



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:31 PM GMT

PDB ID : 1B7T
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

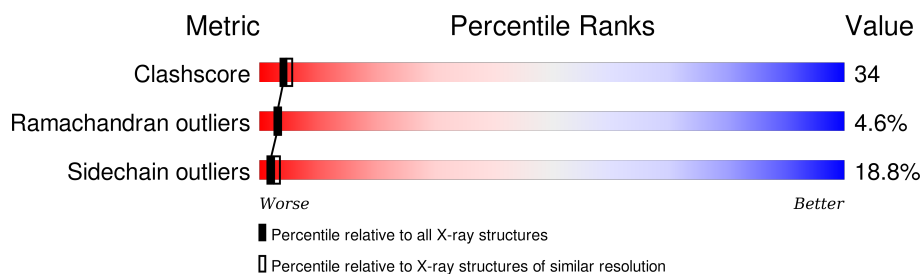
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 (three-letter code: 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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- 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



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN

Chain Y: 29% 44% 15% 12%



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN

Chain Z: 34% 47% 17% 2%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.70 Å 58.90 Å 138.90 Å 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: CA, 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	0.52	1/6155 (0.0%)	0.77	8/8310 (0.1%)
2	Y	0.52	0/1052	0.68	0/1415
3	Z	0.48	0/1206	0.70	1/1626 (0.1%)
All	All	0.52	1/8413 (0.0%)	0.75	9/11351 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	GLN	C-N	-14.33	1.01	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	GLN	O-C-N	-18.76	92.69	122.70
1	A	371	GLN	CA-C-N	13.16	146.15	117.20
1	A	141	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	167	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	A	144	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	664	HIS	N-CA-C	-5.40	96.43	111.00
1	A	371	GLN	C-N-CA	5.23	134.78	121.70
1	A	599	LYS	N-CA-C	5.22	125.09	111.00
3	Z	117	LEU	CA-CB-CG	5.03	126.86	115.30

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	6032	0	5905	380	0
2	Y	1035	0	976	96	0
3	Z	1182	0	1107	111	0
4	A	1	0	0	0	0
4	Y	1	0	0	0	0
5	Z	1	0	0	0	0
6	A	27	0	12	1	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	551	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 34.

All (551) 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:HH11	1:A:236:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:68:ASN:N	2:Y:68:ASN:HD22	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: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:815:ILE:HD11	2:Y:144:PHE:CZ	2.19	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
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
3:Z:67:GLU:O	3:Z:70:PRO:HD2	1.88	0.73
2:Y:80:LEU:HD23	2:Y:80:LEU:N	2.03	0.73
1:A:231:ASN:ND2	1:A:239:ASN:HD21	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Z:87:MET:HE2	3:Z:142:GLU:HG3	1.75	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:OE1	1:A:499:GLU:HA	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
2:Y:29:VAL:C	2:Y:31:ARG:H	1.95	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:499:GLU:C	1:A:501:LYS:H	1.98	0.67
1:A:778:LEU:O	1:A:782:ILE:HG13	1.95	0.67
1:A:29:ASP:H	1:A:33:ASN:ND2	1.92	0.66
1:A:301:LEU:HD11	1:A:385:PHE:HD2	1.60	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:371:GLN:NE2	1:A:400:LYS:CE	2.53	0.65
1:A:533:LEU:O	1:A:533:LEU:HD12	1.96	0.65
3:Z:141:TYR:O	3:Z:145:VAL:HG23	1.95	0.65
1:A:560:ARG:HH11	1:A:560:ARG:HG2	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:459:LEU:HD11	1:A:461:ILE:HD11	1.78	0.64
1:A:162:ASN:O	1:A:166:ASP:HB2	1.97	0.64
1:A:503:GLU:HA	1:A:757:THR:HG23	1.78	0.64
1:A:713:TYR:CE2	1:A:736:LYS:HG3	2.32	0.64
1:A:323:ASP:OD1	1:A:325:VAL:HB	1.97	0.64
1:A:794:ILE:HG22	1:A:795:ARG:N	2.12	0.64
1:A:795:ARG:NH1	3:Z:41:GLY:O	2.30	0.64
1:A:56:ILE:HD11	1:A:71:LYS:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:MET:HE3	1:A:102:ASN:HB3	1.80	0.63
1:A:186:THR:HG23	1:A:458:VAL:CG1	2.28	0.63
1:A:790:ARG:NH1	3:Z:117:LEU:HD23	2.13	0.63
1:A:548:GLN:HB2	1:A:591:ILE:HD11	1.79	0.63
1:A:170:GLN:NE2	1:A:666:HIS:NE2	2.47	0.63
1:A:88:MET:HE2	1:A:102:ASN:HB3	1.80	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
1:A:236:ARG:CG	1:A:236:ARG:HH11	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:718:GLN:HG2	1:A:718:GLN:O	1.99	0.62
1:A:596:GLU:HB3	1:A:601:PRO:HG3	1.81	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
1:A:5:PHE:C	1:A:7:ASP:H	2.03	0.61
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:447:ASP:O	1:A:447:ASP:CG	2.35	0.61
1:A:274:TYR:C	1:A:275:GLN:HG3	2.19	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:36:VAL:HG11	3:Z:68:PHE:HE2	1.64	0.61
3:Z:14:VAL:HG21	3:Z:40:LEU:HD21	1.82	0.61
1:A:301:LEU:HD11	1:A:385:PHE:CD2	2.35	0.61
1:A:124:ASN:HB2	1:A:180:ALA:O	2.00	0.61
3:Z:50:PHE:HE2	3:Z:56:HIS:CD2	2.19	0.60
2:Y:142:VAL:HG12	2:Y:143:LYS:N	2.15	0.60
2:Y:63:ALA:HB1	2:Y:71:MET:HG2	1.82	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	3:Z:24:ARG:CB	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
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:561:MET:O	1:A:581:HIS:HD2	1.87	0.58
1:A:173:LEU:CD2	1:A:173:LEU:N	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
3:Z:49:VAL:HG22	3:Z:50:PHE:CD1	2.37	0.58
1:A:786:GLN:NE2	3:Z:110:LEU:O	2.37	0.58
1:A:503:GLU:HB2	1:A:505:ILE:CD1	2.33	0.58
1:A:272:VAL:O	1:A:281:ASN:ND2	2.37	0.58
1:A:63:ASP:O	1:A:64:SER:HB2	2.04	0.58
1:A:722:ILE:O	1:A:722:ILE:HG12	2.04	0.58
1:A:249:ILE:HG22	1:A:251:PHE:CE1	2.39	0.58
1:A:496:GLU:OE1	1:A:496:GLU:HA	2.04	0.57
1:A:115:TYR:CE2	1:A:150:PRO:HB3	2.39	0.57
1:A:416:MET:O	1:A:420:VAL:HG13	2.04	0.57
3:Z:11:LEU:HD23	3:Z:69:LEU:HD12	1.86	0.57
1:A:437:TRP:HA	1:A:440:ARG:NH1	2.20	0.57
3:Z:131:LEU:HD11	3:Z:144:PHE:HB2	1.86	0.57
1:A:293:ILE:HB	1:A:296:LEU:HD12	1.86	0.57
2:Y:106:ILE:O	2:Y:110:LYS:HG3	2.03	0.57
1:A:400:LYS:HA	1:A:413:GLY:HA2	1.87	0.57
1:A:323:ASP:O	1:A:327:GLU:HG2	2.04	0.57
2:Y:121:ASN:ND2	2:Y:123:ASP:H	2.02	0.57
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
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:738:VAL:O	1:A:742:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:THR:CG2	1:A:412:LYS:H	2.19	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
3:Z:46:ASN:O	3:Z:50:PHE:HD1	1.88	0.56
1:A:650:ARG:HG2	1:A:650:ARG:NH1	2.21	0.56
3:Z:63:LEU:HD22	3:Z:64:PRO:CD	2.37	0.55
1:A:814:ASN:OD1	2:Y:89:ILE:HD11	2.05	0.55
3:Z:58:MET:O	3:Z:60:GLU:N	2.32	0.55
1:A:399:LEU:HD23	1:A:419:VAL:HG21	1.89	0.55
1:A:441:ARG:O	1:A:444:LYS:HB2	2.07	0.55
1:A:561:MET:HE3	1:A:581:HIS:HB2	1.88	0.55
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: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: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:650:ARG:HH11	1:A:650:ARG:HG2	1.71	0.55
1:A:371:GLN:NE2	1:A:400:LYS:CD	2.70	0.54
1:A:335:PHE:O	1:A:340:PHE:HB2	2.06	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:148:ILE:HG13	1:A:149:PRO:CD	2.26	0.54
1:A:104:ARG:NH1	1:A:104:ARG:HG3	2.21	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: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:5:PHE:O	1:A:6:SER:HB3	2.07	0.54
1:A:774:ARG:NH1	1:A:774:ARG:CG	2.64	0.54
2:Y:109:ILE:HG23	2:Y:110:LYS:H	1.73	0.54
1:A:9:ASP:OD2	1:A:139:LYS:HE2	2.08	0.54
1:A:745:GLY:C	1:A:747:GLN:H	2.11	0.54
1:A:570:ARG:O	1:A:573:GLN:HB2	2.08	0.54
1:A:545:LYS:HE2	1:A:549:ASP:OD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:SER:HA	1:A:313:ASN:ND2	2.22	0.53
1:A:598:ASN:O	1:A:644:THR:HB	2.08	0.53
1:A:402:LYS:H	1:A:605:ASN:ND2	2.06	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:306:SER:C	1:A:308:LEU:H	2.12	0.53
1:A:603:ASN:C	1:A:605:ASN:H	2.11	0.53
1:A:319:VAL:O	1:A:320:ASP:C	2.47	0.53
1:A:341:THR:OG1	1:A:343:GLU:HG2	2.07	0.53
2:Y:68:ASN:ND2	2:Y:71:MET:H	2.06	0.53
1:A:415:ASN:HD21	1:A:418:GLN:HB2	1.71	0.53
1:A:603:ASN:C	1:A:605:ASN:N	2.61	0.53
3:Z:15:PHE:C	3:Z:15:PHE:CD1	2.82	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
2:Y:145:THR:O	2:Y:148:ILE:HG22	2.08	0.53
3:Z:9:ASP:O	3:Z:12:LYS:HB2	2.09	0.53
1:A:487:PHE:HD1	1:A:661:TYR:CE1	2.27	0.53
3:Z:4:SER:O	3:Z:8:ILE:HD12	2.09	0.53
1:A:810:VAL:HG12	1:A:811:ILE:N	2.23	0.53
1:A:313:ASN:H	1:A:313:ASN:HD22	1.57	0.53
2:Y:80:LEU:HD23	2:Y:80:LEU:H	1.72	0.53
1:A:29:ASP:H	1:A:33:ASN:HD22	1.56	0.53
1:A:339:GLY:O	1:A:441:ARG:NH2	2.40	0.53
1:A:780:LYS:O	1:A:783:SER:N	2.42	0.52
1:A:338:LEU:HD11	1:A:442:VAL:HG13	1.91	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: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:280:ARG:HD3	1:A:319:VAL:CG2	2.40	0.51
1:A:473:GLU:O	1:A:477:ILE:HG12	2.10	0.51
1:A:464:PHE:HZ	1:A:482:GLU:OE1	1.94	0.51
3:Z:108:HIS:O	3:Z:112:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD23	1:A:87:ASP:O	2.10	0.51
1:A:785:PHE:HZ	3:Z:144:PHE:CE2	2.29	0.51
1:A:499:GLU:C	1:A:501:LYS:N	2.64	0.51
1:A:290:SER:O	1:A:291:ASN:HB2	2.11	0.51
2:Y:29:VAL:C	2:Y:31:ARG:N	2.64	0.51
1:A:503:GLU:HB2	1:A:505:ILE:CG1	2.41	0.51
1:A:484:LEU:O	1:A:487:PHE:HB3	2.09	0.51
1:A:769:ASN:HA	1:A:772:GLU:CG	2.41	0.51
1:A:269:LYS:HE2	1:A:432:ASP:OD2	2.10	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
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:O	2:Y:46:GLN:HG2	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: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:106:ARG:HH11	1:A:106:ARG:HG2	1.75	0.50
2:Y:145:THR:O	2:Y:149:LYS:HB2	2.11	0.50
1:A:791:GLY:HA2	3:Z:38:ARG:HG2	1.92	0.50
1:A:347:SER:HB3	1:A:617:LEU:HD23	1.93	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
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
3:Z:145:VAL:O	3:Z:149:MET:HG3	2.12	0.49
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.26	0.49
1:A:783:SER:HB3	3:Z:45:ARG:HD2	1.95	0.49
1:A:745:GLY:O	1:A:747:GLN:N	2.45	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:599:LYS:HA	1:A:644:THR:HG22	1.95	0.49
1:A:153:PHE:CD1	1:A:192:TYR:CD2	3.01	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
2:Y:20:MET:O	2:Y:23:ALA:HB3	2.13	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:384:ALA:HA	1:A:389:ILE:HD11	1.96	0.48
1:A:95:ASN:O	1:A:97:ALA:N	2.46	0.48
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:830:TYR:C	1:A:830:TYR:CD1	2.87	0.48
1:A:710:ARG:HG2	1:A:710:ARG:NH1	2.27	0.48
1:A:402:LYS:HA	1:A:411:THR:HA	1.96	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: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:833:VAL:HG21	2:Y:27:ILE:HD11	1.95	0.48
1:A:781:ILE:HG12	3:Z:85:ASP:HB3	1.96	0.48
1:A:174:ILE:HD12	1:A:174:ILE:N	2.29	0.48
1:A:442:VAL:HG12	1:A:442:VAL:O	2.14	0.47
1:A:185:ASN:O	1:A:189:VAL:HG23	2.14	0.47
1:A:107:TYR:C	1:A:109:SER:H	2.18	0.47
1:A:804:GLN:HB3	3:Z:21:TRP:CZ2	2.49	0.47
3:Z:15:PHE:O	3:Z:15:PHE:HD1	1.98	0.47
1:A:320:ASP:OD1	1:A:320:ASP:N	2.47	0.47
3:Z:10:ASP:O	3:Z:14:VAL:HG23	2.13	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:390:ASN:HD22	1:A:393:ASP:H	1.58	0.47
1:A:716:PHE:HZ	1:A:743:LEU:HD21	1.80	0.47
3:Z:4:SER:O	3:Z:7:GLU:HB2	2.14	0.47
3:Z:15:PHE:C	3:Z:15:PHE:HD1	2.16	0.47
1:A:319:VAL:HG12	1:A:319:VAL:O	2.14	0.47
2:Y:99:GLN:HA	2:Y:99:GLN:OE1	2.13	0.47
1:A:792:TYR:CE1	3:Z:128:LEU:HD12	2.40	0.47
1:A:384:ALA:HB1	1:A:389:ILE:O	2.15	0.47
1:A:527:MET:O	1:A:528:GLY:O	2.32	0.47
1:A:710:ARG:HG3	1:A:761:PHE:CZ	2.50	0.47
3:Z:12:LYS:O	3:Z:13:ASP:C	2.54	0.47
1:A:477:ILE:O	1:A:480:THR:HB	2.14	0.47
1:A:657:MET:HE3	1:A:657:MET:HA	1.97	0.47
1:A:833:VAL:O	1:A:834:LYS:C	2.53	0.46
2:Y:20:MET:CB	2:Y:73:LEU:HD21	2.45	0.46
3:Z:43:ASN:ND2	3:Z:43:ASN:N	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:PHE:N	1:A:119:PHE:CD1	2.83	0.46
1:A:231:ASN:HB3	1:A:239:ASN:ND2	2.30	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:O	3:Z:15:PHE:CD1	2.68	0.46
1:A:347:SER:HB3	1:A:617:LEU:CD2	2.46	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
2:Y:70:THR:HG22	2:Y:71:MET:N	2.31	0.46
1:A:603:ASN:HB2	1:A:606:VAL:HG23	1.96	0.46
1:A:141:ARG:HA	1:A:157:ASP:OD2	2.16	0.46
1:A:532:ILE:HD12	1:A:555:HIS:HE1	1.81	0.46
3:Z:38:ARG:HA	3:Z:42:ILE:O	2.15	0.46
1:A:5:PHE:C	1:A:7:ASP:N	2.64	0.46
1:A:56:ILE:O	1:A:68:THR:HA	2.16	0.46
1:A:184:GLU:HG3	6:A:999:ADP:C8	2.50	0.46
2:Y:23:ALA:O	2:Y:27:ILE:HD12	2.15	0.46
3:Z:17:LEU:O	3:Z:21:TRP:HD1	1.98	0.46
2:Y:103:LYS:HG2	2:Y:138:LYS:HB2	1.97	0.46
3:Z:99:GLY:HA2	3:Z:141:TYR:CE1	2.51	0.46
1:A:487:PHE:HA	1:A:661:TYR:OH	2.16	0.46
1:A:376:GLY:O	1:A:377:THR:HG23	2.16	0.46
3:Z:24:ARG:HH11	3:Z:24:ARG:HB3	1.80	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: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
1:A:716:PHE:CZ	1:A:743:LEU:HD21	2.52	0.45
1:A:496:GLU:HG3	1:A:500:TYR:CZ	2.50	0.45
1:A:816:ARG:HD2	2:Y:120:PHE:CE1	2.51	0.45
1:A:234:THR:HG22	1:A:236:ARG:N	2.32	0.45
1:A:236:ARG:NH1	1:A:236:ARG:HG3	2.19	0.45
2:Y:91:ASN:C	2:Y:93:PHE:N	2.68	0.45
1:A:125:PRO:O	1:A:679:PRO:HB3	2.15	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
1:A:88:MET:HE2	1:A:102:ASN:CB	2.47	0.45
2:Y:60:LEU:C	2:Y:62:GLU:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:O	1:A:396:LYS:N	2.50	0.45
1:A:222:ALA:O	1:A:226:LEU:HD12	2.16	0.45
2:Y:80:LEU:CD2	2:Y:80:LEU:N	2.75	0.45
2:Y:149:LYS:HD2	2:Y:149:LYS:HA	1.61	0.45
1:A:510:ILE:HG22	1:A:511:ASP:N	2.21	0.45
2:Y:149:LYS:HB3	2:Y:150:GLY:H	1.55	0.45
2:Y:30:ASP:O	2:Y:32:ASP:N	2.50	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
3:Z:120:GLU:HA	3:Z:120:GLU:OE1	2.17	0.45
3:Z:131:LEU:HD22	3:Z:144:PHE:CD1	2.52	0.44
2:Y:93:PHE:C	2:Y:95:MET:H	2.20	0.44
1:A:499:GLU:O	1:A:501:LYS:N	2.50	0.44
2:Y:36:SER:O	2:Y:39:ASP:N	2.47	0.44
3:Z:147:LYS:O	3:Z:150:ALA:N	2.49	0.44
1:A:821:LEU:HG	1:A:821:LEU:O	2.15	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
1:A:35:TRP:NE1	1:A:77:MET:HG2	2.32	0.44
3:Z:42:ILE:CG2	3:Z:43:ASN:N	2.79	0.44
3:Z:36:VAL:HG12	3:Z:37:CYS:N	2.32	0.44
1:A:745:GLY:C	1:A:747:GLN:N	2.71	0.44
1:A:552:TYR:OH	1:A:577:HIS:O	2.29	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:121:ILE:HG23	1:A:671:ILE:HD12	1.98	0.44
3:Z:74:GLY:C	3:Z:76:MET:H	2.21	0.44
1:A:212:GLU:HA	1:A:337:ILE:HA	2.00	0.44
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.87	0.44
1:A:721:SER:C	1:A:723:LEU:H	2.20	0.44
1:A:710:ARG:HG2	1:A:710:ARG:HH11	1.83	0.44
2:Y:103:LYS:C	2:Y:104:LEU:HD23	2.38	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:115:TYR:CE2	1:A:150:PRO:HA	2.53	0.44
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:593:GLY:O	1:A:597:LYS:HG3	2.18	0.43
1:A:275:GLN:NE2	1:A:311:PHE:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:SER:O	1:A:291:ASN:CB	2.66	0.43
3:Z:135:LEU:H	3:Z:135:LEU:HG	1.57	0.43
1:A:721:SER:O	1:A:723:LEU:N	2.50	0.43
1:A:340:PHE:CZ	1:A:441:ARG:HG3	2.53	0.43
2:Y:34:PHE:HE2	2:Y:66:PRO:CB	2.31	0.43
1:A:762:PHE:O	1:A:763:LYS:O	2.37	0.43
2:Y:132:ALA:HA	2:Y:133:PRO:HD3	1.76	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
1:A:537:CYS:HB3	1:A:599:LYS:CD	2.45	0.43
3:Z:14:VAL:CG2	3:Z:40:LEU:HD21	2.45	0.43
1:A:309:TYR:N	1:A:309:TYR:CD1	2.87	0.43
2:Y:68:ASN:C	2:Y:70:THR:H	2.20	0.43
1:A:438:LEU:O	1:A:438:LEU:CD2	2.66	0.43
1:A:650:ARG:HH11	1:A:650:ARG:CG	2.31	0.43
1:A:482:GLU:O	1:A:485:GLN:HB2	2.19	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
1:A:160:TYR:O	1:A:164:VAL:HG23	2.18	0.43
3:Z:122:VAL:HG12	3:Z:123:ASP:N	2.34	0.43
2:Y:60:LEU:C	2:Y:62:GLU:H	2.20	0.43
1:A:13:LEU:HD21	1:A:151:HIS:HD2	1.83	0.43
1:A:753:TYR:C	1:A:754:ARG:HG2	2.40	0.43
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:146:ALA:O	2:Y:149:LYS:N	2.50	0.42
1:A:657:MET:CE	1:A:660:LEU:HD12	2.49	0.42
2:Y:105:ASN:O	2:Y:108:TYR:HB3	2.19	0.42
2:Y:140:ASP:OD1	2:Y:140:ASP:C	2.58	0.42
1:A:501:LYS:HG3	7:A:1051:HOH:O	2.19	0.42
3:Z:12:LYS:HA	3:Z:65:PHE:CE2	2.53	0.42
1:A:275:GLN:NE2	1:A:314:GLN:NE2	2.67	0.42
1:A:221:GLN:C	1:A:224:PRO:HD2	2.40	0.42
1:A:528:GLY:HA3	7:A:1047:HOH:O	2.19	0.42
1:A:394:LEU:C	1:A:396:LYS:N	2.73	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
1:A:438:LEU:CD2	1:A:438:LEU:C	2.88	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:516:LEU:HA	1:A:516:LEU:HD12	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TYR:CD1	1:A:286:TYR:N	2.87	0.42
1:A:811:ILE:O	1:A:815:ILE:HB	2.20	0.42
1:A:483:ARG:HE	1:A:483:ARG:HB3	1.67	0.42
1:A:755:LEU:HB2	1:A:756:GLY:H	1.38	0.42
1:A:486:GLN:HE22	1:A:517:GLN:HE21	1.62	0.42
1:A:803:ASP:O	2:Y:95:MET:SD	2.77	0.42
1:A:581:HIS:ND1	1:A:586:ASN:OD1	2.51	0.42
1:A:280:ARG:HG3	1:A:316:CYS:HB3	2.02	0.42
1:A:768:GLY:O	1:A:772:GLU:HG2	2.20	0.42
1:A:242:ARG:O	1:A:267:LEU:HA	2.20	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
1:A:124:ASN:HA	1:A:125:PRO:HD3	1.84	0.42
2:Y:21:LYS:CA	2:Y:69:PHE:CZ	3.03	0.42
1:A:792:TYR:C	1:A:792:TYR:CD1	2.93	0.42
3:Z:90:PHE:HB3	3:Z:141:TYR:CD2	2.54	0.42
1:A:274:TYR:CD1	1:A:275:GLN:N	2.88	0.42
3:Z:50:PHE:HD1	3:Z:50:PHE:H	1.66	0.42
2:Y:125:MET:CE	2:Y:129:PHE:CE2	3.03	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:305:ASP:HB3	1:A:308:LEU:CD1	2.49	0.42
1:A:107:TYR:CE2	1:A:680:GLY:HA2	2.54	0.42
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
2:Y:44:SER:HB3	2:Y:50:ALA:HB2	2.01	0.41
1:A:233:LYS:HG2	1:A:238:ASN:HA	2.01	0.41
2:Y:79:LYS:C	2:Y:81:SER:H	2.23	0.41
1:A:303:THR:O	1:A:305:ASP:N	2.45	0.41
1:A:691:LEU:O	1:A:692:GLN:C	2.58	0.41
2:Y:94:ALA:HA	2:Y:97:ASP:HB3	2.03	0.41
1:A:397:ALA:HB1	1:A:605:ASN:HB3	2.01	0.41
1:A:321:ASN:O	1:A:322:ILE:HD13	2.21	0.41
2:Y:97:ASP:OD1	2:Y:101:THR:CG2	2.68	0.41
1:A:69:VAL:O	1:A:70:LYS:C	2.58	0.41
2:Y:106:ILE:CG2	2:Y:137:GLY:O	2.66	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
1:A:737:THR:O	1:A:740:GLU:HB3	2.20	0.41
1:A:60:ILE:O	1:A:64:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ASN:O	1:A:644:THR:HG22	2.21	0.41
1:A:598:ASN:O	1:A:644:THR:CG2	2.68	0.41
1:A:803:ASP:N	1:A:803:ASP:OD1	2.53	0.41
1:A:124:ASN:HB3	1:A:673:PRO:HD2	2.02	0.41
2:Y:121:ASN:HD21	2:Y:123:ASP:H	1.68	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
2:Y:68:ASN:C	2:Y:70:THR:N	2.73	0.41
3:Z:17:LEU:O	3:Z:17:LEU:HD12	2.20	0.41
1:A:397:ALA:CB	1:A:605:ASN:HD22	2.33	0.41
3:Z:59:GLY:O	3:Z:60:GLU:C	2.59	0.41
3:Z:45:ARG:O	3:Z:48:ASP:N	2.54	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
1:A:496:GLU:O	1:A:499:GLU:HB2	2.21	0.41
3:Z:15:PHE:HE2	3:Z:65:PHE:HA	1.85	0.41
1:A:287:GLN:O	1:A:290:SER:OG	2.30	0.41
1:A:451:LYS:HG2	1:A:451:LYS:HZ2	1.76	0.41
1:A:785:PHE:CZ	3:Z:144:PHE:HE2	2.39	0.41
1:A:50:SER:HA	3:Z:95:ARG:HH21	1.83	0.41
2:Y:143:LYS:CE	2:Y:143:LYS:HA	2.51	0.41
1:A:223:ASN:N	1:A:224:PRO:CD	2.83	0.41
1:A:194:ALA:O	1:A:198:CYS:HB3	2.21	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
2:Y:93:PHE:C	2:Y:95:MET:N	2.74	0.40
2:Y:121:ASN:HB3	2:Y:124:GLU:OE1	2.20	0.40
1:A:79:PRO:O	1:A:81:LYS:N	2.55	0.40
1:A:519:CYS:SG	1:A:580:LEU:HD22	2.62	0.40
3:Z:16:GLU:O	3:Z:17:LEU:C	2.60	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:131:LEU:HD13	3:Z:144:PHE:CD1	2.44	0.40
3:Z:5:GLN:C	3:Z:7:GLU:N	2.73	0.40
1:A:533:LEU:C	1:A:533:LEU:HD12	2.42	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
1:A:762:PHE:C	1:A:763:LYS:O	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ILE:HG23	1:A:672:ILE:O	2.21	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%)	3	4
2	Y	136/156 (87%)	98 (72%)	32 (24%)	6 (4%)	3	3
3	Z	151/156 (97%)	106 (70%)	35 (23%)	10 (7%)	1	1
All	All	1037/1147 (90%)	820 (79%)	169 (16%)	48 (5%)	3	3

All (48) Ramachandran outliers are listed below:

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

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

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	639/728 (88%)	530 (83%)	109 (17%)	2	4
2	Y	104/133 (78%)	79 (76%)	25 (24%)	1	1
3	Z	120/132 (91%)	92 (77%)	28 (23%)	1	1
All	All	863/993 (87%)	701 (81%)	162 (19%)	2	3

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	31	LYS
1	A	32	LYS
1	A	50	SER
1	A	66	THR
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	145	LYS
1	A	171	SER
1	A	173	LEU
1	A	178	SER
1	A	195	LYS
1	A	217	ASP
1	A	218	GLN
1	A	234	THR
1	A	236	ARG
1	A	237	ASN
1	A	242	ARG
1	A	256	LYS
1	A	266	LEU
1	A	275	GLN
1	A	280	ARG
1	A	284	ILE
1	A	308	LEU
1	A	313	ASN
1	A	314	GLN
1	A	316	CYS
1	A	317	LEU
1	A	318	THR

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Mol	Chain	Res	Type
1	A	338	LEU
1	A	342	LYS
1	A	343	GLU
1	A	345	LYS
1	A	352	THR
1	A	354	SER
1	A	360	GLU
1	A	374	SER
1	A	377	THR
1	A	416	MET
1	A	420	VAL
1	A	423	VAL
1	A	438	LEU
1	A	447	ASP
1	A	451	LYS
1	A	471	SER
1	A	475	LEU
1	A	483	ARG
1	A	485	GLN
1	A	505	ILE
1	A	515	ASP
1	A	518	MET
1	A	519	CYS
1	A	522	LEU
1	A	524	GLU
1	A	527	MET
1	A	531	SER
1	A	553	GLN
1	A	560	ARG
1	A	586	ASN
1	A	590	SER
1	A	592	THR
1	A	596	GLU
1	A	605	ASN
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

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Mol	Chain	Res	Type
1	A	659	ASN
1	A	664	HIS
1	A	681	LEU
1	A	683	ASP
1	A	693	CYS
1	A	709	SER
1	A	710	ARG
1	A	712	ILE
1	A	714	SER
1	A	723	LEU
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	782	ILE
1	A	792	TYR
1	A	794	ILE
1	A	800	LYS
1	A	801	LEU
1	A	802	GLN
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	25	SER
2	Y	29	VAL
2	Y	32	ASP
2	Y	67	LEU
2	Y	68	ASN
2	Y	70	THR
2	Y	74	SER
2	Y	77	SER
2	Y	80	LEU

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Mol	Chain	Res	Type
2	Y	84	ASP
2	Y	85	SER
2	Y	89	ILE
2	Y	90	ARG
2	Y	101	THR
2	Y	103	LYS
2	Y	104	LEU
2	Y	107	GLU
2	Y	115	ASN
2	Y	121	ASN
2	Y	124	GLU
2	Y	134	VAL
2	Y	138	LYS
2	Y	139	PHE
2	Y	143	LYS
2	Y	149	LYS
3	Z	10	ASP
3	Z	15	PHE
3	Z	20	PHE
3	Z	24	ARG
3	Z	28	VAL
3	Z	38	ARG
3	Z	43	ASN
3	Z	44	PRO
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	78	CYS
3	Z	82	THR
3	Z	87	MET
3	Z	91	LYS
3	Z	95	ARG
3	Z	107	ARG
3	Z	119	ASP
3	Z	121	ASP
3	Z	124	GLU
3	Z	125	ILE

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Mol	Chain	Res	Type
3	Z	134	ASP
3	Z	135	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	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	491	HIS
1	A	517	GLN
1	A	555	HIS
1	A	586	ASN
1	A	605	ASN
1	A	769	ASN
1	A	788	HIS
2	Y	68	ASN
2	Y	91	ASN
2	Y	119	ASN
3	Z	108	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
6	ADP	A	999	4	22,29,29	1.27	3 (13%)	27,45,45	2.68	3 (11%)

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
6	ADP	A	999	4	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	999	ADP	C2-N3	2.23	1.36	1.32
6	A	999	ADP	O4'-C1'	2.44	1.44	1.41
6	A	999	ADP	PB-O2B	3.03	1.65	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	999	ADP	N3-C2-N1	-12.92	119.00	128.89
6	A	999	ADP	C4-C5-N7	-2.57	107.12	109.48
6	A	999	ADP	O4'-C1'-N9	2.50	113.34	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	999	ADP	1	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.