:A:695:ARG:O	1:A:744:ILE:HG13	2.03	0.58
1:A:505:ASP:CG	1:A:508:LEU:HD11	2.24	0.58
1:A:737:PHE:HA	1:A:746:PHE:HD1	1.68	0.58
1:A:487:PHE:HB2	1:A:506:PHE:CD2	2.38	0.58
1:A:488:LYS:O	1:A:492:GLU:HG3	2.02	0.58
1:A:521:GLN:NE2	4:A:8333:HOH:O	2.23	0.58
1:A:747:ARG:O	1:A:751:LEU:HB2	2.03	0.58
1:A:532:GLN:HE22	1:A:542:THR:HB	1.69	0.58
1:A:290:ALA:N	4:A:8381:HOH:O	2.35	0.58
1:A:686:ARG:O	1:A:689:ARG:HB2	2.03	0.58
1:A:741:ILE:C	1:A:743:LYS:H	2.06	0.58
1:A:190:LYS:HB3	1:A:194:GLN:NE2	2.17	0.58
1:A:285:LEU:HD12	1:A:298:LEU:HD13	1.85	0.58
1:A:492:GLU:C	1:A:494:TYR:H	2.05	0.58
1:A:693:PRO:C	1:A:695:ARG:H	2.07	0.58
1:A:43:GLU:OE1	1:A:43:GLU:HA	2.03	0.58
1:A:362:GLY:CA	1:A:368:VAL:HG11	2.27	0.58
1:A:552:SER:O	1:A:553:LYS:HB2	2.04	0.57
1:A:494:TYR:O	1:A:496:LYS:N	2.37	0.57
1:A:601:LYS:HD2	1:A:613:ASN:HD21	1.69	0.57
1:A:32:LYS:HA	1:A:32:LYS:HE2	1.85	0.57
1:A:301:PRO:HA	1:A:304:PHE:HD2	1.70	0.57
1:A:732:ILE:HD12	1:A:732:ILE:H	1.70	0.57
1:A:308:ASN:HD22	1:A:308:ASN:C	2.08	0.57
1:A:741:ILE:O	1:A:743:LYS:HG3	2.05	0.57
1:A:32:LYS:HZ3	1:A:51:GLU:HB3	1.69	0.57
1:A:308:ASN:ND2	1:A:309:GLN:HE21	2.03	0.57
1:A:322:GLU:O	1:A:325:LYS:HB2	2.05	0.57
1:A:404:LEU:HD23	1:A:404:LEU:O	2.05	0.57
1:A:656:ILE:CD1	1:A:676:LEU:HD21	2.35	0.57
1:A:696:ILE:HA	1:A:744:ILE:HG12	1.86	0.56
1:A:392:ALA:HB1	1:A:596:LEU:HG	1.86	0.56
1:A:184:GLY:HA2	3:A:999:ADP:O1A	2.05	0.56
1:A:750:GLN:O	1:A:754:ILE:HB	2.05	0.56
1:A:2:ASN:OD1	1:A:5:HIS:ND1	2.38	0.56
1:A:98:ASN:HD22	1:A:100:PRO:CG	2.19	0.56
1:A:40:ASP:O	1:A:43:GLU:N	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:C	1:A:2:ASN:HD22	2.08	0.56
1:A:147:ARG:HG3	1:A:150:GLU:OE1	2.06	0.56
1:A:619:SER:CB	1:A:627:PHE:HE2	2.18	0.56
1:A:744:ILE:HD11	1:A:746:PHE:CB	2.28	0.56
1:A:150:GLU:HG2	4:A:8374:HOH:O	2.06	0.56
1:A:744:ILE:CG1	1:A:745:PHE:N	2.68	0.56
1:A:746:PHE:CG	1:A:751:LEU:HD11	2.41	0.56
1:A:147:ARG:NE	1:A:150:GLU:OE2	2.37	0.56
1:A:368:VAL:CG2	1:A:370:LYS:HE2	2.35	0.56
1:A:382:PHE:HB2	1:A:384:VAL:CG2	2.36	0.56
1:A:752:ALA:O	1:A:753:ARG:HG3	2.06	0.56
1:A:730:LEU:O	1:A:730:LEU:HD23	2.07	0.55
1:A:735:GLU:OE1	1:A:737:PHE:O	2.24	0.55
1:A:7:ARG:NH2	1:A:21:ASP:HB2	2.20	0.55
1:A:535:PHE:CG	1:A:536:PRO:HD2	2.42	0.55
1:A:687:ILE:O	1:A:691:GLY:N	2.39	0.55
1:A:619:SER:HB3	1:A:627:PHE:HE2	1.71	0.55
1:A:750:GLN:O	1:A:754:ILE:N	2.39	0.55
1:A:170:ARG:O	1:A:448:TYR:HE2	1.90	0.55
1:A:398:ILE:N	1:A:405:VAL:O	2.31	0.55
1:A:291:GLU:O	1:A:295:ALA:HB2	2.07	0.55
3:A:999:ADP:O3B	4:A:9951:HOH:O	2.18	0.55
1:A:397:ARG:HB3	1:A:404:LEU:CD2	2.37	0.54
1:A:746:PHE:CE2	1:A:751:LEU:HD21	2.42	0.54
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.37	0.54
1:A:174:SER:O	1:A:651:HIS:HD2	1.89	0.54
1:A:31:ASP:O	1:A:32:LYS:HG2	2.07	0.54
1:A:95:SER:CB	1:A:752:ALA:HB2	2.38	0.54
1:A:687:ILE:C	1:A:689:ARG:H	2.10	0.54
1:A:39:PRO:HD2	1:A:46:SER:O	2.07	0.54
1:A:375:LEU:HD12	1:A:375:LEU:O	2.08	0.54
1:A:693:PRO:CD	1:A:694:ASN:N	2.71	0.54
1:A:97:LEU:HG	1:A:685:ILE:HG23	1.88	0.54
1:A:173:GLN:HB2	1:A:450:ILE:HG12	1.90	0.54
1:A:605:ASP:O	1:A:609:THR:OG1	2.26	0.53
1:A:32:LYS:HZ1	1:A:51:GLU:HB3	1.70	0.53
1:A:99:GLU:CG	1:A:682:LEU:HD13	2.38	0.53
1:A:513:THR:O	1:A:517:ILE:HD12	2.07	0.53
1:A:81:ASN:OD1	1:A:95:SER:HB2	2.09	0.53
1:A:289:THR:O	1:A:291:GLU:N	2.42	0.53
1:A:390:GLU:HG2	1:A:394:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLU:HA	1:A:407:GLN:O	2.08	0.53
1:A:424:ALA:O	1:A:428:ARG:HG3	2.08	0.53
1:A:432:TRP:HE1	1:A:610:LYS:HZ1	1.55	0.53
1:A:284:LEU:HD13	1:A:345:PHE:CD1	2.44	0.53
1:A:696:ILE:HA	1:A:744:ILE:CG2	2.39	0.53
1:A:540:ASP:HB3	1:A:581:ILE:HD13	1.90	0.53
1:A:614:ASP:O	1:A:617:ILE:N	2.33	0.53
1:A:677:ARG:HG2	1:A:682:LEU:HD12	1.91	0.53
1:A:725:ALA:O	1:A:729:HIS:N	2.40	0.53
1:A:4:ILE:HD13	1:A:146:ARG:HH21	1.73	0.53
1:A:375:LEU:HD12	1:A:375:LEU:C	2.29	0.53
1:A:144:LYS:HE2	1:A:199:VAL:HG12	1.90	0.53
1:A:737:PHE:HA	1:A:746:PHE:CD1	2.44	0.53
1:A:35:ILE:HD11	1:A:52:ILE:HD11	1.92	0.52
1:A:311:GLY:N	4:A:8215:HOH:O	2.31	0.52
1:A:548:HIS:ND1	1:A:560:GLU:HG3	2.24	0.52
1:A:677:ARG:CG	1:A:682:LEU:HD12	2.39	0.52
1:A:158:ILE:HD12	1:A:158:ILE:C	2.28	0.52
1:A:344:ILE:O	1:A:348:ILE:HG12	2.09	0.52
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.08	0.52
1:A:362:GLY:H	1:A:368:VAL:HG13	1.73	0.52
1:A:60:PHE:O	1:A:71:GLN:HB2	2.08	0.52
1:A:720:GLN:O	1:A:723:THR:HG22	2.10	0.52
1:A:62:PHE:O	1:A:69:ASP:HB3	2.09	0.52
1:A:590:ASP:N	1:A:591:PRO:HD3	2.24	0.52
1:A:746:PHE:CG	1:A:747:ARG:N	2.76	0.52
1:A:47:TYR:CD1	1:A:47:TYR:N	2.78	0.52
1:A:619:SER:HG	1:A:627:PHE:HE2	1.53	0.52
1:A:38:ASN:N	1:A:38:ASN:OD1	2.42	0.52
1:A:95:SER:HA	1:A:695:ARG:HH22	1.71	0.52
1:A:229:LYS:HG3	1:A:234:ASN:HD22	1.74	0.52
1:A:158:ILE:CD1	1:A:175:LEU:CD2	2.88	0.52
1:A:227:ASN:HA	1:A:236:SER:O	2.10	0.52
1:A:736:GLN:CG	1:A:747:ARG:HD3	2.40	0.52
1:A:737:PHE:HB3	1:A:746:PHE:HE1	1.74	0.52
1:A:535:PHE:CD1	1:A:536:PRO:HD2	2.45	0.52
1:A:594:GLN:O	1:A:597:GLU:HB2	2.10	0.52
1:A:724:ASP:O	1:A:728:LYS:N	2.43	0.52
1:A:747:ARG:O	1:A:751:LEU:HD12	2.10	0.51
1:A:322:GLU:HA	1:A:325:LYS:CE	2.32	0.51
1:A:487:PHE:HB2	1:A:506:PHE:HE2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:O	1:A:492:GLU:HG3	2.09	0.51
1:A:601:LYS:HD3	1:A:613:ASN:ND2	2.25	0.51
1:A:83:ILE:H	1:A:83:ILE:CD1	2.22	0.51
1:A:99:GLU:HG2	1:A:682:LEU:HD13	1.93	0.51
1:A:359:PHE:HB3	1:A:367:ALA:HB1	1.93	0.51
1:A:580:GLU:HG3	1:A:582:GLN:CD	2.31	0.51
1:A:379:SER:HA	1:A:384:VAL:HG23	1.93	0.51
1:A:121:LEU:HD12	1:A:486:MET:HG3	1.92	0.51
1:A:633:GLN:O	1:A:637:GLN:HG3	2.11	0.51
1:A:127:ASN:O	1:A:658:PRO:HG3	2.10	0.51
1:A:219:ASN:N	1:A:220:PRO:HD2	2.25	0.50
1:A:160:ASP:OD1	4:A:8014:HOH:O	2.19	0.50
1:A:580:GLU:OE1	1:A:582:GLN:NE2	2.44	0.50
1:A:37:TYR:OH	1:A:65:SER:HB2	2.11	0.50
1:A:504:ILE:HG23	1:A:504:ILE:O	2.11	0.50
1:A:601:LYS:CD	1:A:613:ASN:ND2	2.75	0.50
1:A:532:GLN:O	1:A:535:PHE:HB3	2.12	0.50
1:A:432:TRP:HE1	1:A:610:LYS:NZ	2.09	0.50
1:A:686:ARG:HD3	1:A:686:ARG:N	2.26	0.50
1:A:98:ASN:ND2	1:A:100:PRO:CG	2.75	0.50
1:A:362:GLY:O	1:A:363:ALA:HB2	2.12	0.50
1:A:746:PHE:HD2	1:A:751:LEU:HD21	1.75	0.50
1:A:687:ILE:HD13	1:A:691:GLY:CA	2.41	0.49
1:A:289:THR:O	1:A:292:GLU:N	2.45	0.49
1:A:62:PHE:CD1	1:A:62:PHE:N	2.80	0.49
1:A:382:PHE:HB3	1:A:384:VAL:HG22	1.95	0.49
1:A:576:GLN:HB2	4:A:8164:HOH:O	2.13	0.49
1:A:691:GLY:C	1:A:693:PRO:HD3	2.32	0.49
1:A:755:GLU:O	1:A:755:GLU:HG3	2.11	0.49
1:A:210:VAL:HG23	1:A:211:LEU:N	2.27	0.49
1:A:211:LEU:HA	1:A:214:GLN:OE1	2.12	0.49
1:A:7:ARG:HA	1:A:12:HIS:CG	2.47	0.49
1:A:490:GLU:O	1:A:494:TYR:CD1	2.66	0.49
1:A:192:VAL:HG11	1:A:452:VAL:HG21	1.94	0.49
1:A:293:LYS:O	1:A:297:HIS:N	2.46	0.49
1:A:71:GLN:O	1:A:71:GLN:HG3	2.13	0.49
1:A:37:TYR:O	1:A:47:TYR:HA	2.13	0.48
1:A:243:ILE:O	1:A:451:GLY:HA2	2.12	0.48
1:A:399:LEU:HD23	1:A:400:ALA:H	1.78	0.48
1:A:289:THR:OG1	1:A:292:GLU:OE2	2.27	0.48
1:A:63:LYS:HD3	1:A:64:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ILE:HD13	1:A:691:GLY:HA3	1.94	0.48
1:A:274:THR:N	1:A:310:SER:O	2.36	0.48
1:A:285:LEU:HD11	1:A:298:LEU:HD13	1.96	0.48
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.96	0.48
1:A:2:ASN:HD21	1:A:4:ILE:HB	1.78	0.48
1:A:722:ALA:HA	1:A:725:ALA:CB	2.43	0.48
1:A:285:LEU:HD21	1:A:304:PHE:CD2	2.48	0.47
1:A:736:GLN:OE1	1:A:747:ARG:HD3	2.14	0.47
1:A:262:LEU:HA	4:A:8077:HOH:O	2.14	0.47
1:A:408:HIS:HD2	1:A:409:LEU:N	2.12	0.47
1:A:486:MET:HE3	1:A:486:MET:HB3	1.79	0.47
1:A:701:PHE:HE2	1:A:754:ILE:CG2	2.26	0.47
1:A:99:GLU:N	1:A:100:PRO:CD	2.77	0.47
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.14	0.47
1:A:532:GLN:HE22	1:A:542:THR:CB	2.27	0.47
1:A:582:GLN:HG2	4:A:8240:HOH:O	2.14	0.47
1:A:37:TYR:CZ	1:A:48:GLU:HB2	2.50	0.47
1:A:47:TYR:H	1:A:47:TYR:HD1	1.63	0.47
1:A:81:ASN:HA	1:A:96:TYR:HD2	1.79	0.47
1:A:85:PHE:O	1:A:88:VAL:HG13	2.14	0.47
1:A:97:LEU:HD12	1:A:685:ILE:HG21	1.96	0.47
1:A:509:ASP:N	1:A:509:ASP:OD1	2.48	0.47
1:A:285:LEU:O	1:A:293:LYS:HE2	2.15	0.47
1:A:90:ASP:OD1	1:A:92:SER:OG	2.25	0.47
1:A:321:SER:HG	1:A:322:GLU:H	1.62	0.47
1:A:505:ASP:HB2	1:A:508:LEU:CD1	2.44	0.47
1:A:10:ASP:OD2	1:A:14:TYR:HE2	1.97	0.47
1:A:327:THR:HG22	1:A:331:MET:HE2	1.96	0.46
1:A:743:LYS:C	1:A:744:ILE:HG22	2.34	0.46
1:A:616:ASN:HD22	1:A:616:ASN:N	2.13	0.46
1:A:187:GLU:HG2	3:A:999:ADP:O1A	2.15	0.46
1:A:605:ASP:OD1	1:A:607:VAL:N	2.44	0.46
1:A:686:ARG:HA	1:A:689:ARG:CD	2.40	0.46
1:A:410:ASN:ND2	4:A:8354:HOH:O	2.27	0.46
1:A:496:LYS:CG	1:A:497:GLU:H	2.28	0.46
1:A:746:PHE:CD2	1:A:751:LEU:CD1	2.96	0.46
1:A:473:TYR:OH	1:A:518:ASP:OD2	2.25	0.46
1:A:580:GLU:HB2	1:A:582:GLN:NE2	2.26	0.46
1:A:66:ASP:OD1	1:A:66:ASP:N	2.47	0.46
1:A:184:GLY:HA2	3:A:999:ADP:PA	2.55	0.46
1:A:272:SER:O	1:A:310:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:LEU:O	1:A:642:MET:HG2	2.15	0.46
1:A:701:PHE:CE2	1:A:754:ILE:CG2	2.99	0.46
1:A:687:ILE:C	1:A:689:ARG:N	2.69	0.46
1:A:74:LYS:O	1:A:77:ALA:HB3	2.16	0.46
1:A:737:PHE:CB	1:A:746:PHE:CE1	2.97	0.46
1:A:289:THR:C	1:A:291:GLU:N	2.69	0.45
1:A:371:ASP:OD2	1:A:373:THR:OG1	2.26	0.45
1:A:217:GLN:HE21	1:A:330:ALA:HA	1.81	0.45
1:A:741:ILE:O	1:A:741:ILE:HG22	2.15	0.45
1:A:142:ILE:O	1:A:142:ILE:HG22	2.16	0.45
1:A:533:SER:HB3	1:A:589:LYS:HD2	1.98	0.45
1:A:601:LYS:CD	1:A:613:ASN:HD21	2.30	0.45
1:A:726:VAL:CG1	1:A:727:LEU:N	2.79	0.45
1:A:35:ILE:CG2	1:A:36:TRP:N	2.80	0.45
1:A:140:VAL:HG11	1:A:198:SER:OG	2.16	0.45
1:A:219:ASN:N	1:A:220:PRO:CD	2.79	0.45
1:A:38:ASN:C	1:A:40:ASP:H	2.20	0.45
1:A:158:ILE:CD1	1:A:175:LEU:HD21	2.47	0.45
1:A:388:VAL:HG12	1:A:388:VAL:O	2.16	0.45
1:A:97:LEU:HD12	1:A:685:ILE:CG2	2.46	0.45
1:A:379:SER:O	1:A:383:GLY:N	2.48	0.45
1:A:369:LEU:HB2	1:A:394:MET:CE	2.47	0.45
1:A:137:GLN:NE2	1:A:140:VAL:HB	2.32	0.45
1:A:191:LYS:HD3	1:A:191:LYS:HA	1.74	0.45
1:A:693:PRO:HD2	1:A:694:ASN:H	1.82	0.45
1:A:491:GLN:O	1:A:494:TYR:HB2	2.16	0.45
1:A:306:TYR:OH	1:A:422:VAL:HG21	2.17	0.44
1:A:747:ARG:C	1:A:749:GLY:H	2.19	0.44
1:A:81:ASN:HA	1:A:96:TYR:CD2	2.52	0.44
1:A:273:GLU:C	1:A:274:THR:CG2	2.83	0.44
1:A:396:PRO:HD2	1:A:407:GLN:O	2.17	0.44
1:A:656:ILE:HD11	1:A:676:LEU:CD2	2.47	0.44
1:A:746:PHE:CD2	1:A:751:LEU:CD2	2.98	0.44
1:A:32:LYS:HD3	1:A:51:GLU:OE1	2.18	0.44
1:A:686:ARG:O	1:A:689:ARG:HD3	2.18	0.44
1:A:693:PRO:CG	1:A:694:ASN:N	2.79	0.44
1:A:697:ILE:O	1:A:699:ALA:N	2.50	0.44
1:A:747:ARG:HE	1:A:748:ALA:H	1.66	0.44
1:A:752:ALA:C	1:A:753:ARG:HG3	2.38	0.44
1:A:584:TRP:CD1	1:A:584:TRP:N	2.84	0.44
1:A:701:PHE:CE2	1:A:754:ILE:HG22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:GLN:CD	1:A:747:ARG:CD	2.70	0.44
1:A:368:VAL:CG2	1:A:370:LYS:HG3	2.43	0.44
1:A:491:GLN:HE21	1:A:491:GLN:CA	2.27	0.44
1:A:693:PRO:O	1:A:695:ARG:N	2.49	0.44
1:A:37:TYR:CE1	1:A:48:GLU:CB	3.01	0.43
1:A:687:ILE:CD1	1:A:691:GLY:CA	2.95	0.43
1:A:685:ILE:CG2	1:A:686:ARG:N	2.79	0.43
1:A:293:LYS:HA	1:A:298:LEU:HB2	2.01	0.43
1:A:565:LYS:NZ	4:A:8097:HOH:O	2.51	0.43
1:A:580:GLU:CG	1:A:582:GLN:NE2	2.81	0.43
1:A:273:GLU:O	1:A:274:THR:CG2	2.58	0.43
1:A:544:ILE:O	1:A:544:ILE:HG13	2.19	0.43
1:A:158:ILE:HD13	1:A:175:LEU:HD21	2.00	0.43
1:A:619:SER:OG	1:A:627:PHE:HE2	2.01	0.43
1:A:389:LEU:O	1:A:392:ALA:HB3	2.18	0.43
1:A:505:ASP:HB2	1:A:508:LEU:HD11	2.00	0.43
1:A:746:PHE:CD2	1:A:751:LEU:CG	3.01	0.43
1:A:98:ASN:ND2	1:A:100:PRO:CD	2.64	0.43
1:A:280:ILE:HD11	1:A:345:PHE:HE1	1.84	0.43
1:A:581:ILE:HD12	1:A:581:ILE:C	2.39	0.43
1:A:210:VAL:HG23	1:A:211:LEU:H	1.84	0.43
1:A:243:ILE:O	1:A:452:VAL:N	2.40	0.43
1:A:687:ILE:HD13	1:A:687:ILE:O	2.18	0.43
1:A:2:ASN:HD22	1:A:3:PRO:N	2.16	0.43
1:A:685:ILE:HG13	4:A:8197:HOH:O	2.18	0.43
1:A:732:ILE:CD1	1:A:732:ILE:H	2.32	0.43
1:A:746:PHE:CE2	1:A:751:LEU:CD2	3.01	0.42
1:A:354:LEU:O	1:A:418:ARG:NH1	2.50	0.42
1:A:685:ILE:O	1:A:688:THR:HB	2.19	0.42
1:A:158:ILE:CD1	1:A:175:LEU:HD23	2.47	0.42
1:A:308:ASN:ND2	1:A:308:ASN:C	2.72	0.42
1:A:315:ILE:O	1:A:318:VAL:HB	2.19	0.42
1:A:590:ASP:N	1:A:591:PRO:CD	2.82	0.42
1:A:736:GLN:O	1:A:747:ARG:HB2	2.19	0.42
1:A:35:ILE:CG1	1:A:52:ILE:HD11	2.50	0.42
1:A:136:THR:O	1:A:139:MET:N	2.52	0.42
1:A:732:ILE:CD1	1:A:732:ILE:N	2.78	0.42
1:A:121:LEU:CD1	1:A:486:MET:HG3	2.49	0.42
1:A:693:PRO:HG2	1:A:694:ASN:H	1.82	0.42
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.71	0.42
1:A:305:ASN:HA	1:A:308:ASN:CG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:O	1:A:71:GLN:HB3	2.19	0.42
1:A:97:LEU:HD13	1:A:97:LEU:HA	1.79	0.42
1:A:285:LEU:HD12	1:A:298:LEU:CD1	2.48	0.42
1:A:697:ILE:N	1:A:744:ILE:HG21	2.34	0.42
1:A:390:GLU:HG2	1:A:394:MET:CE	2.48	0.42
1:A:362:GLY:CA	1:A:368:VAL:CG1	2.95	0.41
1:A:746:PHE:CB	1:A:751:LEU:HD11	2.46	0.41
1:A:505:ASP:HB2	1:A:508:LEU:CD2	2.50	0.41
1:A:217:GLN:C	1:A:220:PRO:HD2	2.40	0.41
1:A:247:PHE:N	1:A:247:PHE:CD1	2.88	0.41
1:A:425:LEU:O	1:A:429:LEU:HB2	2.20	0.41
1:A:521:GLN:HA	1:A:522:PRO:HA	1.86	0.41
1:A:285:LEU:HD12	1:A:285:LEU:HA	1.58	0.41
1:A:676:LEU:O	1:A:682:LEU:HG	2.20	0.41
1:A:683:GLU:O	1:A:685:ILE:N	2.54	0.41
1:A:37:TYR:CE1	1:A:48:GLU:HB3	2.56	0.41
1:A:136:THR:O	1:A:139:MET:HB2	2.21	0.41
1:A:442:CYS:SG	1:A:443:GLN:N	2.94	0.41
1:A:227:ASN:CA	1:A:236:SER:O	2.69	0.41
1:A:687:ILE:HD12	1:A:691:GLY:HA3	2.00	0.41
1:A:741:ILE:C	1:A:743:LYS:N	2.73	0.41
1:A:389:LEU:O	1:A:393:LEU:N	2.49	0.41
1:A:431:LEU:HG	4:A:8413:HOH:O	2.20	0.41
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.62	0.41
1:A:56:THR:O	1:A:58:ASP:N	2.54	0.41
1:A:104:HIS:O	1:A:108:VAL:HG23	2.21	0.41
1:A:167:LEU:HD21	1:A:251:GLY:HA3	2.02	0.41
1:A:440:VAL:HG12	1:A:441:LEU:HD23	2.03	0.41
1:A:754:ILE:HG21	1:A:754:ILE:HD13	1.65	0.41
1:A:2:ASN:CG	1:A:5:HIS:ND1	2.74	0.41
1:A:19:GLN:HB3	1:A:21:ASP:OD1	2.20	0.41
1:A:153:PRO:O	1:A:154:HIS:HB2	2.20	0.41
1:A:289:THR:C	1:A:291:GLU:H	2.23	0.41
1:A:535:PHE:HA	1:A:536:PRO:HD3	1.58	0.41
1:A:609:THR:O	1:A:613:ASN:N	2.50	0.41
1:A:696:ILE:CB	1:A:744:ILE:HG23	2.50	0.41
1:A:720:GLN:N	1:A:723:THR:HB	2.36	0.41
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.56	0.40
1:A:319:SER:OG	1:A:321:SER:OG	2.27	0.40
1:A:354:LEU:O	1:A:418:ARG:HD3	2.20	0.40
1:A:504:ILE:HA	1:A:504:ILE:HD12	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:GLY:O	1:A:741:ILE:HG12	2.21	0.40
1:A:59:SER:HB3	1:A:73:LYS:HA	2.02	0.40
1:A:127:ASN:ND2	3:A:999:ADP:O4'	2.38	0.40
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.21	0.40
1:A:428:ARG:HD3	1:A:611:LEU:O	2.20	0.40
1:A:687:ILE:CG2	1:A:688:THR:N	2.83	0.40
1:A:730:LEU:C	1:A:732:ILE:HD12	2.42	0.40
1:A:743:LYS:H	1:A:743:LYS:HG3	1.69	0.40

There are no symmetry-related clashes.

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	707/762 (93%)	609 (86%)	76 (11%)	22 (3%)	4 1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	373	THR
1	A	535	PHE
1	A	691	GLY
1	A	741	ILE
1	A	57	SER
1	A	86	ASP
1	A	290	ALA
1	A	363	ALA
1	A	688	THR
1	A	693	PRO
1	A	694	ASN
1	A	698	TYR

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Mol	Chain	Res	Type
1	A	753	ARG
1	A	410	ASN
1	A	735	GLU
1	A	743	LYS
1	A	64	THR
1	A	536	PRO
1	A	493	GLU
1	A	744	ILE
1	A	692	PHE

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	609/666 (91%)	525 (86%)	84 (14%)	3 2

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	10	ASP
1	A	13	LYS
1	A	22	SER
1	A	31	ASP
1	A	32	LYS
1	A	38	ASN
1	A	46	SER
1	A	47	TYR
1	A	49	CYS
1	A	54	SER
1	A	59	SER
1	A	63	LYS
1	A	66	ASP
1	A	68	GLN
1	A	69	ASP
1	A	76	ASP

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Mol	Chain	Res	Type
1	A	89	GLU
1	A	92	SER
1	A	97	LEU
1	A	98	ASN
1	A	203	ASN
1	A	219	ASN
1	A	244	GLU
1	A	259	GLN
1	A	274	THR
1	A	285	LEU
1	A	298	LEU
1	A	305	ASN
1	A	308	ASN
1	A	337	SER
1	A	372	LYS
1	A	379	SER
1	A	381	VAL
1	A	384	VAL
1	A	398	ILE
1	A	399	LEU
1	A	403	ASP
1	A	404	LEU
1	A	405	VAL
1	A	407	GLN
1	A	429	LEU
1	A	436	LYS
1	A	446	LYS
1	A	463	VAL
1	A	486	MET
1	A	487	PHE
1	A	491	GLN
1	A	492	GLU
1	A	495	LEU
1	A	505	ASP
1	A	520	ARG
1	A	533	SER
1	A	542	THR
1	A	562	ARG
1	A	580	GLU
1	A	582	GLN
1	A	601	LYS
1	A	604	SER

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Mol	Chain	Res	Type
1	A	606	ASN
1	A	609	THR
1	A	616	ASN
1	A	617	ILE
1	A	626	ASN
1	A	661	LYS
1	A	668	GLU
1	A	669	ASP
1	A	685	ILE
1	A	686	ARG
1	A	687	ILE
1	A	689	ARG
1	A	701	PHE
1	A	720	GLN
1	A	723	THR
1	A	726	VAL
1	A	730	LEU
1	A	733	ASP
1	A	735	GLU
1	A	738	ARG
1	A	743	LYS
1	A	744	ILE
1	A	746	PHE
1	A	750	GLN
1	A	754	ILE

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	68	GLN
1	A	98	ASN
1	A	137	GLN
1	A	217	GLN
1	A	234	ASN
1	A	235	ASN
1	A	259	GLN
1	A	283	GLN
1	A	308	ASN
1	A	329	GLN
1	A	376	ASN
1	A	408	HIS

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Mol	Chain	Res	Type
1	A	439	ASN
1	A	468	GLN
1	A	479	GLN
1	A	483	ASN
1	A	491	GLN
1	A	521	GLN
1	A	532	GLN
1	A	616	ASN
1	A	694	ASN
1	A	736	GLN
1	A	750	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	ADP	A	999	2	24,29,29	1.42	4 (16%)	29,45,45	1.88	8 (27%)

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
3	ADP	A	999	2	-	3/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ADP	C2'-C1'	-3.43	1.48	1.53
3	A	999	ADP	C2-N1	3.13	1.39	1.33
3	A	999	ADP	C6-N6	-2.43	1.25	1.34
3	A	999	ADP	O4'-C1'	-2.43	1.37	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ADP	C5-C6-N6	5.71	129.03	120.35
3	A	999	ADP	C5-C6-N1	-3.23	113.02	120.35
3	A	999	ADP	C1'-N9-C4	-2.96	121.45	126.64
3	A	999	ADP	C2-N1-C6	2.88	123.69	118.75
3	A	999	ADP	O3B-PB-O3A	2.69	113.64	104.64
3	A	999	ADP	N3-C2-N1	-2.30	125.08	128.68
3	A	999	ADP	O3'-C3'-C2'	2.27	119.17	111.82
3	A	999	ADP	O4'-C4'-C3'	-2.04	101.09	105.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	ADP	PA-O3A-PB-O2B
3	A	999	ADP	PA-O3A-PB-O1B
3	A	999	ADP	C5'-O5'-PA-O1A

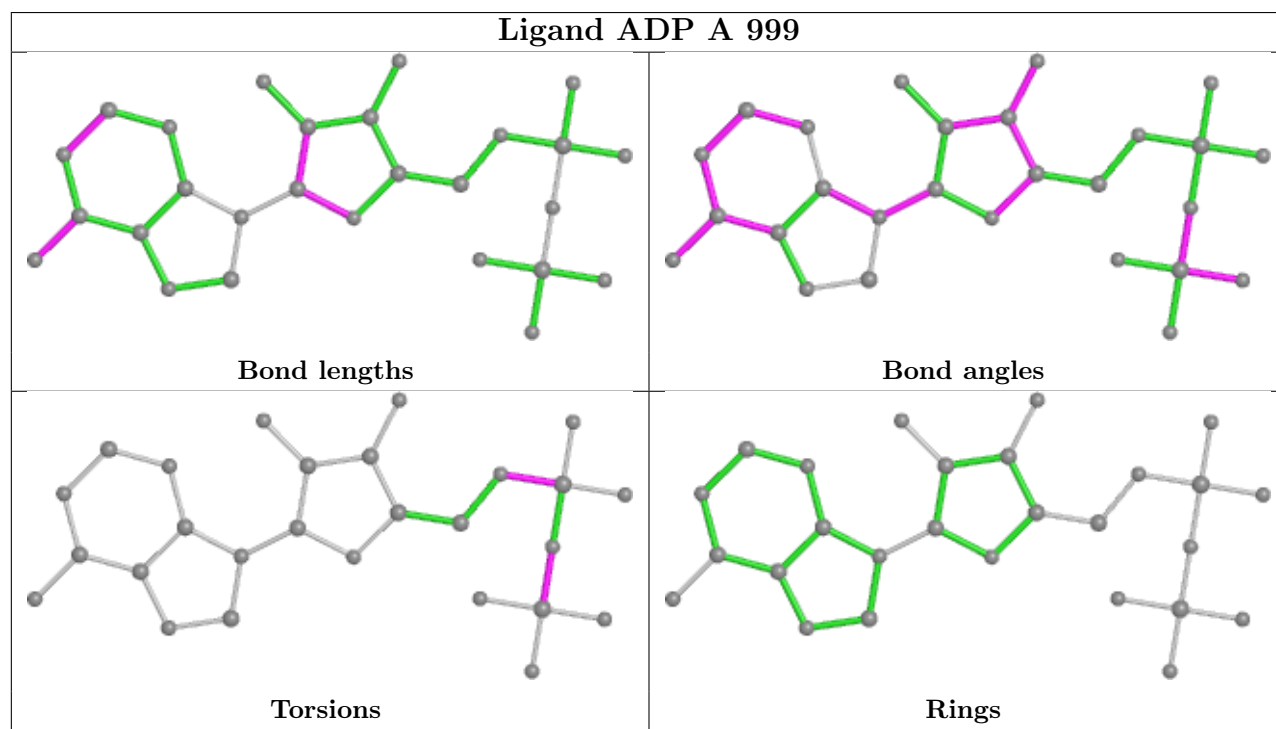
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ADP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.