



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:10 PM UTC

PDB ID : 1MNE / pdb_00001mne
Title : TRUNCATED HEAD OF MYOSIN FROM DICTYOSTELIUM DIS-
COIDEUM COMPLEXED WITH MG-PYROPHOSPHATE
Authors : Smith, C.A.; Rayment, I.
Deposited on : 1995-04-20
Resolution : 2.70 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
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

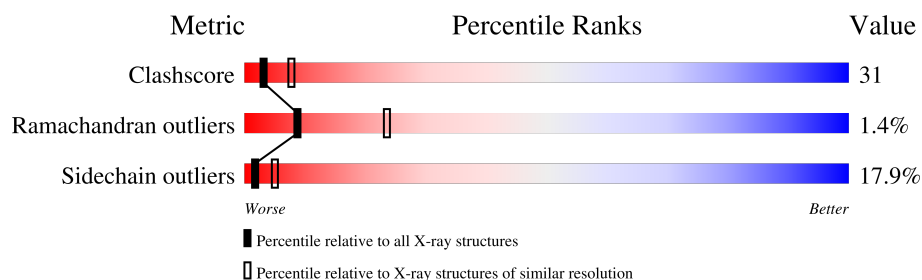
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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% 41% 13% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6027 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	0	0
			5869	3728	1012	1113	16			

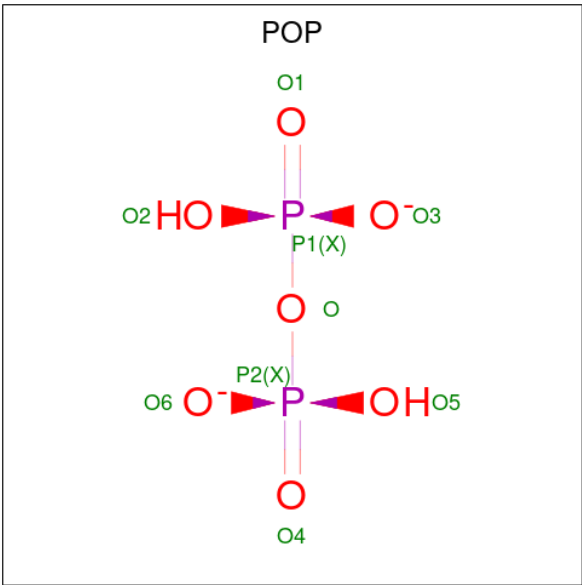
There are 7 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is water.

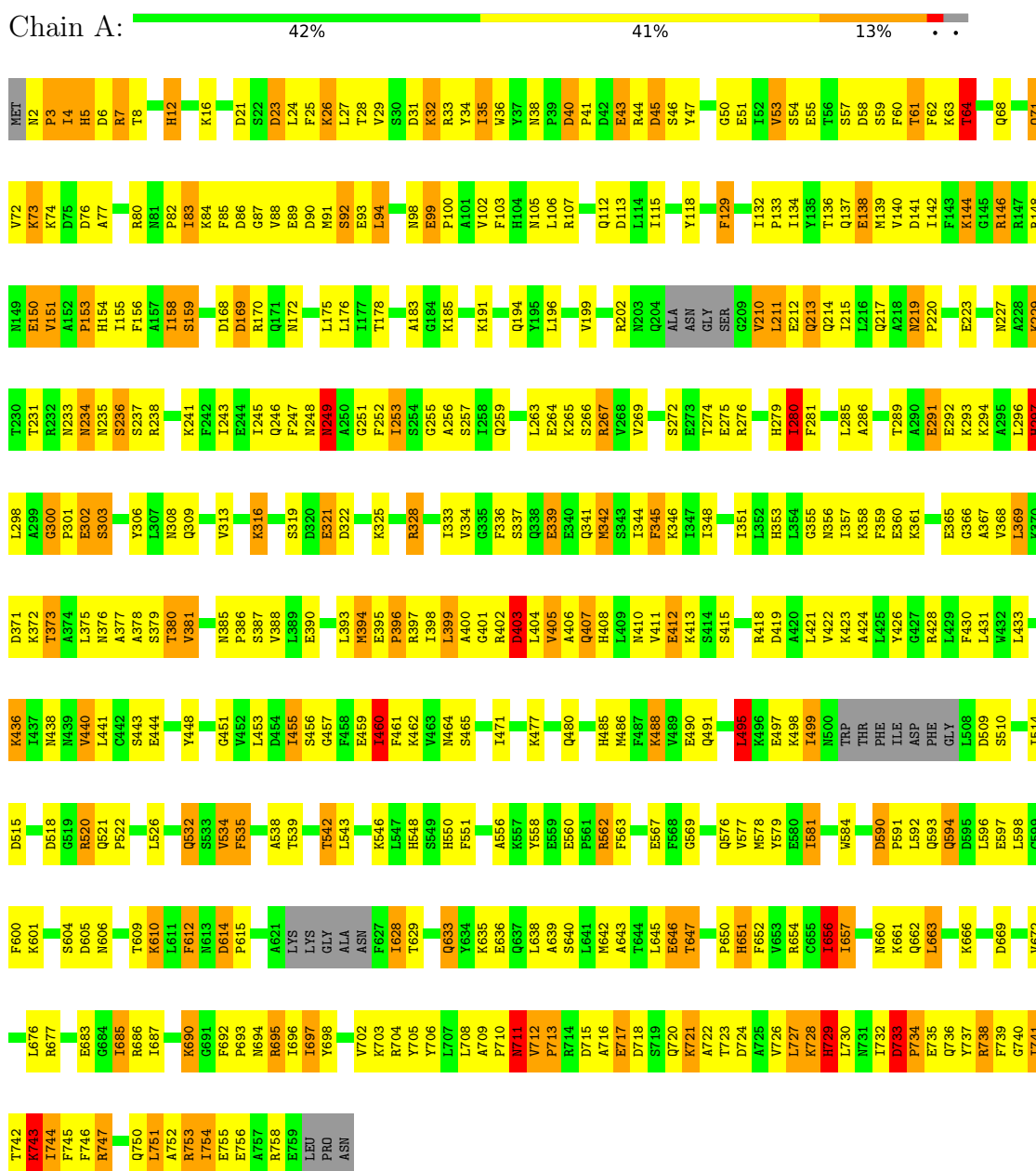
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		

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



4 Data and refinement statistics

Xtriage (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	105.20Å 182.10Å 54.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6027	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: POP, MG

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	1.07	1/5978 (0.0%)	1.70	91/8073 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ILE	CA-CB	-6.05	1.49	1.54

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	HIS	CA-CB-CG	-13.85	99.95	113.80
1	A	729	HIS	CA-CB-CG	-11.40	102.39	113.80
1	A	345	PHE	CA-CB-CG	-10.75	103.05	113.80
1	A	535	PHE	CA-CB-CG	-9.80	104.00	113.80
1	A	628	ILE	N-CA-C	9.38	121.25	108.11
1	A	40	ASP	CA-C-N	9.19	128.93	119.56
1	A	40	ASP	C-N-CA	9.19	128.93	119.56
1	A	356	ASN	CA-CB-CG	-8.77	103.83	112.60
1	A	651	HIS	CA-CB-CG	-8.69	105.11	113.80
1	A	660	ASN	CA-CB-CG	-8.48	104.12	112.60
1	A	12	HIS	CA-CB-CG	-8.32	105.48	113.80
1	A	712	VAL	O-C-N	7.74	129.92	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	PRO	CB-CA-C	-7.56	102.11	111.64
1	A	234	ASN	CA-CB-CG	-7.53	105.07	112.60
1	A	365	GLU	N-CA-C	-7.44	104.71	114.31
1	A	733	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	25	PHE	CA-CB-CG	7.33	121.13	113.80
1	A	133	PRO	CB-CA-C	-7.25	103.22	113.09
1	A	711	ASN	O-C-N	7.25	132.24	122.59
1	A	656	ILE	N-CA-C	7.08	118.02	108.11
1	A	515	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	219	ASN	CA-CB-CG	-6.98	105.62	112.60
1	A	94	LEU	N-CA-CB	6.95	120.17	110.17
1	A	129	PHE	CA-CB-CG	-6.85	106.95	113.80
1	A	168	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	21	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	210	VAL	CB-CA-C	-6.58	103.38	111.87
1	A	440	VAL	CB-CA-C	-6.58	103.40	112.02
1	A	146	ARG	N-CA-CB	6.55	120.25	110.29
1	A	606	ASN	CA-CB-CG	-6.55	106.05	112.60
1	A	509	ASP	N-CA-C	-6.50	104.28	111.82
1	A	210	VAL	N-CA-C	6.46	116.50	110.42
1	A	711	ASN	CB-CA-C	-6.29	97.89	110.42
1	A	713	PRO	N-CA-CB	6.28	109.84	103.25
1	A	103	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	280	ILE	N-CA-CB	6.16	121.39	111.23
1	A	31	ASP	CA-C-N	6.14	130.03	120.75
1	A	31	ASP	C-N-CA	6.14	130.03	120.75
1	A	249	ASN	CA-CB-CG	-6.03	106.57	112.60
1	A	26	LYS	N-CA-C	6.02	117.84	111.28
1	A	590	ASP	CB-CA-C	6.00	116.35	110.71
1	A	733	ASP	CA-C-N	5.87	127.18	119.84
1	A	733	ASP	C-N-CA	5.87	127.18	119.84
1	A	153	PRO	N-CA-CB	5.86	108.44	103.35
1	A	717	GLU	N-CA-CB	5.83	119.53	110.44
1	A	663	LEU	CA-C-N	5.78	127.06	119.84
1	A	663	LEU	C-N-CA	5.78	127.06	119.84
1	A	43	GLU	N-CA-CB	5.76	118.98	109.88
1	A	361	LYS	CB-CA-C	-5.64	108.30	116.54
1	A	606	ASN	CB-CA-C	5.64	121.65	110.42
1	A	460	ILE	N-CA-CB	-5.62	105.66	112.35
1	A	495	LEU	N-CA-CB	5.59	118.41	110.13
1	A	600	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	76	ASP	CA-CB-CG	5.58	118.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	CA-CB-CG	-5.58	107.02	112.60
1	A	629	THR	N-CA-CB	5.48	118.62	110.29
1	A	62	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	38	ASN	CB-CA-C	-5.46	105.52	110.44
1	A	743	LYS	CA-C-N	-5.46	116.05	122.93
1	A	743	LYS	C-N-CA	-5.46	116.05	122.93
1	A	556	ALA	N-CA-C	5.44	119.54	113.01
1	A	279	HIS	N-CA-CB	5.44	118.04	109.94
1	A	403	ASP	CA-C-N	-5.43	115.20	122.42
1	A	403	ASP	C-N-CA	-5.43	115.20	122.42
1	A	107	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	A	169	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	393	LEU	CA-C-N	-5.42	112.54	121.92
1	A	393	LEU	C-N-CA	-5.42	112.54	121.92
1	A	462	LYS	N-CA-C	-5.42	105.02	111.03
1	A	534	VAL	CA-C-O	5.42	124.11	118.96
1	A	605	ASP	N-CA-CB	5.39	117.94	109.69
1	A	303	SER	CA-C-N	-5.39	114.63	122.44
1	A	303	SER	C-N-CA	-5.39	114.63	122.44
1	A	276	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	300	GLY	CA-C-N	5.34	126.52	119.84
1	A	300	GLY	C-N-CA	5.34	126.52	119.84
1	A	612	PHE	N-CA-CB	5.28	118.01	110.67
1	A	115	ILE	N-CA-C	5.26	119.56	112.98
1	A	28	THR	CA-C-N	-5.25	113.62	120.91
1	A	28	THR	C-N-CA	-5.25	113.62	120.91
1	A	151	VAL	N-CA-C	5.25	117.60	108.95
1	A	669	ASP	N-CA-C	5.24	117.40	111.11
1	A	3	PRO	N-CA-CB	5.22	108.70	103.48
1	A	86	ASP	N-CA-CB	5.18	117.69	109.71
1	A	733	ASP	CB-CA-C	5.14	120.31	110.17
1	A	485	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	590	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	99	GLU	O-C-N	5.07	124.38	120.38
1	A	461	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	614	ASP	CA-C-O	5.06	124.24	119.59
1	A	334	VAL	CB-CA-C	5.03	118.93	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	606	ASN	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	HIS	Sidechain
1	A	403	ASP	Mainchain
1	A	729	HIS	Sidechain

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	5869	0	5740	362	1
2	A	1	0	0	0	0
3	A	9	0	0	2	0
4	A	148	0	0	11	0
All	All	6027	0	5740	362	1

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 31.

All (362) 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:499:ILE:HD13	1:A:738:ARG:HB3	1.37	1.06
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.39	1.00
1:A:397:ARG:HA	1:A:406:ALA:HA	1.48	0.93
1:A:628:ILE:CB	1:A:628:ILE:CD1	2.48	0.91
1:A:638:LEU:CB	1:A:638:LEU:CD1	2.50	0.90
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.04	0.88
1:A:146:ARG:HG3	1:A:151:VAL:HG11	1.59	0.84
1:A:412:GLU:HG2	1:A:413:LYS:N	1.96	0.81
1:A:64:THR:HG23	1:A:68:GLN:O	1.81	0.81
1:A:727:LEU:HD12	1:A:732:ILE:HD13	1.64	0.80
1:A:289:THR:O	1:A:293:LYS:HG3	1.82	0.80
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.63	0.80
1:A:91:MET:HE1	1:A:106:LEU:HD13	1.63	0.79
1:A:499:ILE:HD13	1:A:738:ARG:CB	2.11	0.79
1:A:718:ASP:OD1	1:A:721:LYS:HB2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLN:O	1:A:598:LEU:HG	1.84	0.78
1:A:497:GLU:OE1	1:A:742:THR:HB	1.84	0.78
1:A:91:MET:CE	1:A:106:LEU:HD13	2.13	0.77
1:A:247:PHE:CE2	1:A:253:ILE:HG12	2.20	0.77
1:A:753:ARG:HG2	1:A:753:ARG:HH11	1.50	0.76
1:A:238:ARG:HD3	1:A:264:GLU:OE2	1.85	0.76
1:A:385:ASN:O	1:A:388:VAL:HB	1.85	0.76
1:A:280:ILE:N	1:A:280:ILE:HD12	2.02	0.75
1:A:296:LEU:HD21	1:A:342:MET:HE1	1.66	0.75
1:A:397:ARG:HD2	1:A:404:LEU:HD21	1.68	0.75
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.96	0.74
1:A:697:ILE:HD13	1:A:743:LYS:HG3	1.70	0.74
1:A:4:ILE:HD13	1:A:146:ARG:NH2	2.03	0.73
1:A:337:SER:O	1:A:341:GLN:HG3	1.88	0.73
1:A:499:ILE:HD12	1:A:745:PHE:CD2	2.24	0.72
1:A:639:ALA:HA	4:A:836:HOH:O	1.88	0.72
1:A:210:VAL:O	1:A:214:GLN:HG3	1.91	0.71
1:A:683:GLU:HG3	1:A:686:ARG:NH1	2.05	0.71
1:A:403:ASP:HB3	1:A:405:VAL:CG2	2.21	0.70
1:A:87:GLY:H	1:A:105:ASN:ND2	1.90	0.70
1:A:710:PRO:HD2	1:A:729:HIS:CE1	2.27	0.70
1:A:139:MET:HA	1:A:142:ILE:HD12	1.73	0.70
1:A:733:ASP:OD2	1:A:735:GLU:HB2	1.92	0.70
1:A:60:PHE:CE1	1:A:74:LYS:HG2	2.27	0.70
1:A:215:ILE:HG13	1:A:441:LEU:HD22	1.72	0.70
1:A:510:SER:O	1:A:514:ILE:HD12	1.92	0.69
1:A:730:LEU:HB2	1:A:732:ILE:CD1	2.22	0.69
1:A:280:ILE:HD12	1:A:280:ILE:H	1.57	0.69
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.23	0.69
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.74	0.68
1:A:319:SER:OG	1:A:321:GLU:HG2	1.93	0.68
1:A:477:LYS:HE2	4:A:893:HOH:O	1.93	0.68
1:A:217:GLN:HG3	1:A:333:ILE:HG21	1.76	0.68
1:A:377:ALA:O	1:A:381:VAL:HG13	1.93	0.67
1:A:372:LYS:O	1:A:376:ASN:ND2	2.28	0.67
1:A:499:ILE:HD12	1:A:745:PHE:CG	2.29	0.66
1:A:215:ILE:HG13	1:A:441:LEU:CD2	2.24	0.66
1:A:33:ARG:NH1	4:A:856:HOH:O	2.28	0.66
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.30	0.66
1:A:58:ASP:N	1:A:58:ASP:OD2	2.28	0.66
1:A:736:GLN:HG3	1:A:750:GLN:OE1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:ILE:HD11	1:A:751:LEU:HD21	1.77	0.66
1:A:26:LYS:HA	1:A:29:VAL:HG23	1.79	0.65
1:A:548:HIS:CE1	1:A:560:GLU:HG3	2.31	0.65
1:A:2:ASN:HB3	1:A:5:HIS:HD2	1.60	0.65
1:A:229:LYS:HE2	1:A:274:THR:O	1.96	0.64
1:A:297:HIS:ND1	1:A:297:HIS:N	2.46	0.64
1:A:344:ILE:O	1:A:348:ILE:HG12	1.97	0.64
1:A:322:ASP:OD1	1:A:325:LYS:NZ	2.28	0.64
1:A:539:THR:O	1:A:542:THR:HB	1.98	0.64
1:A:146:ARG:HG3	1:A:151:VAL:CG1	2.27	0.63
1:A:219:ASN:N	1:A:220:PRO:HD2	2.11	0.63
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.28	0.63
1:A:2:ASN:HB3	1:A:5:HIS:CD2	2.32	0.62
1:A:397:ARG:CG	1:A:406:ALA:HB2	2.30	0.62
1:A:397:ARG:HD2	1:A:404:LEU:CD2	2.29	0.61
1:A:397:ARG:HG2	1:A:406:ALA:HB2	1.81	0.61
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.30	0.61
1:A:359:PHE:HB2	1:A:411:VAL:HG13	1.82	0.60
1:A:548:HIS:ND1	1:A:560:GLU:HG3	2.16	0.60
1:A:241:LYS:HA	1:A:259:GLN:O	2.01	0.60
1:A:698:TYR:O	1:A:702:VAL:HG23	2.02	0.60
1:A:702:VAL:O	1:A:706:TYR:HB3	2.02	0.60
1:A:754:ILE:HG22	1:A:755:GLU:N	2.15	0.60
1:A:711:ASN:HB3	1:A:712:VAL:HG23	1.82	0.60
1:A:723:THR:O	1:A:727:LEU:HD22	2.01	0.60
1:A:175:LEU:HG	1:A:651:HIS:HB2	1.82	0.59
1:A:342:MET:O	1:A:345:PHE:HB2	2.01	0.59
1:A:367:ALA:N	1:A:408:HIS:HE1	2.01	0.59
1:A:87:GLY:H	1:A:105:ASN:HD21	1.51	0.59
1:A:263:LEU:HD12	1:A:264:GLU:H	1.67	0.58
1:A:712:VAL:HG12	1:A:713:PRO:O	2.04	0.58
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.84	0.58
1:A:84:LYS:HD3	1:A:755:GLU:CD	2.29	0.58
1:A:185:LYS:HG3	3:A:999:POP:O2	2.03	0.58
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.37	0.58
1:A:308:ASN:OD1	1:A:309:GLN:HG2	2.03	0.58
1:A:721:LYS:O	1:A:724:ASP:HB3	2.02	0.58
1:A:293:LYS:HA	1:A:298:LEU:HB2	1.86	0.57
1:A:176:LEU:N	1:A:176:LEU:HD12	2.19	0.57
1:A:60:PHE:CD1	1:A:74:LYS:HG2	2.39	0.57
1:A:170:ARG:HB3	1:A:448:TYR:OH	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ARG:HG2	1:A:705:TYR:CZ	2.39	0.57
1:A:750:GLN:HA	4:A:873:HOH:O	2.05	0.57
1:A:183:ALA:HA	1:A:657:ILE:HG13	1.86	0.57
1:A:263:LEU:HD12	1:A:264:GLU:N	2.20	0.57
1:A:705:TYR:HD1	1:A:708:LEU:HD11	1.70	0.57
1:A:690:LYS:NZ	1:A:690:LYS:HB2	2.19	0.56
1:A:711:ASN:CB	1:A:712:VAL:HG23	2.35	0.56
1:A:686:ARG:HB3	4:A:881:HOH:O	2.04	0.56
1:A:139:MET:CA	1:A:142:ILE:HD12	2.36	0.56
1:A:185:LYS:HE2	4:A:946:HOH:O	2.05	0.56
1:A:499:ILE:HG23	1:A:738:ARG:HG3	1.87	0.56
1:A:601:LYS:HE3	1:A:612:PHE:O	2.06	0.56
1:A:730:LEU:HB2	1:A:732:ILE:HD12	1.88	0.56
1:A:139:MET:HA	1:A:142:ILE:CD1	2.36	0.56
1:A:581:ILE:O	1:A:581:ILE:HG13	2.04	0.56
1:A:138:GLU:O	1:A:142:ILE:HD12	2.05	0.56
1:A:498:LYS:O	1:A:498:LYS:HG2	2.06	0.56
1:A:736:GLN:HB3	1:A:750:GLN:HG2	1.88	0.56
1:A:176:LEU:HD22	1:A:652:PHE:CE2	2.40	0.56
1:A:82:PRO:O	1:A:85:PHE:HD1	1.88	0.56
1:A:98:ASN:OD1	1:A:100:PRO:HD2	2.06	0.56
1:A:302:GLU:H	1:A:302:GLU:CD	2.14	0.55
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.14	0.55
1:A:170:ARG:O	1:A:448:TYR:HE2	1.89	0.55
1:A:532:GLN:CA	1:A:532:GLN:HE21	2.17	0.55
1:A:692:PHE:CE2	1:A:747:ARG:NH1	2.75	0.55
1:A:32:LYS:HB3	1:A:34:TYR:CE2	2.42	0.55
1:A:153:PRO:O	1:A:154:HIS:HB2	2.06	0.55
1:A:718:ASP:CG	1:A:721:LYS:HB2	2.32	0.55
1:A:399:LEU:HD12	1:A:400:ALA:N	2.21	0.55
1:A:366:GLY:HA3	1:A:408:HIS:CE1	2.42	0.55
1:A:4:ILE:HD13	1:A:146:ARG:CZ	2.37	0.54
1:A:214:GLN:HB2	1:A:441:LEU:HD21	1.89	0.54
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.25	0.54
1:A:219:ASN:O	1:A:223:GLU:HG3	2.08	0.54
1:A:236:SER:HB2	3:A:999:POP:O5	2.08	0.54
1:A:418:ARG:C	1:A:418:ARG:HD2	2.32	0.54
1:A:296:LEU:HD21	1:A:342:MET:CE	2.36	0.54
1:A:385:ASN:OD1	1:A:386:PRO:HD2	2.07	0.54
1:A:510:SER:C	1:A:514:ILE:HD12	2.32	0.54
1:A:90:ASP:HA	1:A:118:TYR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:C	1:A:170:ARG:HG2	2.31	0.54
1:A:191:LYS:O	1:A:194:GLN:HB3	2.08	0.53
1:A:636:GLU:O	1:A:639:ALA:HB3	2.08	0.53
1:A:730:LEU:CD1	1:A:732:ILE:HD11	2.38	0.53
1:A:367:ALA:H	1:A:408:HIS:HE1	1.56	0.53
1:A:576:GLN:HG3	1:A:577:VAL:N	2.22	0.53
1:A:730:LEU:HB2	1:A:732:ILE:HD11	1.89	0.53
1:A:704:ARG:HG2	1:A:705:TYR:CE1	2.44	0.53
1:A:656:ILE:HD11	1:A:676:LEU:HD23	1.91	0.53
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.44	0.53
1:A:371:ASP:OD2	1:A:372:LYS:N	2.42	0.53
1:A:526:LEU:HB2	4:A:819:HOH:O	2.08	0.53
1:A:752:ALA:O	1:A:756:GLU:HG3	2.09	0.53
1:A:59:SER:HB2	1:A:72:VAL:O	2.09	0.52
1:A:155:ILE:O	1:A:158:ILE:HG22	2.10	0.52
1:A:336:PHE:CE2	1:A:436:LYS:HG2	2.45	0.52
1:A:712:VAL:HG12	1:A:713:PRO:N	2.24	0.52
1:A:697:ILE:CD1	1:A:743:LYS:HG3	2.37	0.52
1:A:727:LEU:HD12	1:A:732:ILE:CD1	2.36	0.52
1:A:33:ARG:NH2	1:A:55:GLU:OE2	2.40	0.52
1:A:341:GLN:HA	1:A:344:ILE:HD12	1.92	0.52
1:A:695:ARG:HD3	1:A:745:PHE:CZ	2.45	0.52
1:A:419:ASP:O	1:A:423:LYS:HG3	2.09	0.52
1:A:741:ILE:HG22	1:A:742:THR:N	2.24	0.52
1:A:32:LYS:HE3	1:A:51:GLU:OE1	2.10	0.52
1:A:112:GLN:O	1:A:113:ASP:HB2	2.10	0.52
1:A:61:THR:OG1	1:A:71:GLN:HG2	2.10	0.51
1:A:499:ILE:CD1	1:A:738:ARG:HB3	2.26	0.51
1:A:534:VAL:HG12	1:A:534:VAL:O	2.08	0.51
1:A:367:ALA:H	1:A:408:HIS:CE1	2.29	0.51
1:A:692:PHE:O	1:A:695:ARG:NE	2.41	0.51
1:A:321:GLU:H	1:A:321:GLU:CD	2.17	0.51
1:A:737:TYR:HB2	1:A:744:ILE:HD11	1.92	0.51
1:A:2:ASN:ND2	1:A:5:HIS:NE2	2.56	0.51
1:A:546:LYS:O	1:A:550:HIS:HD2	1.94	0.51
1:A:695:ARG:HD3	1:A:745:PHE:CE2	2.46	0.51
1:A:289:THR:HB	1:A:291:GLU:OE2	2.11	0.51
1:A:495:LEU:CD1	1:A:495:LEU:N	2.74	0.51
1:A:543:LEU:CD2	1:A:581:ILE:HD11	2.41	0.51
1:A:712:VAL:CG1	1:A:713:PRO:N	2.74	0.51
1:A:53:VAL:HG12	1:A:54:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:GLY:HA2	1:A:577:VAL:O	2.12	0.50
1:A:90:ASP:OD2	1:A:92:SER:OG	2.29	0.50
1:A:562:ARG:NH1	1:A:563:PHE:CZ	2.80	0.50
1:A:88:VAL:HB	1:A:93:GLU:OE1	2.12	0.50
1:A:386:PRO:O	1:A:390:GLU:HB2	2.10	0.50
1:A:155:ILE:O	1:A:159:SER:OG	2.30	0.49
1:A:234:ASN:N	1:A:234:ASN:HD22	2.10	0.49
1:A:202:ARG:HD3	1:A:252:PHE:CB	2.43	0.49
1:A:440:VAL:HG12	1:A:441:LEU:HG	1.94	0.49
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.94	0.49
1:A:342:MET:CE	1:A:346:LYS:HG3	2.43	0.49
1:A:590:ASP:N	1:A:591:PRO:CD	2.76	0.49
1:A:150:GLU:HB3	1:A:151:VAL:HG13	1.93	0.49
1:A:64:THR:HG23	1:A:68:GLN:C	2.38	0.49
1:A:709:ALA:HB1	1:A:729:HIS:HB2	1.94	0.49
1:A:538:ALA:HB1	1:A:542:THR:HG21	1.93	0.49
1:A:724:ASP:O	1:A:728:LYS:HB2	2.13	0.49
1:A:730:LEU:HD13	1:A:732:ILE:HD11	1.94	0.49
1:A:477:LYS:NZ	4:A:835:HOH:O	2.39	0.48
1:A:643:ALA:O	1:A:647:THR:HG23	2.13	0.48
1:A:698:TYR:OH	1:A:739:PHE:HD2	1.96	0.48
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.46	0.48
1:A:138:GLU:C	1:A:142:ILE:HD12	2.37	0.48
1:A:241:LYS:O	1:A:453:LEU:HD12	2.14	0.48
1:A:730:LEU:CB	1:A:732:ILE:HD11	2.42	0.48
1:A:403:ASP:HB3	1:A:405:VAL:HG22	1.93	0.48
1:A:424:ALA:O	1:A:428:ARG:HG3	2.14	0.48
1:A:98:ASN:O	1:A:102:VAL:HG23	2.14	0.48
1:A:477:LYS:HE3	4:A:814:HOH:O	2.14	0.48
1:A:102:VAL:HG21	1:A:685:ILE:HD13	1.96	0.48
1:A:306:TYR:CE1	1:A:355:GLY:HA3	2.49	0.48
1:A:367:ALA:N	1:A:408:HIS:CE1	2.82	0.48
1:A:497:GLU:CD	1:A:742:THR:HB	2.38	0.47
1:A:296:LEU:O	1:A:298:LEU:HD23	2.14	0.47
1:A:243:ILE:O	1:A:451:GLY:HA2	2.15	0.47
1:A:464:ASN:HB2	1:A:578:MET:O	2.15	0.47
1:A:266:SER:O	1:A:269:VAL:HG22	2.13	0.47
1:A:520:ARG:O	1:A:521:GLN:HG2	2.14	0.47
1:A:176:LEU:N	1:A:176:LEU:CD1	2.77	0.47
1:A:219:ASN:N	1:A:220:PRO:CD	2.78	0.47
1:A:375:LEU:O	1:A:379:SER:OG	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:C	1:A:695:ARG:HG2	2.39	0.47
1:A:708:LEU:HD23	1:A:758:ARG:O	2.15	0.47
1:A:249:ASN:ND2	1:A:249:ASN:H	2.13	0.47
1:A:656:ILE:CD1	1:A:676:LEU:HD21	2.45	0.47
1:A:300:GLY:O	1:A:303:SER:OG	2.29	0.47
1:A:178:THR:HG22	1:A:455:ILE:HG22	1.96	0.46
1:A:633:GLN:HE21	1:A:633:GLN:HB3	1.36	0.46
1:A:136:THR:O	1:A:140:VAL:N	2.42	0.46
1:A:248:ASN:O	1:A:251:GLY:N	2.47	0.46
1:A:281:PHE:O	1:A:285:LEU:HG	2.16	0.46
1:A:430:PHE:HA	1:A:433:LEU:HD12	1.97	0.46
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.98	0.46
1:A:705:TYR:HD1	1:A:708:LEU:CD1	2.26	0.46
1:A:99:GLU:N	1:A:100:PRO:HD2	2.31	0.46
1:A:35:ILE:O	1:A:50:GLY:N	2.48	0.46
1:A:213:GLN:O	1:A:217:GLN:HG2	2.15	0.46
1:A:654:ARG:NH1	4:A:816:HOH:O	2.31	0.46
1:A:146:ARG:HB3	1:A:150:GLU:HB3	1.98	0.46
1:A:399:LEU:HD12	1:A:401:GLY:N	2.31	0.45
1:A:576:GLN:CG	1:A:577:VAL:N	2.79	0.45
1:A:459:GLU:C	1:A:460:ILE:HG12	2.42	0.45
1:A:369:LEU:HB2	1:A:394:MET:HE1	1.98	0.45
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.72	0.45
1:A:342:MET:HE3	1:A:346:LYS:HG3	1.98	0.45
1:A:397:ARG:HG3	1:A:406:ALA:HB2	1.99	0.45
1:A:376:ASN:O	1:A:380:THR:OG1	2.35	0.45
1:A:542:THR:HG22	1:A:543:LEU:N	2.32	0.45
1:A:698:TYR:CE1	1:A:720:GLN:HG2	2.51	0.45
1:A:397:ARG:C	1:A:398:ILE:HD12	2.42	0.45
1:A:590:ASP:N	1:A:591:PRO:HD3	2.32	0.45
1:A:233:ASN:OD1	1:A:235:ASN:N	2.28	0.45
1:A:233:ASN:OD1	1:A:234:ASN:N	2.49	0.45
1:A:296:LEU:O	1:A:297:HIS:HB2	2.17	0.45
1:A:490:GLU:OE2	1:A:695:ARG:NH1	2.34	0.45
1:A:610:LYS:HB3	1:A:610:LYS:HE2	1.26	0.45
1:A:690:LYS:NZ	1:A:690:LYS:CB	2.79	0.45
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.64	0.45
1:A:246:GLN:HB2	1:A:255:GLY:C	2.41	0.45
1:A:337:SER:OG	1:A:339:GLU:HG2	2.17	0.45
1:A:597:GLU:O	1:A:601:LYS:HG3	2.16	0.45
1:A:223:GLU:O	1:A:227:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:O	1:A:256:ALA:HB2	2.17	0.44
1:A:339:GLU:HG2	1:A:339:GLU:H	1.36	0.44
1:A:418:ARG:O	1:A:421:LEU:HB3	2.17	0.44
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.82	0.44
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.99	0.44
1:A:231:THR:HG23	1:A:275:GLU:OE2	2.18	0.44
1:A:292:GLU:OE1	1:A:328:ARG:NH1	2.48	0.44
1:A:499:ILE:CD1	1:A:745:PHE:CG	2.98	0.44
1:A:672:VAL:O	1:A:676:LEU:HG	2.16	0.44
1:A:726:VAL:HG12	1:A:730:LEU:HD12	1.99	0.44
1:A:551:PHE:HB2	1:A:558:TYR:CD2	2.53	0.44
1:A:396:PRO:O	1:A:398:ILE:HD12	2.17	0.44
1:A:741:ILE:HG22	1:A:742:THR:OG1	2.17	0.44
1:A:129:PHE:HD1	1:A:663:LEU:O	2.01	0.44
1:A:247:PHE:HE2	1:A:253:ILE:HG12	1.77	0.44
1:A:518:ASP:HB2	1:A:635:LYS:HD2	1.99	0.44
1:A:521:GLN:HA	1:A:522:PRO:HA	1.70	0.44
1:A:614:ASP:OD1	1:A:615:PRO:HD2	2.16	0.44
1:A:4:ILE:CD1	1:A:146:ARG:NH2	2.78	0.44
1:A:642:MET:O	1:A:646:GLU:HB2	2.18	0.44
1:A:734:PRO:HA	1:A:737:TYR:CZ	2.53	0.44
1:A:715:ASP:O	1:A:716:ALA:HB2	2.17	0.44
1:A:2:ASN:HD22	1:A:5:HIS:CD2	2.35	0.44
1:A:23:ASP:N	1:A:23:ASP:OD1	2.51	0.44
1:A:144:LYS:HG2	1:A:199:VAL:HG12	2.00	0.44
1:A:91:MET:HE2	1:A:106:LEU:HD13	1.96	0.43
1:A:395:GLU:HA	1:A:407:GLN:O	2.18	0.43
1:A:280:ILE:N	1:A:280:ILE:CD1	2.77	0.43
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.81	0.43
1:A:656:ILE:CD1	1:A:676:LEU:CD2	2.96	0.43
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.73	0.43
1:A:535:PHE:CD2	1:A:535:PHE:N	2.86	0.43
1:A:709:ALA:CB	1:A:729:HIS:HB2	2.49	0.43
1:A:241:LYS:HD2	1:A:243:ILE:HD11	2.00	0.43
1:A:322:ASP:HA	1:A:325:LYS:HE3	2.01	0.43
1:A:397:ARG:HB3	1:A:404:LEU:HD21	2.01	0.43
1:A:170:ARG:HB3	1:A:448:TYR:CZ	2.54	0.43
1:A:301:PRO:C	1:A:303:SER:N	2.76	0.43
1:A:345:PHE:N	1:A:345:PHE:CD1	2.74	0.43
1:A:385:ASN:HD22	1:A:388:VAL:HG23	1.83	0.43
1:A:488:LYS:HB2	1:A:488:LYS:HE3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:OD2	1:A:41:PRO:HD2	2.18	0.43
1:A:257:SER:HA	1:A:438:ASN:OD1	2.19	0.43
1:A:683:GLU:O	1:A:687:ILE:HG13	2.19	0.43
1:A:129:PHE:CE1	1:A:662:GLN:HA	2.54	0.42
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.72	0.42
1:A:471:ILE:HG23	1:A:471:ILE:HD12	1.70	0.42
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.19	0.42
1:A:567:GLU:HA	1:A:579:TYR:O	2.20	0.42
1:A:142:ILE:HG22	1:A:142:ILE:O	2.20	0.42
1:A:286:ALA:O	1:A:321:GLU:HB3	2.20	0.42
1:A:656:ILE:HD11	1:A:676:LEU:CD2	2.49	0.42
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.50	0.42
1:A:693:PRO:HD2	1:A:746:PHE:O	2.20	0.42
1:A:134:ILE:HG22	1:A:139:MET:HE3	2.02	0.42
1:A:398:ILE:O	1:A:398:ILE:HG22	2.17	0.42
1:A:696:ILE:O	1:A:744:ILE:N	2.49	0.42
1:A:345:PHE:HD1	1:A:345:PHE:HA	1.53	0.42
1:A:562:ARG:NH1	1:A:563:PHE:CE1	2.88	0.42
1:A:584:TRP:N	1:A:584:TRP:CD1	2.87	0.42
1:A:7:ARG:HA	1:A:12:HIS:CG	2.55	0.42
1:A:36:TRP:NE1	1:A:80:ARG:HG3	2.34	0.42
1:A:155:ILE:HG23	1:A:156:PHE:N	2.34	0.42
1:A:421:LEU:HA	1:A:592:LEU:HD11	2.02	0.42
1:A:532:GLN:HE21	1:A:532:GLN:N	2.18	0.41
1:A:376:ASN:O	1:A:379:SER:HB2	2.20	0.41
1:A:698:TYR:OH	1:A:740:GLY:O	2.20	0.41
1:A:698:TYR:CE1	1:A:720:GLN:CG	3.03	0.41
1:A:366:GLY:CA	1:A:408:HIS:CE1	3.03	0.41
1:A:726:VAL:CG1	1:A:730:LEU:HD11	2.49	0.41
1:A:698:TYR:CE2	1:A:720:GLN:HG2	2.55	0.41
1:A:706:TYR:CD1	1:A:706:TYR:C	2.99	0.41
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.84	0.41
1:A:353:HIS:HB2	1:A:378:ALA:HB2	2.03	0.41
1:A:211:LEU:HB3	1:A:212:GLU:H	1.50	0.41
1:A:495:LEU:N	1:A:495:LEU:HD13	2.36	0.41
1:A:722:ALA:C	1:A:724:ASP:N	2.78	0.41
1:A:238:ARG:HH11	1:A:264:GLU:CD	2.29	0.41
1:A:348:ILE:HD13	1:A:348:ILE:HA	1.89	0.41
1:A:373:THR:O	1:A:376:ASN:N	2.54	0.41
1:A:457:GLY:HA3	4:A:865:HOH:O	2.20	0.41
1:A:696:ILE:O	1:A:743:LYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.46	0.41
1:A:84:LYS:HD3	1:A:755:GLU:OE2	2.21	0.41
1:A:293:LYS:CA	1:A:298:LEU:HB2	2.50	0.41
1:A:359:PHE:HE1	1:A:415:SER:HA	1.86	0.41
1:A:697:ILE:HD13	1:A:743:LYS:CG	2.47	0.41
1:A:738:ARG:HB2	1:A:745:PHE:HB2	2.01	0.41
1:A:267:ARG:O	1:A:267:ARG:HG3	2.21	0.40
1:A:727:LEU:CD1	1:A:732:ILE:HD13	2.44	0.40
1:A:137:GLN:NE2	1:A:141:ASP:OD2	2.54	0.40
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.57	0.40
1:A:433:LEU:O	1:A:436:LYS:HB3	2.22	0.40
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.56	0.40
1:A:61:THR:O	1:A:61:THR:HG22	2.21	0.40
1:A:144:LYS:HG2	1:A:199:VAL:CG1	2.51	0.40
1:A:698:TYR:CE1	1:A:740:GLY:O	2.75	0.40
1:A:172:ASN:OD1	1:A:448:TYR:HA	2.22	0.40
1:A:175:LEU:C	1:A:176:LEU:HD12	2.46	0.40
1:A:727:LEU:HA	1:A:732:ILE:HD12	2.03	0.40
1:A:733:ASP:HA	1:A:734:PRO:HD3	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLU:O	1:A:402:ARG:NH2[2_665]	2.07	0.13

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	734/762 (96%)	675 (92%)	49 (7%)	10 (1%)	9	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ASN
1	A	373	THR
1	A	144	LYS
1	A	410	ASN
1	A	7	ARG
1	A	64	THR
1	A	249	ASN
1	A	650	PRO
1	A	734	PRO
1	A	83	ILE

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	625/665 (94%)	513 (82%)	112 (18%)	2 5

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	HIS
1	A	8	THR
1	A	16	LYS
1	A	23	ASP
1	A	24	LEU
1	A	27	LEU
1	A	32	LYS
1	A	35	ILE
1	A	43	GLU
1	A	44	ARG
1	A	46	SER
1	A	53	VAL
1	A	57	SER
1	A	61	THR

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Mol	Chain	Res	Type
1	A	63	LYS
1	A	64	THR
1	A	71	GLN
1	A	73	LYS
1	A	83	ILE
1	A	89	GLU
1	A	92	SER
1	A	94	LEU
1	A	138	GLU
1	A	148	ARG
1	A	150	GLU
1	A	158	ILE
1	A	159	SER
1	A	211	LEU
1	A	213	GLN
1	A	229	LYS
1	A	236	SER
1	A	237	SER
1	A	245	ILE
1	A	249	ASN
1	A	253	ILE
1	A	265	LYS
1	A	267	ARG
1	A	272	SER
1	A	280	ILE
1	A	291	GLU
1	A	294	LYS
1	A	302	GLU
1	A	313	VAL
1	A	316	LYS
1	A	321	GLU
1	A	328	ARG
1	A	339	GLU
1	A	342	MET
1	A	351	ILE
1	A	357	ILE
1	A	358	LYS
1	A	360	GLU
1	A	368	VAL
1	A	369	LEU
1	A	380	THR
1	A	381	VAL

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Mol	Chain	Res	Type
1	A	387	SER
1	A	394	MET
1	A	399	LEU
1	A	405	VAL
1	A	407	GLN
1	A	412	GLU
1	A	422	VAL
1	A	436	LYS
1	A	443	SER
1	A	444	GLU
1	A	455	ILE
1	A	456	SER
1	A	460	ILE
1	A	465	SER
1	A	480	GLN
1	A	486	MET
1	A	488	LYS
1	A	491	GLN
1	A	495	LEU
1	A	499	ILE
1	A	520	ARG
1	A	532	GLN
1	A	542	THR
1	A	562	ARG
1	A	581	ILE
1	A	594	GLN
1	A	604	SER
1	A	609	THR
1	A	610	LYS
1	A	633	GLN
1	A	640	SER
1	A	646	GLU
1	A	647	THR
1	A	656	ILE
1	A	657	ILE
1	A	661	LYS
1	A	666	LYS
1	A	685	ILE
1	A	690	LYS
1	A	695	ARG
1	A	697	ILE
1	A	703	LYS

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Mol	Chain	Res	Type
1	A	717	GLU
1	A	721	LYS
1	A	727	LEU
1	A	728	LYS
1	A	733	ASP
1	A	738	ARG
1	A	741	ILE
1	A	743	LYS
1	A	744	ILE
1	A	747	ARG
1	A	751	LEU
1	A	753	ARG
1	A	754	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	171	GLN
1	A	219	ASN
1	A	234	ASN
1	A	259	GLN
1	A	283	GLN
1	A	408	HIS
1	A	439	ASN
1	A	479	GLN
1	A	480	GLN
1	A	485	HIS
1	A	541	ASN
1	A	550	HIS
1	A	613	ASN
1	A	633	GLN
1	A	637	GLN
1	A	731	ASN
1	A	736	GLN

5.3.3 RNA ⓘ

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 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	POP	A	999	2	6,8,8	1.34	0	12,13,13	1.01	1 (8%)

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	POP	A	999	2	-	1/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	POP	O2-P1-O	2.02	111.40	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	POP	P2-O-P1-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	POP	2	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

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.