



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:53 PM UTC

PDB ID : 1B7T / pdb_00001b7t
Title : MYOSIN DIGESTED BY PAPAIN
Authors : Houdusse, A.; Kalabokis, V.; Himmel, D.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on : 1999-01-15
Resolution : 2.50 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

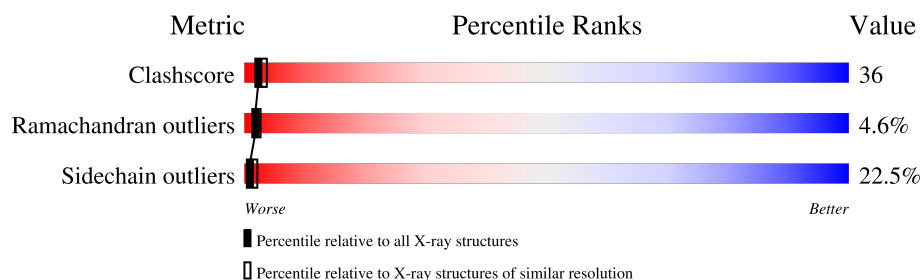
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	835	
2	Y	156	
3	Z	156	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8383 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 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	766	Total	C	N	O	S	0	0	0
			6032	3847	1032	1117	36			

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	138	Total	C	N	O	S	0	0	0
			1035	660	165	203	7			

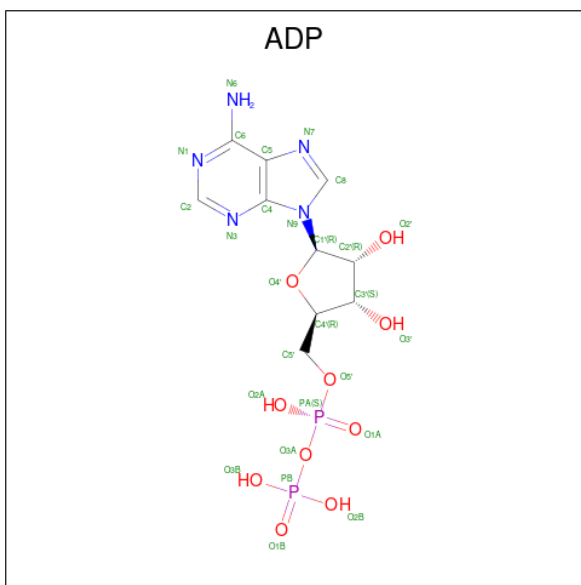
- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	153	Total	C	N	O	S	0	0	0
			1182	754	191	230	7			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	Y	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Z	1	Total Ca 1 1	0	0

- Molecule 7 is water.

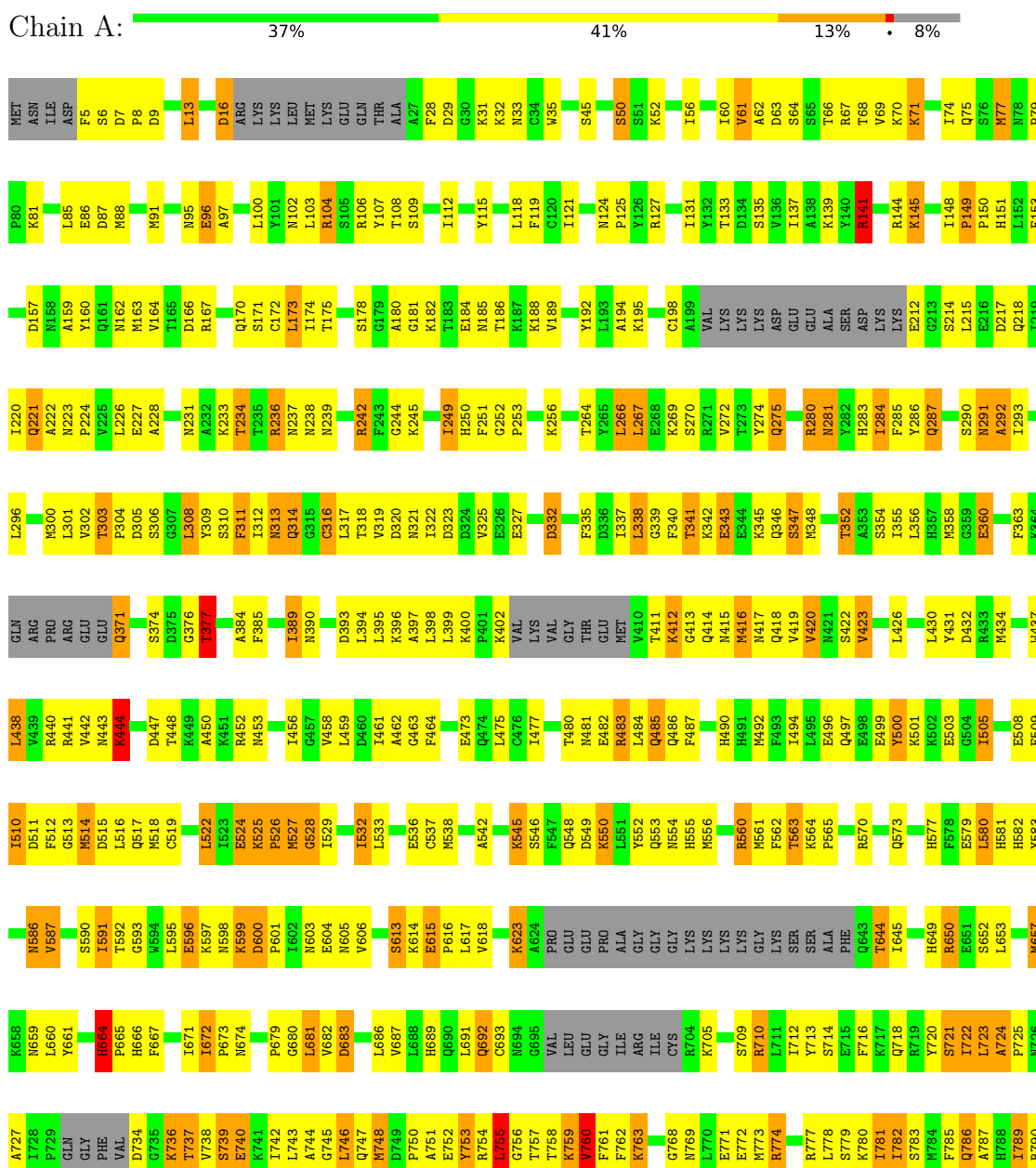
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	80	Total O 80 80	0	0
7	Y	8	Total O 8 8	0	0
7	Z	16	Total O 16 16	0	0

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 HEAVY CHAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.70Å 58.90Å 138.90Å 89.10° 90.00° 73.50°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	80.5 (30.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 4.0	Depositor
R, R_{free}	0.224 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8383	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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: MG, ADP, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	1/6155 (0.0%)	1.15	51/8310 (0.6%)
2	Y	0.59	1/1052 (0.1%)	1.15	12/1415 (0.8%)
3	Z	0.53	0/1206	1.09	10/1626 (0.6%)
All	All	0.63	2/8413 (0.0%)	1.14	73/11351 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	GLN	C-N	-23.01	1.01	1.33
2	Y	149	LYS	CA-C	6.63	1.57	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	GLN	O-C-N	-18.95	92.69	123.00
1	A	815	ILE	N-CA-C	-11.94	101.02	112.96
1	A	423	VAL	N-CA-C	-9.68	101.43	110.53
3	Z	73	GLU	N-CA-C	-9.07	101.48	111.36
1	A	599	LYS	N-CA-C	8.75	125.09	113.72
1	A	664	HIS	CA-C-N	8.48	128.41	119.85
1	A	664	HIS	C-N-CA	8.48	128.41	119.85
1	A	799	LYS	N-CA-C	-8.12	102.37	111.14
1	A	514	MET	N-CA-C	-7.83	104.25	113.88
1	A	270	SER	N-CA-C	7.82	120.70	111.71
1	A	371	GLN	CA-C-N	7.76	134.78	122.59
1	A	371	GLN	C-N-CA	7.76	134.78	122.59
2	Y	114	GLU	N-CA-C	7.26	118.89	110.97
2	Y	124	GLU	N-CA-C	-7.01	103.63	111.28
1	A	346	GLN	N-CA-C	-6.84	105.21	113.97
3	Z	126	ILE	N-CA-C	-6.82	103.68	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	SER	N-CA-C	-6.82	103.93	111.36
1	A	802	GLN	N-CA-C	-6.78	104.65	113.12
1	A	524	GLU	N-CA-C	6.53	121.52	112.45
3	Z	11	LEU	N-CA-C	-6.46	104.16	111.07
2	Y	16	GLN	N-CA-C	-6.39	104.17	112.23
1	A	28	PHE	N-CA-C	6.21	118.52	108.34
1	A	252	GLY	CA-C-N	6.18	127.57	119.84
1	A	252	GLY	C-N-CA	6.18	127.57	119.84
2	Y	43	ILE	N-CA-C	6.07	116.81	110.62
1	A	422	SER	N-CA-C	-6.05	105.73	113.23
3	Z	65	PHE	N-CA-C	-6.05	105.73	113.23
1	A	740	GLU	N-CA-C	-6.00	104.73	111.28
1	A	786	GLN	N-CA-C	-5.99	105.05	112.90
3	Z	79	GLU	N-CA-C	5.99	119.04	110.24
2	Y	86	GLU	N-CA-C	-5.97	105.48	112.89
2	Y	68	ASN	N-CA-C	-5.86	102.98	110.53
1	A	281	ASN	N-CA-C	-5.83	101.33	110.36
1	A	303	THR	N-CA-C	-5.81	100.20	109.04
1	A	554	ASN	N-CA-C	5.81	120.49	113.41
1	A	587	VAL	N-CA-C	5.79	116.85	107.71
1	A	604	GLU	N-CA-C	-5.73	105.99	112.87
1	A	245	LYS	N-CA-C	5.72	117.72	108.34
1	A	787	ALA	N-CA-C	-5.71	104.98	111.14
1	A	664	HIS	N-CA-C	-5.63	96.43	108.93
3	Z	112	ALA	N-CA-C	5.59	120.23	112.45
3	Z	49	VAL	N-CA-C	5.55	116.19	110.36
2	Y	15	LYS	N-CA-C	-5.54	106.69	113.50
1	A	760	VAL	CB-CA-C	-5.53	103.64	111.21
2	Y	134	VAL	N-CA-C	5.49	115.70	107.51
1	A	363	PHE	N-CA-C	5.49	115.53	108.34
1	A	444	LYS	N-CA-C	-5.46	105.23	111.07
3	Z	21	TRP	N-CA-C	5.45	119.02	112.38
1	A	759	LYS	N-CA-C	5.42	117.31	109.07
1	A	806	ILE	N-CA-C	-5.41	105.81	110.74
3	Z	71	ALA	N-CA-C	-5.39	105.49	111.36
1	A	141	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	A	287	GLN	N-CA-C	-5.32	105.40	111.14
2	Y	146	ALA	N-CA-C	-5.30	105.15	111.03
1	A	443	ASN	N-CA-C	-5.30	106.66	113.23
2	Y	149	LYS	O-C-N	5.27	126.02	121.65
3	Z	22	ASP	N-CA-C	-5.25	103.72	111.81
1	A	525	LYS	CA-C-N	5.24	126.39	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	LYS	C-N-CA	5.24	126.39	119.84
1	A	167	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	135	SER	N-CA-C	-5.21	105.49	111.07
1	A	563	THR	N-CA-C	5.18	117.51	108.76
1	A	332	ASP	N-CA-C	-5.16	105.57	111.14
1	A	144	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	672	ILE	CA-C-N	5.10	124.89	119.28
1	A	672	ILE	C-N-CA	5.10	124.89	119.28
1	A	667	PHE	N-CA-C	5.09	117.27	109.07
1	A	753	TYR	N-CA-C	5.08	115.87	108.14
1	A	721	SER	N-CA-C	-5.05	105.47	111.69
1	A	283	HIS	N-CA-C	5.02	117.41	111.33
2	Y	13	PRO	N-CA-CB	5.02	108.52	103.00
2	Y	92	ALA	N-CA-C	-5.02	106.26	112.38
1	A	292	ALA	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6032	0	5905	403	0
2	Y	1035	0	976	104	0
3	Z	1182	0	1107	117	0
4	A	1	0	0	0	0
4	Y	1	0	0	0	0
5	A	27	0	12	1	0
6	Z	1	0	0	0	0
7	A	80	0	0	7	0
7	Y	8	0	0	1	0
7	Z	16	0	0	2	0
All	All	8383	0	8000	588	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 36.

All (588) 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:231:ASN:HD22	1:A:239:ASN:ND2	1.52	1.06
1:A:148:ILE:HG13	1:A:149:PRO:HD2	1.40	1.03
1:A:525:LYS:HD2	1:A:526:PRO:HD2	1.37	1.01
1:A:371:GLN:NE2	1:A:400:LYS:HE2	1.76	0.99
1:A:371:GLN:HE21	1:A:400:LYS:HE2	1.28	0.98
1:A:774:ARG:HG2	1:A:774:ARG:HH11	1.34	0.90
1:A:231:ASN:HD22	1:A:239:ASN:HD21	1.12	0.90
1:A:266:LEU:HD21	1:A:649:HIS:ND1	1.88	0.89
2:Y:106:ILE:HD11	2:Y:110:LYS:HE2	1.53	0.89
1:A:236:ARG:HG3	1:A:236:ARG:HH11	1.39	0.88
1:A:505:ILE:HG22	1:A:754:ARG:HB3	1.56	0.88
1:A:390:ASN:ND2	1:A:393:ASP:H	1.72	0.86
1:A:88:MET:CE	1:A:102:ASN:HB3	2.06	0.85
1:A:371:GLN:HE21	1:A:400:LYS:CE	1.90	0.84
3:Z:3:LEU:HD21	3:Z:76:MET:SD	2.17	0.84
2:Y:68:ASN:H	2:Y:68:ASN:ND2	1.70	0.84
1:A:581:HIS:CE1	1:A:586:ASN:HD21	1.94	0.84
2:Y:68:ASN:HD22	2:Y:68:ASN:N	1.75	0.84
1:A:510:ILE:HG22	1:A:511:ASP:H	1.42	0.83
1:A:716:PHE:CE2	1:A:739:SER:HB3	2.14	0.83
1:A:415:ASN:ND2	1:A:418:GLN:HB2	1.95	0.82
1:A:355:ILE:HA	1:A:358:MET:HG3	1.62	0.82
1:A:250:HIS:HB3	1:A:452:ARG:HG2	1.62	0.82
1:A:522:LEU:HD12	1:A:580:LEU:HD21	1.62	0.81
2:Y:68:ASN:H	2:Y:68:ASN:HD22	1.27	0.80
1:A:186:THR:HG23	1:A:458:VAL:HG11	1.64	0.80
2:Y:16:GLN:O	2:Y:20:MET:HG2	1.83	0.78
1:A:755:LEU:HA	7:A:1068:HOH:O	1.83	0.78
1:A:35:TRP:HB2	1:A:75:GLN:HB2	1.63	0.78
1:A:815:ILE:HD11	2:Y:144:PHE:CZ	2.19	0.78
1:A:829:LEU:HA	1:A:832:LYS:HE3	1.66	0.78
3:Z:4:SER:OG	3:Z:7:GLU:HG3	1.84	0.78
1:A:503:GLU:HB2	1:A:505:ILE:HD11	1.66	0.77
1:A:716:PHE:CD2	1:A:739:SER:HB3	2.20	0.76
1:A:173:LEU:N	1:A:173:LEU:HD23	2.01	0.76
2:Y:116:MET:HG2	3:Z:21:TRP:O	1.85	0.75
1:A:789:ILE:HG23	3:Z:125:ILE:HD13	1.67	0.75
1:A:774:ARG:HH11	1:A:774:ARG:CG	1.98	0.75
1:A:792:TYR:HE1	3:Z:128:LEU:HD12	1.52	0.75
3:Z:87:MET:HE2	3:Z:142:GLU:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLN:HE22	1:A:517:GLN:NE2	1.84	0.74
3:Z:45:ARG:O	3:Z:48:ASP:HB2	1.87	0.74
1:A:234:THR:HG22	1:A:237:ASN:H	1.52	0.74
1:A:371:GLN:HE21	1:A:400:LYS:HG2	1.52	0.74
1:A:310:SER:HA	1:A:313:ASN:HD21	1.53	0.73
1:A:88:MET:HE3	1:A:102:ASN:HB3	1.69	0.73
2:Y:80:LEU:HD23	2:Y:80:LEU:N	2.03	0.73
3:Z:67:GLU:O	3:Z:70:PRO:HD2	1.88	0.73
1:A:231:ASN:ND2	1:A:239:ASN:HD21	1.85	0.73
2:Y:29:VAL:C	2:Y:31:ARG:H	1.95	0.73
1:A:360:GLU:HA	1:A:360:GLU:OE1	1.89	0.72
1:A:546:SER:O	1:A:550:LYS:HB2	1.89	0.72
1:A:537:CYS:HB3	1:A:599:LYS:HD2	1.71	0.71
1:A:499:GLU:C	1:A:501:LYS:H	1.98	0.71
3:Z:131:LEU:HD13	3:Z:144:PHE:HD1	1.55	0.71
1:A:801:LEU:O	3:Z:17:LEU:HD11	1.89	0.71
3:Z:63:LEU:HD22	3:Z:64:PRO:HD2	1.71	0.71
1:A:411:THR:HG22	1:A:412:LYS:N	2.05	0.71
1:A:555:HIS:HB2	1:A:562:PHE:CD2	2.26	0.70
1:A:490:HIS:O	1:A:494:ILE:HG12	1.92	0.70
2:Y:93:PHE:HB3	2:Y:141:TYR:CD2	2.26	0.70
1:A:512:PHE:O	1:A:514:MET:HG2	1.91	0.70
1:A:163:MET:HB2	1:A:170:GLN:HG2	1.74	0.69
1:A:50:SER:HA	3:Z:95:ARG:NH2	2.07	0.69
1:A:615:GLU:HG2	1:A:618:VAL:HG23	1.75	0.69
3:Z:33:LEU:HD12	3:Z:33:LEU:O	1.93	0.69
1:A:371:GLN:HE21	1:A:400:LYS:CD	2.05	0.69
2:Y:115:ASN:HA	2:Y:119:ASN:HD22	1.56	0.68
1:A:815:ILE:HD11	2:Y:144:PHE:HZ	1.56	0.68
1:A:499:GLU:HA	1:A:499:GLU:OE1	1.94	0.68
1:A:371:GLN:NE2	1:A:400:LYS:HG2	2.08	0.68
1:A:505:ILE:CG2	1:A:754:ARG:HB3	2.24	0.68
1:A:231:ASN:ND2	1:A:239:ASN:ND2	2.36	0.68
1:A:774:ARG:HG2	7:A:1056:HOH:O	1.93	0.68
3:Z:15:PHE:CD2	3:Z:65:PHE:HD2	2.11	0.68
2:Y:79:LYS:HB3	2:Y:80:LEU:HD23	1.76	0.67
1:A:508:GLU:HG3	1:A:509:PHE:H	1.59	0.67
2:Y:106:ILE:HG22	2:Y:137:GLY:O	1.94	0.67
1:A:133:THR:O	1:A:137:ILE:HG13	1.93	0.67
2:Y:55:GLU:O	2:Y:59:MET:HB2	1.95	0.67
1:A:778:LEU:O	1:A:782:ILE:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:H	1:A:33:ASN:ND2	1.92	0.66
1:A:447:ASP:CG	1:A:447:ASP:O	2.35	0.66
1:A:301:LEU:HD11	1:A:385:PHE:HD2	1.60	0.66
1:A:5:PHE:C	1:A:7:ASP:H	2.03	0.66
1:A:371:GLN:HE21	1:A:400:LYS:CG	2.07	0.66
1:A:721:SER:HA	1:A:742:ILE:HD13	1.77	0.66
1:A:818:TRP:CE3	1:A:819:LEU:HD23	2.31	0.66
1:A:274:TYR:C	1:A:275:GLN:HG3	2.19	0.65
1:A:371:GLN:NE2	1:A:400:LYS:CE	2.53	0.65
1:A:533:LEU:HD12	1:A:533:LEU:O	1.96	0.65
3:Z:141:TYR:O	3:Z:145:VAL:HG23	1.95	0.65
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.62	0.65
1:A:411:THR:CG2	1:A:412:LYS:N	2.59	0.65
1:A:777:ARG:O	1:A:781:ILE:HD12	1.96	0.65
1:A:162:ASN:O	1:A:166:ASP:HB2	1.97	0.64
1:A:459:LEU:HD11	1:A:461:ILE:HD11	1.78	0.64
1:A:503:GLU:HA	1:A:757:THR:HG23	1.78	0.64
1:A:323:ASP:OD1	1:A:325:VAL:HB	1.97	0.64
1:A:713:TYR:CE2	1:A:736:LYS:HG3	2.32	0.64
1:A:56:ILE:HD11	1:A:71:LYS:HG3	1.79	0.64
1:A:795:ARG:NH1	3:Z:41:GLY:O	2.30	0.64
1:A:16:ASP:OD1	1:A:16:ASP:N	2.31	0.63
1:A:786:GLN:HG2	3:Z:117:LEU:HG	1.79	0.63
1:A:186:THR:HG23	1:A:458:VAL:CG1	2.28	0.63
1:A:548:GLN:HB2	1:A:591:ILE:HD11	1.79	0.63
1:A:790:ARG:NH1	3:Z:117:LEU:HD23	2.13	0.63
1:A:170:GLN:NE2	1:A:666:HIS:NE2	2.47	0.63
1:A:280:ARG:HD3	1:A:319:VAL:HG23	1.81	0.63
1:A:713:TYR:CE1	1:A:760:VAL:HG22	2.33	0.62
1:A:824:TRP:HE3	1:A:827:TRP:HB2	1.64	0.62
2:Y:125:MET:HE1	2:Y:129:PHE:HE2	1.64	0.62
1:A:794:ILE:HG22	1:A:795:ARG:N	2.12	0.62
1:A:236:ARG:HH11	1:A:236:ARG:CG	2.08	0.62
1:A:508:GLU:HG3	1:A:509:PHE:N	2.14	0.62
1:A:797:ALA:HA	7:A:1069:HOH:O	1.99	0.62
1:A:596:GLU:HB3	1:A:601:PRO:HG3	1.81	0.62
1:A:718:GLN:HG2	1:A:718:GLN:O	1.99	0.62
1:A:159:ALA:O	1:A:170:GLN:HG3	1.99	0.62
1:A:750:PRO:HA	1:A:753:TYR:CE1	2.35	0.62
1:A:809:SER:HA	7:Y:762:HOH:O	2.00	0.62
3:Z:73:GLU:HB2	7:Z:759:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LEU:HD23	1:A:438:LEU:O	1.99	0.61
1:A:483:ARG:HG3	1:A:653:LEU:HD21	1.82	0.61
1:A:104:ARG:HG3	1:A:104:ARG:HH11	1.65	0.61
1:A:112:ILE:HD13	1:A:125:PRO:HG3	1.80	0.61
3:Z:14:VAL:HG21	3:Z:40:LEU:HD21	1.82	0.61
3:Z:36:VAL:HG11	3:Z:68:PHE:HE2	1.64	0.61
1:A:124:ASN:HB2	1:A:180:ALA:O	2.00	0.61
1:A:301:LEU:HD11	1:A:385:PHE:CD2	2.35	0.61
2:Y:125:MET:HE1	2:Y:129:PHE:CE2	2.36	0.60
3:Z:50:PHE:HE2	3:Z:56:HIS:CD2	2.19	0.60
1:A:244:GLY:O	1:A:264:THR:HA	2.01	0.60
1:A:305:ASP:HB3	1:A:308:LEU:HD13	1.83	0.60
2:Y:63:ALA:HB1	2:Y:71:MET:HG2	1.82	0.60
1:A:320:ASP:O	1:A:321:ASN:HB2	2.02	0.60
1:A:792:TYR:HE1	3:Z:128:LEU:CD1	2.14	0.60
1:A:536:GLU:HA	1:A:536:GLU:OE1	2.02	0.59
2:Y:142:VAL:HG12	2:Y:143:LYS:N	2.15	0.59
2:Y:36:SER:H	2:Y:39:ASP:HB2	1.67	0.59
1:A:45:SER:O	1:A:61:VAL:HG23	2.02	0.59
1:A:358:MET:SD	1:A:426:LEU:HD23	2.42	0.59
2:Y:121:ASN:O	2:Y:125:MET:HG2	2.02	0.59
2:Y:29:VAL:O	2:Y:31:ARG:N	2.36	0.59
3:Z:24:ARG:CB	3:Z:24:ARG:HH11	2.15	0.59
3:Z:96:GLU:HB2	7:Z:754:HOH:O	2.03	0.59
1:A:740:GLU:O	1:A:744:ALA:HB2	2.03	0.58
1:A:721:SER:HA	1:A:742:ILE:CD1	2.34	0.58
1:A:745:GLY:C	1:A:747:GLN:H	2.11	0.58
3:Z:42:ILE:HG22	3:Z:43:ASN:N	2.18	0.58
1:A:227:GLU:O	1:A:231:ASN:HB2	2.03	0.58
3:Z:70:PRO:HA	3:Z:73:GLU:HB3	1.86	0.58
1:A:431:TYR:HA	1:A:434:MET:HE3	1.84	0.58
1:A:561:MET:O	1:A:581:HIS:HD2	1.87	0.58
1:A:173:LEU:N	1:A:173:LEU:CD2	2.66	0.58
3:Z:29:ASP:OD2	3:Z:58:MET:SD	2.61	0.58
1:A:266:LEU:HD21	1:A:649:HIS:CE1	2.38	0.58
1:A:306:SER:C	1:A:308:LEU:H	2.12	0.58
3:Z:49:VAL:HG22	3:Z:50:PHE:CD1	2.37	0.58
1:A:319:VAL:O	1:A:320:ASP:C	2.47	0.58
1:A:786:GLN:NE2	3:Z:110:LEU:O	2.37	0.58
1:A:603:ASN:C	1:A:605:ASN:H	2.11	0.58
1:A:249:ILE:HG22	1:A:251:PHE:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:O	1:A:281:ASN:ND2	2.37	0.58
1:A:503:GLU:HB2	1:A:505:ILE:CD1	2.33	0.58
1:A:115:TYR:CE2	1:A:150:PRO:HB3	2.39	0.57
1:A:496:GLU:HA	1:A:496:GLU:OE1	2.04	0.57
1:A:603:ASN:C	1:A:605:ASN:N	2.61	0.57
1:A:63:ASP:O	1:A:64:SER:HB2	2.04	0.57
1:A:416:MET:O	1:A:420:VAL:HG13	2.04	0.57
1:A:722:ILE:HG12	1:A:722:ILE:O	2.04	0.57
3:Z:11:LEU:HD23	3:Z:69:LEU:HD12	1.86	0.57
3:Z:15:PHE:CD1	3:Z:15:PHE:C	2.82	0.57
1:A:437:TRP:HA	1:A:440:ARG:NH1	2.20	0.57
1:A:293:ILE:HB	1:A:296:LEU:HD12	1.86	0.57
3:Z:131:LEU:HD11	3:Z:144:PHE:HB2	1.86	0.57
1:A:556:MET:HE3	1:A:556:MET:HA	1.87	0.57
2:Y:106:ILE:O	2:Y:110:LYS:HG3	2.03	0.57
1:A:323:ASP:O	1:A:327:GLU:HG2	2.04	0.57
1:A:400:LYS:HA	1:A:413:GLY:HA2	1.87	0.57
2:Y:121:ASN:ND2	2:Y:123:ASP:H	2.02	0.57
1:A:561:MET:HE3	1:A:581:HIS:HB2	1.86	0.56
2:Y:109:ILE:HG23	2:Y:110:LYS:N	2.20	0.56
1:A:805:ARG:HG2	3:Z:20:PHE:CE1	2.40	0.56
1:A:720:TYR:O	1:A:742:ILE:HD13	2.05	0.56
1:A:724:ALA:N	1:A:725:PRO:HD3	2.20	0.56
1:A:725:PRO:HB3	3:Z:88:GLU:CG	2.36	0.56
2:Y:64:PRO:HG2	2:Y:71:MET:HE1	1.87	0.56
1:A:818:TRP:CZ3	1:A:819:LEU:HD23	2.40	0.56
1:A:266:LEU:HD11	1:A:649:HIS:CE1	2.40	0.56
1:A:785:PHE:O	1:A:789:ILE:HG13	2.05	0.56
1:A:411:THR:CG2	1:A:412:LYS:H	2.19	0.56
1:A:738:VAL:O	1:A:742:ILE:HG13	2.05	0.56
2:Y:103:LYS:O	2:Y:104:LEU:HD23	2.05	0.56
3:Z:49:VAL:O	3:Z:52:VAL:HG23	2.05	0.56
1:A:499:GLU:C	1:A:501:LYS:N	2.64	0.56
1:A:650:ARG:NH1	1:A:650:ARG:HG2	2.21	0.56
3:Z:46:ASN:O	3:Z:50:PHE:HD1	1.88	0.56
1:A:814:ASN:OD1	2:Y:89:ILE:HD11	2.05	0.55
3:Z:63:LEU:HD22	3:Z:64:PRO:CD	2.37	0.55
1:A:399:LEU:HD23	1:A:419:VAL:HG21	1.89	0.55
3:Z:58:MET:O	3:Z:60:GLU:N	2.32	0.55
1:A:441:ARG:O	1:A:444:LYS:HB2	2.07	0.55
1:A:5:PHE:C	1:A:7:ASP:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLN:HB3	7:A:1051:HOH:O	2.06	0.55
2:Y:58:ALA:O	2:Y:62:GLU:HG3	2.07	0.55
1:A:389:ILE:HG23	1:A:613:SER:HB2	1.88	0.55
1:A:689:HIS:O	1:A:692:GLN:HB2	2.07	0.55
1:A:716:PHE:HE2	1:A:739:SER:HB3	1.69	0.55
2:Y:102:LYS:O	2:Y:103:LYS:HD2	2.07	0.55
2:Y:103:LYS:N	2:Y:141:TYR:HE1	2.05	0.55
1:A:650:ARG:HG2	1:A:650:ARG:HH11	1.71	0.55
1:A:335:PHE:O	1:A:340:PHE:HB2	2.06	0.54
1:A:371:GLN:NE2	1:A:400:LYS:CD	2.70	0.54
2:Y:26:MET:O	2:Y:43:ILE:HD12	2.07	0.54
1:A:348:MET:O	1:A:352:THR:HG23	2.06	0.54
2:Y:112:LEU:O	2:Y:116:MET:HB2	2.07	0.54
3:Z:105:GLU:O	3:Z:109:VAL:HG23	2.07	0.54
1:A:104:ARG:HG3	1:A:104:ARG:NH1	2.21	0.54
1:A:148:ILE:HG13	1:A:149:PRO:CD	2.26	0.54
1:A:503:GLU:CB	1:A:505:ILE:HD11	2.35	0.54
1:A:759:LYS:HG3	1:A:761:PHE:HE1	1.73	0.54
3:Z:49:VAL:CG2	3:Z:50:PHE:N	2.71	0.54
1:A:5:PHE:O	1:A:6:SER:HB3	2.07	0.54
1:A:300:MET:O	1:A:301:LEU:HB2	2.06	0.54
1:A:795:ARG:HD3	3:Z:38:ARG:O	2.08	0.54
1:A:9:ASP:OD2	1:A:139:LYS:HE2	2.08	0.54
1:A:774:ARG:CG	1:A:774:ARG:NH1	2.64	0.54
2:Y:109:ILE:HG23	2:Y:110:LYS:H	1.73	0.54
1:A:545:LYS:HE2	1:A:549:ASP:OD2	2.08	0.54
1:A:570:ARG:O	1:A:573:GLN:HB2	2.08	0.54
1:A:818:TRP:CG	2:Y:148:ILE:HG13	2.43	0.54
2:Y:40:ILE:HD11	2:Y:60:LEU:HD21	1.90	0.54
1:A:310:SER:HA	1:A:313:ASN:ND2	2.22	0.53
1:A:402:LYS:H	1:A:605:ASN:ND2	2.06	0.53
1:A:598:ASN:O	1:A:644:THR:HB	2.08	0.53
1:A:807:GLY:O	2:Y:92:ALA:HB1	2.08	0.53
1:A:813:ARG:NH2	2:Y:84:ASP:OD1	2.41	0.53
1:A:657:MET:HA	1:A:657:MET:HE3	1.90	0.53
1:A:341:THR:OG1	1:A:343:GLU:HG2	2.07	0.53
1:A:415:ASN:HD21	1:A:418:GLN:HB2	1.71	0.53
2:Y:68:ASN:ND2	2:Y:71:MET:H	2.06	0.53
1:A:284:ILE:O	1:A:287:GLN:N	2.41	0.53
1:A:683:ASP:O	1:A:687:VAL:HG23	2.08	0.53
1:A:830:TYR:CD1	1:A:830:TYR:C	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:145:THR:O	2:Y:148:ILE:HG22	2.08	0.53
1:A:487:PHE:HD1	1:A:661:TYR:CE1	2.27	0.53
3:Z:9:ASP:O	3:Z:12:LYS:HB2	2.09	0.53
1:A:29:ASP:H	1:A:33:ASN:HD22	1.56	0.53
1:A:313:ASN:HD22	1:A:313:ASN:H	1.57	0.53
1:A:810:VAL:HG12	1:A:811:ILE:N	2.23	0.53
2:Y:80:LEU:HD23	2:Y:80:LEU:H	1.72	0.53
3:Z:4:SER:O	3:Z:8:ILE:HD12	2.09	0.53
1:A:339:GLY:O	1:A:441:ARG:NH2	2.40	0.53
1:A:107:TYR:C	1:A:109:SER:H	2.18	0.52
3:Z:15:PHE:C	3:Z:15:PHE:HD1	2.16	0.52
1:A:338:LEU:HD11	1:A:442:VAL:HG13	1.91	0.52
1:A:780:LYS:O	1:A:783:SER:N	2.42	0.52
2:Y:85:SER:HB2	2:Y:88:THR:H	1.74	0.52
3:Z:147:LYS:O	3:Z:150:ALA:HB3	2.10	0.52
1:A:796:LYS:HB2	3:Z:152:PRO:HB3	1.92	0.52
1:A:85:LEU:N	1:A:102:ASN:HD21	2.08	0.52
3:Z:44:PRO:CB	3:Z:75:LEU:HD22	2.39	0.52
1:A:88:MET:HE2	1:A:102:ASN:HB3	1.91	0.52
1:A:148:ILE:CG1	1:A:149:PRO:HD2	2.26	0.52
1:A:223:ASN:HB2	1:A:224:PRO:HD3	1.91	0.52
1:A:397:ALA:HB1	1:A:605:ASN:HD22	1.75	0.52
1:A:461:ILE:HG22	1:A:462:ALA:N	2.25	0.52
1:A:615:GLU:OE2	1:A:616:PRO:HD2	2.10	0.51
1:A:720:TYR:O	1:A:742:ILE:HG21	2.10	0.51
1:A:91:MET:HE1	1:A:102:ASN:HB2	1.92	0.51
1:A:280:ARG:HD3	1:A:319:VAL:CG2	2.40	0.51
1:A:464:PHE:HZ	1:A:482:GLU:OE1	1.94	0.51
1:A:473:GLU:O	1:A:477:ILE:HG12	2.10	0.51
3:Z:12:LYS:O	3:Z:13:ASP:C	2.54	0.51
1:A:833:VAL:O	1:A:834:LYS:C	2.53	0.51
3:Z:108:HIS:O	3:Z:112:ALA:HB3	2.11	0.51
1:A:85:LEU:HD23	1:A:87:ASP:O	2.10	0.51
1:A:290:SER:O	1:A:291:ASN:HB2	2.11	0.51
1:A:785:PHE:HZ	3:Z:144:PHE:CE2	2.29	0.51
1:A:269:LYS:HE2	1:A:432:ASP:OD2	2.10	0.51
1:A:484:LEU:O	1:A:487:PHE:HB3	2.09	0.51
1:A:503:GLU:HB2	1:A:505:ILE:CG1	2.41	0.51
1:A:769:ASN:HA	1:A:772:GLU:CG	2.41	0.51
1:A:723:LEU:HD21	1:A:773:MET:CB	2.40	0.51
3:Z:87:MET:CE	3:Z:142:GLU:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ASN:ND2	1:A:681:LEU:HD23	2.26	0.51
3:Z:114:GLY:O	3:Z:116:ARG:N	2.44	0.51
2:Y:46:GLN:HG2	2:Y:46:GLN:O	2.10	0.50
1:A:723:LEU:HD21	1:A:773:MET:HB3	1.93	0.50
3:Z:36:VAL:HG11	3:Z:68:PHE:CE2	2.45	0.50
3:Z:109:VAL:HG13	3:Z:113:LEU:HD12	1.93	0.50
3:Z:121:ASP:OD1	3:Z:121:ASP:N	2.42	0.50
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.75	0.50
1:A:137:ILE:HG23	1:A:192:TYR:CE2	2.47	0.50
1:A:284:ILE:HD11	1:A:431:TYR:OH	2.11	0.50
1:A:791:GLY:HA2	3:Z:38:ARG:HG2	1.92	0.50
2:Y:145:THR:O	2:Y:149:LYS:HB2	2.11	0.50
2:Y:29:VAL:C	2:Y:31:ARG:N	2.64	0.50
2:Y:93:PHE:C	2:Y:95:MET:H	2.20	0.50
1:A:347:SER:HB3	1:A:617:LEU:HD23	1.93	0.50
2:Y:60:LEU:C	2:Y:62:GLU:N	2.69	0.50
2:Y:91:ASN:C	2:Y:93:PHE:N	2.68	0.50
1:A:415:ASN:ND2	1:A:418:GLN:OE1	2.44	0.49
3:Z:111:THR:O	3:Z:116:ARG:HG2	2.12	0.49
1:A:745:GLY:C	1:A:747:GLN:N	2.71	0.49
3:Z:29:ASP:OD2	3:Z:58:MET:HA	2.12	0.49
1:A:725:PRO:HB3	3:Z:88:GLU:HG2	1.94	0.49
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.26	0.49
3:Z:145:VAL:O	3:Z:149:MET:HG3	2.12	0.49
2:Y:60:LEU:C	2:Y:62:GLU:H	2.20	0.49
1:A:745:GLY:O	1:A:747:GLN:N	2.45	0.49
1:A:783:SER:HB3	3:Z:45:ARG:HD2	1.95	0.49
1:A:358:MET:SD	1:A:426:LEU:CD2	3.01	0.49
3:Z:15:PHE:CE1	3:Z:19:ASP:HB2	2.47	0.49
1:A:153:PHE:CD1	1:A:192:TYR:CD2	3.01	0.49
1:A:599:LYS:HA	1:A:644:THR:HG22	1.95	0.49
3:Z:49:VAL:HG22	3:Z:50:PHE:HD1	1.76	0.49
1:A:352:THR:HG22	1:A:434:MET:SD	2.53	0.49
3:Z:46:ASN:O	3:Z:50:PHE:CD1	2.66	0.49
3:Z:74:GLY:C	3:Z:76:MET:H	2.21	0.49
2:Y:103:LYS:C	2:Y:104:LEU:HD23	2.38	0.48
1:A:721:SER:C	1:A:723:LEU:H	2.20	0.48
2:Y:20:MET:O	2:Y:23:ALA:HB3	2.13	0.48
1:A:95:ASN:O	1:A:97:ALA:N	2.46	0.48
1:A:384:ALA:HA	1:A:389:ILE:HD11	1.96	0.48
2:Y:122:LYS:O	2:Y:125:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HB2	1:A:456:ILE:HG12	1.95	0.48
1:A:438:LEU:O	1:A:442:VAL:HG23	2.14	0.48
1:A:402:LYS:HA	1:A:411:THR:HA	1.96	0.48
1:A:710:ARG:NH1	1:A:710:ARG:HG2	2.27	0.48
3:Z:15:PHE:CD2	3:Z:65:PHE:CD2	2.98	0.48
3:Z:85:ASP:N	3:Z:85:ASP:OD1	2.47	0.48
1:A:184:GLU:O	1:A:188:LYS:HG2	2.13	0.48
1:A:287:GLN:O	1:A:290:SER:OG	2.30	0.48
1:A:414:GLN:HB3	1:A:418:GLN:HB3	1.95	0.48
2:Y:38:GLU:O	2:Y:42:ALA:HB2	2.14	0.48
1:A:174:ILE:N	1:A:174:ILE:HD12	2.29	0.48
1:A:781:ILE:HG12	3:Z:85:ASP:HB3	1.96	0.48
1:A:833:VAL:HG21	2:Y:27:ILE:HD11	1.95	0.48
1:A:185:ASN:O	1:A:189:VAL:HG23	2.14	0.47
1:A:442:VAL:HG12	1:A:442:VAL:O	2.14	0.47
1:A:320:ASP:N	1:A:320:ASP:OD1	2.47	0.47
1:A:804:GLN:HB3	3:Z:21:TRP:CZ2	2.49	0.47
2:Y:68:ASN:C	2:Y:70:THR:H	2.20	0.47
3:Z:10:ASP:O	3:Z:14:VAL:HG23	2.13	0.47
3:Z:15:PHE:HD1	3:Z:15:PHE:O	1.98	0.47
1:A:753:TYR:C	1:A:754:ARG:HG2	2.40	0.47
2:Y:140:ASP:C	2:Y:140:ASP:OD1	2.58	0.47
3:Z:48:ASP:O	3:Z:51:ALA:HB3	2.15	0.47
1:A:352:THR:HA	1:A:355:ILE:HD12	1.96	0.47
2:Y:37:LYS:HG3	2:Y:60:LEU:HD12	1.96	0.47
1:A:221:GLN:C	1:A:224:PRO:HD2	2.40	0.47
1:A:390:ASN:HD22	1:A:393:ASP:H	1.58	0.47
1:A:319:VAL:O	1:A:319:VAL:HG12	2.14	0.47
1:A:438:LEU:C	1:A:438:LEU:CD2	2.88	0.47
1:A:716:PHE:HZ	1:A:743:LEU:HD21	1.80	0.47
2:Y:99:GLN:HA	2:Y:99:GLN:OE1	2.13	0.47
3:Z:4:SER:O	3:Z:7:GLU:HB2	2.14	0.47
1:A:384:ALA:HB1	1:A:389:ILE:O	2.15	0.47
1:A:792:TYR:CD1	1:A:792:TYR:C	2.93	0.47
1:A:792:TYR:CE1	3:Z:128:LEU:HD12	2.40	0.47
1:A:527:MET:O	1:A:528:GLY:O	2.32	0.47
2:Y:79:LYS:C	2:Y:81:SER:H	2.23	0.47
1:A:430:LEU:HG	1:A:434:MET:HE2	1.96	0.47
1:A:477:ILE:O	1:A:480:THR:HB	2.14	0.47
1:A:710:ARG:HG3	1:A:761:PHE:CZ	2.50	0.47
2:Y:20:MET:CB	2:Y:73:LEU:HD21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:43:ASN:N	3:Z:43:ASN:ND2	2.63	0.46
1:A:394:LEU:C	1:A:396:LYS:N	2.73	0.46
1:A:769:ASN:O	1:A:772:GLU:HB2	2.15	0.46
1:A:720:TYR:OH	1:A:771:GLU:HG2	2.15	0.46
3:Z:36:VAL:O	3:Z:39:CYS:HB2	2.16	0.46
1:A:69:VAL:O	1:A:70:LYS:C	2.58	0.46
1:A:119:PHE:N	1:A:119:PHE:CD1	2.83	0.46
1:A:691:LEU:O	1:A:692:GLN:C	2.58	0.46
1:A:231:ASN:HB3	1:A:239:ASN:ND2	2.30	0.46
1:A:347:SER:HB3	1:A:617:LEU:CD2	2.46	0.46
1:A:756:GLY:HA3	1:A:759:LYS:O	2.16	0.46
2:Y:115:ASN:CA	2:Y:119:ASN:HD22	2.25	0.46
3:Z:15:PHE:CD1	3:Z:15:PHE:O	2.68	0.46
1:A:710:ARG:HH11	1:A:710:ARG:CG	2.27	0.46
1:A:815:ILE:HD11	2:Y:144:PHE:CE1	2.49	0.46
1:A:141:ARG:HA	1:A:157:ASP:OD2	2.16	0.46
1:A:603:ASN:HB2	1:A:606:VAL:HG23	1.96	0.46
2:Y:70:THR:HG22	2:Y:71:MET:N	2.31	0.46
1:A:532:ILE:HD12	1:A:555:HIS:HE1	1.81	0.46
2:Y:93:PHE:C	2:Y:95:MET:N	2.74	0.46
3:Z:38:ARG:HA	3:Z:42:ILE:O	2.15	0.46
1:A:56:ILE:O	1:A:68:THR:HA	2.16	0.46
1:A:184:GLU:HG3	5:A:999:ADP:C8	2.50	0.46
3:Z:59:GLY:O	3:Z:60:GLU:C	2.59	0.46
1:A:376:GLY:O	1:A:377:THR:HG23	2.16	0.46
1:A:487:PHE:HA	1:A:661:TYR:OH	2.16	0.46
2:Y:23:ALA:O	2:Y:27:ILE:HD12	2.15	0.46
2:Y:103:LYS:HG2	2:Y:138:LYS:HB2	1.97	0.46
3:Z:17:LEU:O	3:Z:21:TRP:HD1	1.98	0.46
3:Z:99:GLY:HA2	3:Z:141:TYR:CE1	2.51	0.46
1:A:496:GLU:CD	1:A:710:ARG:HH21	2.22	0.45
2:Y:68:ASN:C	2:Y:70:THR:N	2.73	0.45
3:Z:24:ARG:HH11	3:Z:24:ARG:HB3	1.80	0.45
1:A:119:PHE:N	1:A:119:PHE:HD1	2.14	0.45
1:A:463:GLY:HA2	1:A:481:ASN:OD1	2.15	0.45
2:Y:109:ILE:HG13	2:Y:113:LEU:HD11	1.98	0.45
3:Z:44:PRO:CG	3:Z:75:LEU:HD22	2.46	0.45
1:A:496:GLU:HG3	1:A:500:TYR:CZ	2.50	0.45
1:A:716:PHE:CZ	1:A:743:LEU:HD21	2.52	0.45
1:A:816:ARG:HD2	2:Y:120:PHE:CE1	2.51	0.45
1:A:125:PRO:O	1:A:679:PRO:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HG22	1:A:236:ARG:N	2.32	0.45
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.19	0.45
1:A:725:PRO:HB3	3:Z:88:GLU:HG3	1.99	0.45
2:Y:21:LYS:HA	2:Y:69:PHE:CZ	2.52	0.45
3:Z:16:GLU:O	3:Z:17:LEU:C	2.60	0.45
1:A:222:ALA:O	1:A:226:LEU:HD12	2.16	0.45
1:A:394:LEU:O	1:A:396:LYS:N	2.50	0.45
1:A:533:LEU:HD12	1:A:533:LEU:C	2.42	0.45
1:A:762:PHE:C	1:A:763:LYS:O	2.58	0.45
2:Y:80:LEU:N	2:Y:80:LEU:CD2	2.75	0.45
2:Y:149:LYS:HA	2:Y:149:LYS:HD2	1.61	0.45
1:A:510:ILE:HG22	1:A:511:ASP:N	2.21	0.45
2:Y:30:ASP:O	2:Y:32:ASP:N	2.50	0.45
2:Y:149:LYS:HB3	2:Y:150:GLY:H	1.55	0.45
3:Z:5:GLN:C	3:Z:7:GLU:N	2.73	0.45
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.31	0.45
1:A:253:PRO:HG3	1:A:453:ASN:HD21	1.80	0.45
1:A:686:LEU:O	1:A:689:HIS:HB3	2.17	0.45
1:A:499:GLU:O	1:A:501:LYS:N	2.50	0.44
1:A:821:LEU:O	1:A:821:LEU:HG	2.15	0.44
2:Y:36:SER:O	2:Y:39:ASP:N	2.47	0.44
3:Z:131:LEU:HD22	3:Z:144:PHE:CD1	2.52	0.44
3:Z:147:LYS:O	3:Z:150:ALA:N	2.49	0.44
1:A:85:LEU:H	1:A:102:ASN:HD21	1.64	0.44
1:A:565:PRO:HA	1:A:579:GLU:HG3	1.99	0.44
2:Y:20:MET:HB3	2:Y:73:LEU:HD21	1.99	0.44
3:Z:128:LEU:C	3:Z:130:ASP:H	2.25	0.44
1:A:35:TRP:NE1	1:A:77:MET:HG2	2.32	0.44
1:A:552:TYR:OH	1:A:577:HIS:O	2.29	0.44
2:Y:91:ASN:C	2:Y:93:PHE:H	2.25	0.44
3:Z:36:VAL:HG12	3:Z:37:CYS:N	2.32	0.44
3:Z:42:ILE:CG2	3:Z:43:ASN:N	2.79	0.44
1:A:121:ILE:HG23	1:A:671:ILE:HD12	1.98	0.44
1:A:266:LEU:CD2	1:A:649:HIS:ND1	2.70	0.44
3:Z:14:VAL:HG21	3:Z:40:LEU:CD2	2.46	0.44
1:A:212:GLU:HA	1:A:337:ILE:HA	2.00	0.44
1:A:644:THR:O	1:A:645:ILE:C	2.61	0.44
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.87	0.44
1:A:79:PRO:C	1:A:81:LYS:H	2.26	0.44
1:A:710:ARG:HG2	1:A:710:ARG:HH11	1.83	0.44
3:Z:120:GLU:OE1	3:Z:120:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CE2	1:A:150:PRO:HA	2.53	0.44
1:A:250:HIS:CB	1:A:452:ARG:HG2	2.41	0.44
1:A:801:LEU:HB3	3:Z:17:LEU:HD21	2.00	0.44
1:A:563:THR:O	1:A:564:LYS:C	2.60	0.43
1:A:593:GLY:O	1:A:597:LYS:HG3	2.18	0.43
1:A:657:MET:HE1	1:A:660:LEU:HD12	2.01	0.43
1:A:716:PHE:CD1	1:A:720:TYR:HD2	2.36	0.43
2:Y:13:PRO:O	2:Y:17:ILE:HG13	2.17	0.43
1:A:275:GLN:NE2	1:A:311:PHE:O	2.52	0.43
3:Z:135:LEU:H	3:Z:135:LEU:HG	1.57	0.43
1:A:582:HIS:O	1:A:583:TYR:C	2.62	0.43
1:A:290:SER:O	1:A:291:ASN:CB	2.66	0.43
1:A:340:PHE:CZ	1:A:441:ARG:HG3	2.53	0.43
1:A:473:GLU:CD	1:A:473:GLU:H	2.25	0.43
1:A:721:SER:O	1:A:723:LEU:N	2.50	0.43
1:A:762:PHE:O	1:A:763:LYS:O	2.37	0.43
2:Y:34:PHE:HE2	2:Y:66:PRO:CB	2.31	0.43
2:Y:132:ALA:HA	2:Y:133:PRO:HD3	1.76	0.43
1:A:309:TYR:CD1	1:A:309:TYR:N	2.87	0.43
1:A:537:CYS:HB3	1:A:599:LYS:CD	2.45	0.43
1:A:748:MET:HG2	1:A:753:TYR:CE1	2.54	0.43
2:Y:63:ALA:HB1	2:Y:71:MET:SD	2.59	0.43
2:Y:115:ASN:C	2:Y:119:ASN:HD22	2.25	0.43
3:Z:14:VAL:CG2	3:Z:40:LEU:HD21	2.45	0.43
1:A:160:TYR:O	1:A:164:VAL:HG23	2.18	0.43
1:A:417:ASN:C	1:A:419:VAL:N	2.74	0.43
1:A:438:LEU:O	1:A:438:LEU:CD2	2.66	0.43
1:A:482:GLU:O	1:A:485:GLN:HB2	2.19	0.43
1:A:650:ARG:HH11	1:A:650:ARG:CG	2.31	0.43
2:Y:34:PHE:CE2	2:Y:66:PRO:HB3	2.54	0.43
2:Y:97:ASP:OD1	2:Y:101:THR:HG23	2.19	0.43
3:Z:122:VAL:HG12	3:Z:123:ASP:N	2.34	0.43
1:A:13:LEU:HD21	1:A:151:HIS:HD2	1.83	0.43
2:Y:30:ASP:OD1	2:Y:30:ASP:C	2.61	0.43
1:A:657:MET:CE	1:A:660:LEU:HD12	2.49	0.42
1:A:743:LEU:O	1:A:748:MET:HB3	2.18	0.42
2:Y:13:PRO:HB2	2:Y:16:GLN:CB	2.49	0.42
2:Y:70:THR:C	2:Y:72:PHE:N	2.77	0.42
2:Y:105:ASN:O	2:Y:108:TYR:HB3	2.19	0.42
2:Y:146:ALA:O	2:Y:149:LYS:N	2.50	0.42
1:A:86:GLU:CD	1:A:150:PRO:HD3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLN:NE2	1:A:314:GLN:NE2	2.67	0.42
1:A:501:LYS:HG3	7:A:1051:HOH:O	2.19	0.42
1:A:528:GLY:HA3	7:A:1047:HOH:O	2.19	0.42
2:Y:48:GLY:O	2:Y:49:ARG:C	2.60	0.42
3:Z:12:LYS:HA	3:Z:65:PHE:CE2	2.53	0.42
1:A:286:TYR:CD1	1:A:286:TYR:N	2.87	0.42
1:A:516:LEU:HD12	1:A:516:LEU:HA	1.86	0.42
1:A:757:THR:OG1	1:A:758:THR:N	2.52	0.42
1:A:785:PHE:CZ	3:Z:144:PHE:CE2	3.07	0.42
2:Y:36:SER:O	2:Y:39:ASP:HB2	2.19	0.42
3:Z:119:ASP:O	3:Z:123:ASP:OD1	2.37	0.42
1:A:438:LEU:HD23	1:A:438:LEU:C	2.43	0.42
1:A:483:ARG:HE	1:A:483:ARG:HB3	1.67	0.42
1:A:811:ILE:O	1:A:815:ILE:HB	2.20	0.42
1:A:396:LYS:C	1:A:398:LEU:H	2.27	0.42
1:A:486:GLN:HE22	1:A:517:GLN:HE21	1.62	0.42
1:A:755:LEU:HB2	1:A:756:GLY:H	1.38	0.42
1:A:803:ASP:O	2:Y:95:MET:SD	2.77	0.42
1:A:242:ARG:O	1:A:267:LEU:HA	2.20	0.42
1:A:280:ARG:HG3	1:A:316:CYS:HB3	2.02	0.42
1:A:581:HIS:ND1	1:A:586:ASN:OD1	2.51	0.42
1:A:768:GLY:O	1:A:772:GLU:HG2	2.20	0.42
1:A:124:ASN:HA	1:A:125:PRO:HD3	1.84	0.42
1:A:599:LYS:O	1:A:600:ASP:HB3	2.20	0.42
1:A:713:TYR:CD1	1:A:760:VAL:HG22	2.54	0.42
2:Y:21:LYS:CA	2:Y:69:PHE:CZ	3.03	0.42
1:A:79:PRO:C	1:A:81:LYS:N	2.78	0.42
1:A:274:TYR:CD1	1:A:275:GLN:N	2.88	0.42
3:Z:18:PHE:C	3:Z:20:PHE:N	2.78	0.42
3:Z:50:PHE:HD1	3:Z:50:PHE:H	1.66	0.42
3:Z:90:PHE:HB3	3:Z:141:TYR:CD2	2.54	0.42
1:A:13:LEU:HD13	1:A:131:ILE:CG2	2.50	0.42
1:A:228:ALA:HB2	7:A:1036:HOH:O	2.19	0.42
1:A:107:TYR:CE2	1:A:680:GLY:HA2	2.54	0.42
1:A:305:ASP:HB3	1:A:308:LEU:CD1	2.49	0.42
1:A:448:THR:C	1:A:450:ALA:H	2.28	0.42
1:A:233:LYS:HG2	1:A:238:ASN:HA	2.01	0.41
1:A:292:ALA:C	1:A:293:ILE:HG13	2.45	0.41
1:A:522:LEU:HD13	1:A:529:ILE:HD11	2.02	0.41
1:A:759:LYS:HG3	1:A:761:PHE:CE1	2.53	0.41
1:A:769:ASN:HA	1:A:772:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:44:SER:HB3	2:Y:50:ALA:HB2	2.01	0.41
1:A:303:THR:O	1:A:305:ASP:N	2.45	0.41
2:Y:94:ALA:HA	2:Y:97:ASP:HB3	2.03	0.41
1:A:284:ILE:O	1:A:285:PHE:C	2.63	0.41
1:A:321:ASN:O	1:A:322:ILE:HD13	2.21	0.41
1:A:397:ALA:HB1	1:A:605:ASN:HB3	2.01	0.41
2:Y:97:ASP:OD1	2:Y:101:THR:CG2	2.68	0.41
3:Z:20:PHE:CD1	3:Z:20:PHE:C	2.97	0.41
1:A:60:ILE:O	1:A:64:SER:HA	2.21	0.41
1:A:118:LEU:C	1:A:119:PHE:HD1	2.29	0.41
1:A:737:THR:O	1:A:740:GLU:HB3	2.20	0.41
1:A:794:ILE:HD12	1:A:794:ILE:HA	1.80	0.41
2:Y:90:ARG:HD3	2:Y:142:VAL:HG22	2.01	0.41
2:Y:106:ILE:CG2	2:Y:137:GLY:O	2.66	0.41
1:A:124:ASN:HB3	1:A:673:PRO:HD2	2.02	0.41
1:A:598:ASN:O	1:A:644:THR:CG2	2.68	0.41
1:A:598:ASN:O	1:A:644:THR:HG22	2.21	0.41
1:A:803:ASP:OD1	1:A:803:ASP:N	2.53	0.41
2:Y:52:ASP:O	2:Y:53:ASP:C	2.63	0.41
2:Y:121:ASN:HD21	2:Y:123:ASP:H	1.68	0.41
1:A:214:SER:O	1:A:215:LEU:C	2.64	0.41
1:A:582:HIS:HD2	1:A:587:VAL:CG2	2.33	0.41
2:Y:139:PHE:O	2:Y:139:PHE:CG	2.73	0.41
1:A:397:ALA:CB	1:A:605:ASN:HD22	2.33	0.41
3:Z:17:LEU:O	3:Z:17:LEU:HD12	2.20	0.41
1:A:496:GLU:O	1:A:499:GLU:HB2	2.21	0.41
1:A:664:HIS:O	1:A:666:HIS:CD2	2.74	0.41
1:A:666:HIS:CD2	1:A:666:HIS:N	2.89	0.41
3:Z:15:PHE:HE2	3:Z:65:PHE:HA	1.85	0.41
3:Z:45:ARG:O	3:Z:48:ASP:N	2.54	0.41
1:A:50:SER:HA	3:Z:95:ARG:HH21	1.83	0.41
1:A:172:CYS:C	1:A:173:LEU:HD23	2.44	0.41
1:A:194:ALA:O	1:A:198:CYS:HB3	2.21	0.41
1:A:223:ASN:N	1:A:224:PRO:CD	2.83	0.41
1:A:785:PHE:CZ	3:Z:144:PHE:HE2	2.39	0.41
2:Y:143:LYS:CE	2:Y:143:LYS:HA	2.51	0.41
3:Z:45:ARG:O	3:Z:46:ASN:C	2.63	0.41
1:A:522:LEU:CD1	1:A:580:LEU:HD21	2.40	0.41
1:A:734:ASP:HB3	1:A:737:THR:OG1	2.21	0.41
1:A:79:PRO:O	1:A:81:LYS:N	2.55	0.40
2:Y:121:ASN:HB3	2:Y:124:GLU:OE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:CYS:SG	1:A:580:LEU:HD22	2.62	0.40
1:A:780:LYS:O	1:A:781:ILE:C	2.64	0.40
3:Z:46:ASN:O	3:Z:47:GLU:C	2.64	0.40
3:Z:125:ILE:O	3:Z:129:THR:HG23	2.21	0.40
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.76	0.40
2:Y:63:ALA:HA	2:Y:64:PRO:HD2	1.94	0.40
3:Z:128:LEU:C	3:Z:130:ASP:N	2.79	0.40
3:Z:131:LEU:HD13	3:Z:144:PHE:CD1	2.44	0.40
1:A:7:ASP:OD1	1:A:8:PRO:HD2	2.22	0.40
3:Z:96:GLU:HA	3:Z:96:GLU:OE1	2.20	0.40
3:Z:140:LYS:HE2	3:Z:140:LYS:HB3	1.78	0.40
1:A:221:GLN:O	1:A:224:PRO:HD2	2.21	0.40
1:A:665:PRO:C	1:A:666:HIS:CD2	3.00	0.40
1:A:672:ILE:HG23	1:A:672:ILE:O	2.21	0.40
1:A:751:ALA:C	1:A:753:TYR:H	2.29	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	750/835 (90%)	616 (82%)	102 (14%)	32 (4%)	2	2
2	Y	136/156 (87%)	98 (72%)	32 (24%)	6 (4%)	2	2
3	Z	151/156 (97%)	106 (70%)	35 (23%)	10 (7%)	1	1
All	All	1037/1147 (90%)	820 (79%)	169 (16%)	48 (5%)	2	2

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	GLY
1	A	542	ALA

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Mol	Chain	Res	Type
1	A	623	LYS
1	A	692	GLN
1	A	722	ILE
1	A	752	GLU
1	A	755	LEU
1	A	834	LYS
2	Y	31	ARG
3	Z	42	ILE
3	Z	75	LEU
3	Z	116	ARG
1	A	62	ALA
1	A	96	GLU
1	A	145	LYS
1	A	291	ASN
1	A	528	GLY
1	A	746	LEU
1	A	763	LYS
2	Y	30	ASP
2	Y	66	PRO
2	Y	80	LEU
3	Z	115	GLU
1	A	52	LYS
1	A	149	PRO
1	A	395	LEU
1	A	500	TYR
1	A	727	ALA
3	Z	25	ASP
3	Z	59	GLY
3	Z	124	GLU
1	A	311	PHE
1	A	377	THR
1	A	705	LYS
2	Y	42	ALA
1	A	108	THR
1	A	412	LYS
1	A	526	PRO
1	A	600	ASP
3	Z	118	SER
1	A	103	LEU
3	Z	128	LEU
1	A	304	PRO
1	A	810	VAL

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Mol	Chain	Res	Type
3	Z	101	ILE
1	A	181	GLY
2	Y	64	PRO
1	A	724	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	639/728 (88%)	507 (79%)	132 (21%)	1	2
2	Y	104/133 (78%)	75 (72%)	29 (28%)	0	1
3	Z	120/132 (91%)	87 (72%)	33 (28%)	0	1
All	All	863/993 (87%)	669 (78%)	194 (22%)	1	1

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	ASP
1	A	31	LYS
1	A	32	LYS
1	A	50	SER
1	A	61	VAL
1	A	66	THR
1	A	67	ARG
1	A	71	LYS
1	A	74	ILE
1	A	77	MET
1	A	96	GLU
1	A	100	LEU
1	A	104	ARG
1	A	127	ARG
1	A	141	ARG
1	A	145	LYS
1	A	171	SER

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	175	THR
1	A	178	SER
1	A	182	LYS
1	A	195	LYS
1	A	217	ASP
1	A	218	GLN
1	A	220	ILE
1	A	221	GLN
1	A	234	THR
1	A	236	ARG
1	A	242	ARG
1	A	249	ILE
1	A	256	LYS
1	A	266	LEU
1	A	267	LEU
1	A	275	GLN
1	A	280	ARG
1	A	284	ILE
1	A	302	VAL
1	A	308	LEU
1	A	312	ILE
1	A	313	ASN
1	A	314	GLN
1	A	316	CYS
1	A	317	LEU
1	A	318	THR
1	A	332	ASP
1	A	338	LEU
1	A	341	THR
1	A	342	LYS
1	A	343	GLU
1	A	345	LYS
1	A	352	THR
1	A	354	SER
1	A	356	LEU
1	A	360	GLU
1	A	374	SER
1	A	377	THR
1	A	389	ILE
1	A	416	MET
1	A	420	VAL

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Mol	Chain	Res	Type
1	A	423	VAL
1	A	438	LEU
1	A	444	LYS
1	A	475	LEU
1	A	483	ARG
1	A	485	GLN
1	A	492	MET
1	A	505	ILE
1	A	510	ILE
1	A	515	ASP
1	A	518	MET
1	A	522	LEU
1	A	524	GLU
1	A	527	MET
1	A	532	ILE
1	A	538	MET
1	A	545	LYS
1	A	550	LYS
1	A	553	GLN
1	A	560	ARG
1	A	580	LEU
1	A	586	ASN
1	A	590	SER
1	A	591	ILE
1	A	592	THR
1	A	596	GLU
1	A	613	SER
1	A	614	LYS
1	A	615	GLU
1	A	623	LYS
1	A	644	THR
1	A	650	ARG
1	A	652	SER
1	A	657	MET
1	A	659	ASN
1	A	664	HIS
1	A	681	LEU
1	A	682	VAL
1	A	683	ASP
1	A	693	CYS
1	A	709	SER
1	A	710	ARG

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Mol	Chain	Res	Type
1	A	712	ILE
1	A	714	SER
1	A	723	LEU
1	A	736	LYS
1	A	737	THR
1	A	739	SER
1	A	746	LEU
1	A	748	MET
1	A	755	LEU
1	A	760	VAL
1	A	774	ARG
1	A	779	SER
1	A	781	ILE
1	A	782	ILE
1	A	789	ILE
1	A	792	TYR
1	A	794	ILE
1	A	800	LYS
1	A	801	LEU
1	A	802	GLN
1	A	803	ASP
1	A	805	ARG
1	A	814	ASN
1	A	815	ILE
1	A	816	ARG
1	A	817	LYS
1	A	819	LEU
1	A	820	VAL
1	A	821	LEU
1	A	829	LEU
2	Y	17	ILE
2	Y	25	SER
2	Y	29	VAL
2	Y	67	LEU
2	Y	68	ASN
2	Y	70	THR
2	Y	74	SER
2	Y	77	SER
2	Y	80	LEU
2	Y	84	ASP
2	Y	85	SER
2	Y	89	ILE

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Mol	Chain	Res	Type
2	Y	90	ARG
2	Y	95	MET
2	Y	101	THR
2	Y	103	LYS
2	Y	104	LEU
2	Y	107	GLU
2	Y	114	GLU
2	Y	115	ASN
2	Y	121	ASN
2	Y	124	GLU
2	Y	130	LYS
2	Y	134	VAL
2	Y	138	LYS
2	Y	139	PHE
2	Y	142	VAL
2	Y	143	LYS
2	Y	149	LYS
3	Z	7	GLU
3	Z	14	VAL
3	Z	15	PHE
3	Z	24	ARG
3	Z	28	VAL
3	Z	33	LEU
3	Z	38	ARG
3	Z	43	ASN
3	Z	49	VAL
3	Z	52	VAL
3	Z	61	LYS
3	Z	62	SER
3	Z	63	LEU
3	Z	68	PHE
3	Z	73	GLU
3	Z	76	MET
3	Z	82	THR
3	Z	87	MET
3	Z	91	LYS
3	Z	92	THR
3	Z	95	ARG
3	Z	109	VAL
3	Z	117	LEU
3	Z	119	ASP
3	Z	121	ASP

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Mol	Chain	Res	Type
3	Z	122	VAL
3	Z	124	GLU
3	Z	125	ILE
3	Z	126	ILE
3	Z	128	LEU
3	Z	135	LEU
3	Z	139	VAL
3	Z	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	49	GLN
1	A	102	ASN
1	A	158	ASN
1	A	162	ASN
1	A	170	GLN
1	A	221	GLN
1	A	237	ASN
1	A	238	ASN
1	A	239	ASN
1	A	313	ASN
1	A	314	GLN
1	A	371	GLN
1	A	390	ASN
1	A	414	GLN
1	A	421	ASN
1	A	453	ASN
1	A	485	GLN
1	A	486	GLN
1	A	491	HIS
1	A	497	GLN
1	A	517	GLN
1	A	555	HIS
1	A	586	ASN
1	A	605	ASN
1	A	678	GLN
1	A	769	ASN
1	A	788	HIS
2	Y	68	ASN
2	Y	91	ASN

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Mol	Chain	Res	Type
2	Y	119	ASN
3	Z	108	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are 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	$\# Z > 2$
5	ADP	A	999	4	28,29,29	1.39	5 (17%)	43,45,45	1.95	8 (18%)

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
5	ADP	A	999	4	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	ADP	C5-N7	-3.29	1.33	1.39
5	A	999	ADP	PB-O2B	2.91	1.65	1.54
5	A	999	ADP	C1'-N9	2.33	1.52	1.46
5	A	999	ADP	C5-C4	2.19	1.43	1.39
5	A	999	ADP	C4-N9	-2.14	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	ADP	N3-C2-N1	-6.33	119.00	128.58
5	A	999	ADP	C5-C4-N3	-5.16	119.62	126.72
5	A	999	ADP	C2-N3-C4	4.46	122.73	111.83
5	A	999	ADP	N3-C4-N9	3.50	133.12	127.17
5	A	999	ADP	C5-N7-C8	3.11	108.34	103.45
5	A	999	ADP	C4-C5-N7	-3.03	107.12	110.58
5	A	999	ADP	N9-C8-N7	-3.02	109.65	113.94
5	A	999	ADP	O4'-C1'-N9	2.73	113.34	108.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	999	ADP	PA-O3A-PB-O1B
5	A	999	ADP	PA-O3A-PB-O2B
5	A	999	ADP	PA-O3A-PB-O3B

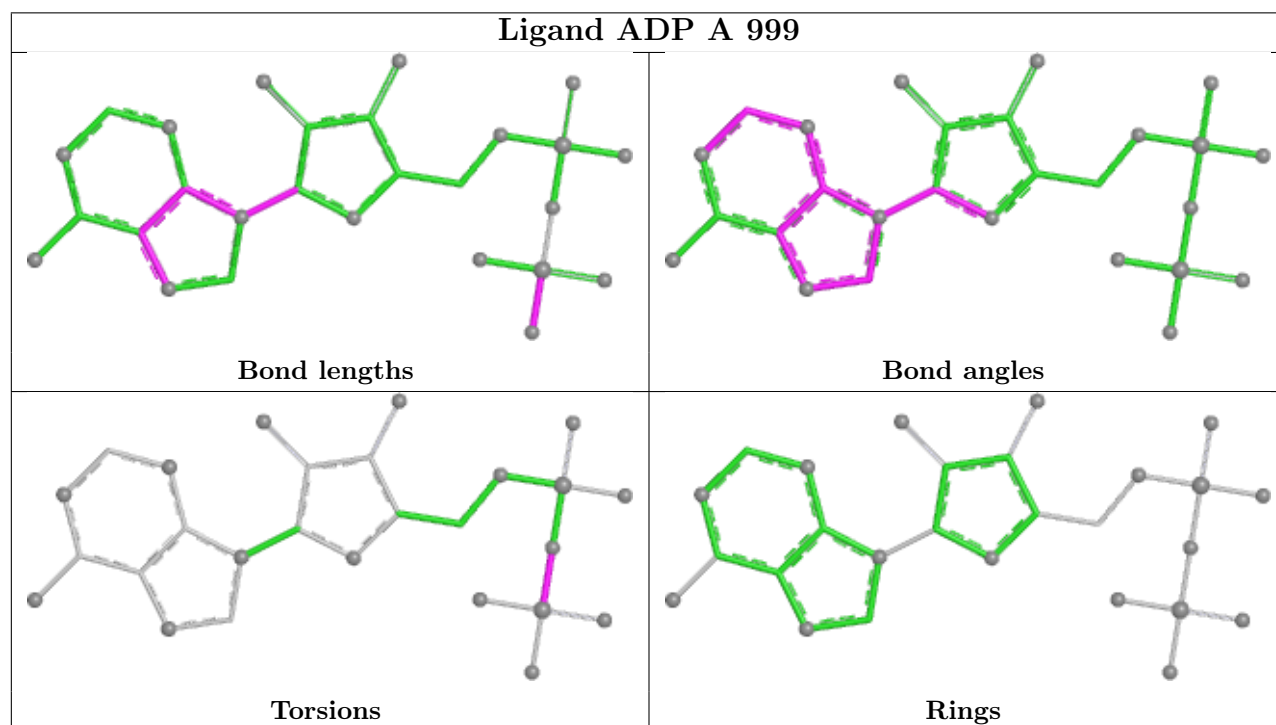
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	999	ADP	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	371:GLN	C	372:ALA	N	1.01

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.