WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 07:48 PM EST

PDB ID	:	1MNE
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:

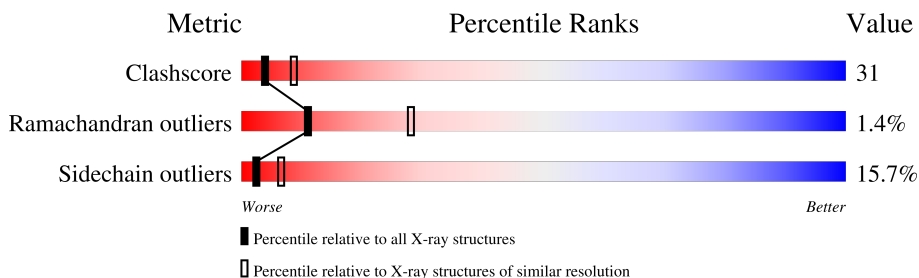|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Clashscore		31
Ramachandran outliers		1.4%
Sidechain outliers		15.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	41% 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.

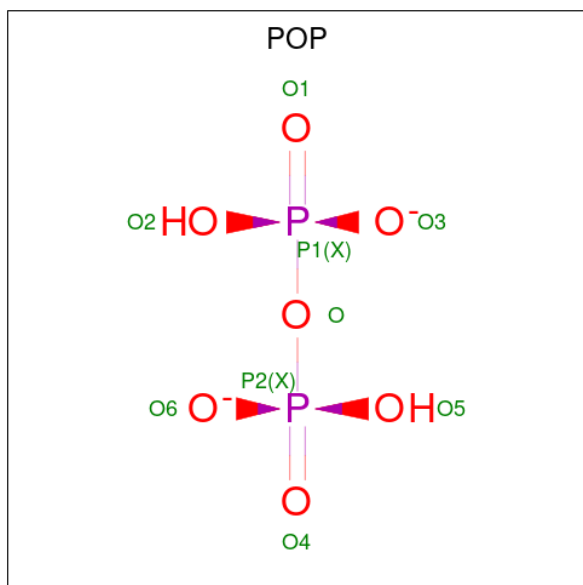| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	0	0
			5869	3728	1012	1113	16			

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).

POP

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total 148	O 148	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
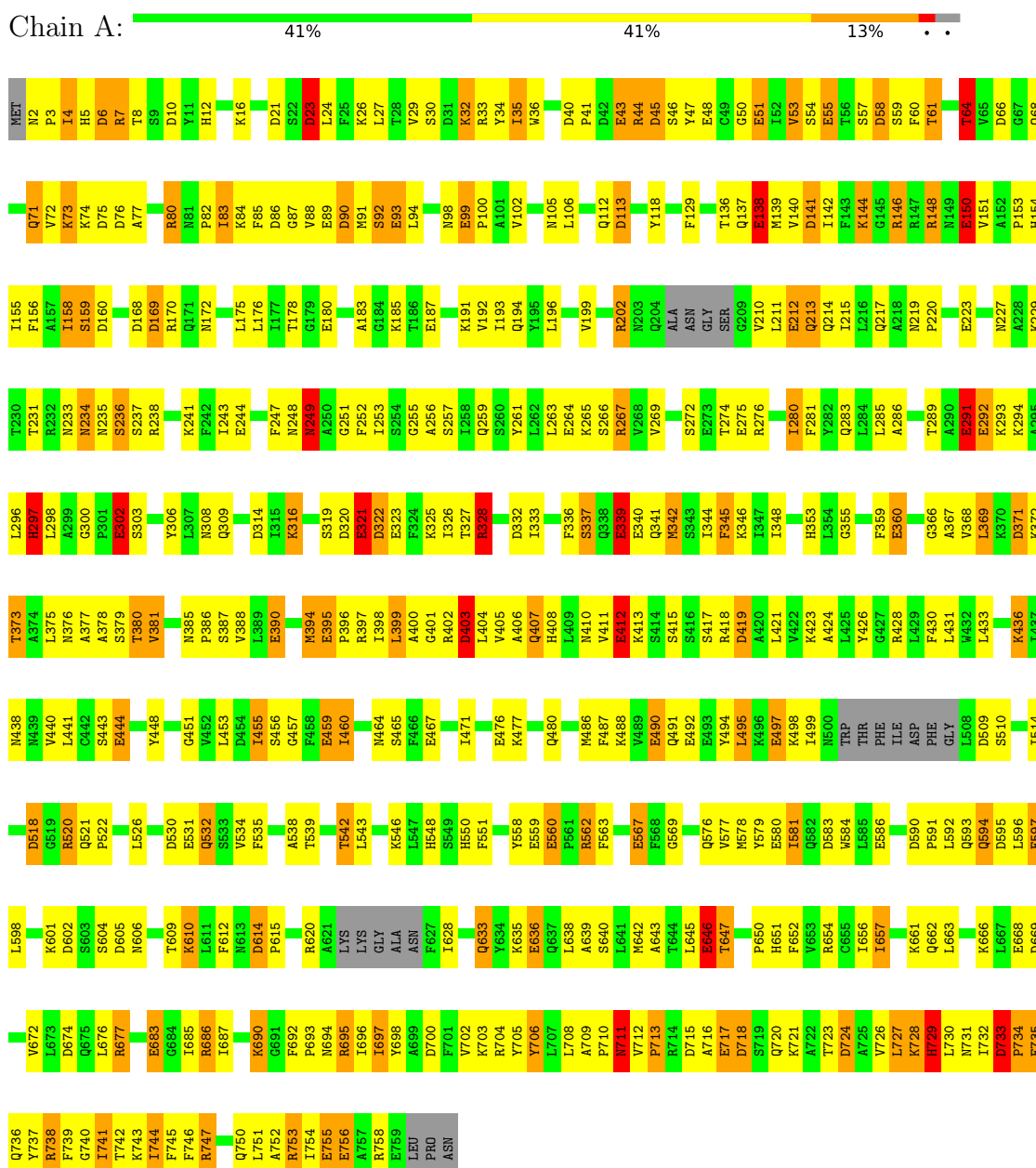
4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.93	46/5978 (0.8%)	1.41	87/8073 (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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	GLU	CD-OE2	6.16	1.32	1.25
1	A	497	GLU	CD-OE2	6.00	1.32	1.25
1	A	187	GLU	CD-OE2	5.88	1.32	1.25
1	A	43	GLU	CD-OE2	5.83	1.32	1.25
1	A	150	GLU	CD-OE2	5.83	1.32	1.25
1	A	412	GLU	CD-OE2	5.82	1.32	1.25
1	A	636	GLU	CD-OE2	5.80	1.32	1.25
1	A	180	GLU	CD-OE2	5.79	1.32	1.25
1	A	580	GLU	CD-OE2	5.77	1.31	1.25
1	A	390	GLU	CD-OE2	5.77	1.31	1.25
1	A	668	GLU	CD-OE2	5.75	1.31	1.25
1	A	302	GLU	CD-OE2	5.74	1.31	1.25
1	A	321	GLU	CD-OE2	5.72	1.31	1.25
1	A	212	GLU	CD-OE2	5.72	1.31	1.25
1	A	444	GLU	CD-OE2	5.68	1.31	1.25
1	A	735	GLU	CD-OE2	5.67	1.31	1.25
1	A	89	GLU	CD-OE2	5.66	1.31	1.25
1	A	48	GLU	CD-OE2	5.60	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	GLU	CD-OE2	5.58	1.31	1.25
1	A	755	GLU	CD-OE2	5.57	1.31	1.25
1	A	683	GLU	CD-OE2	5.55	1.31	1.25
1	A	291	GLU	CD-OE2	5.55	1.31	1.25
1	A	756	GLU	CD-OE2	5.55	1.31	1.25
1	A	476	GLU	CD-OE2	5.54	1.31	1.25
1	A	55	GLU	CD-OE2	5.54	1.31	1.25
1	A	99	GLU	CD-OE2	5.54	1.31	1.25
1	A	339	GLU	CD-OE2	5.52	1.31	1.25
1	A	360	GLU	CD-OE2	5.51	1.31	1.25
1	A	395	GLU	CD-OE2	5.50	1.31	1.25
1	A	531	GLU	CD-OE2	5.50	1.31	1.25
1	A	586	GLU	CD-OE2	5.50	1.31	1.25
1	A	93	GLU	CD-OE2	5.48	1.31	1.25
1	A	340	GLU	CD-OE2	5.46	1.31	1.25
1	A	467	GLU	CD-OE2	5.45	1.31	1.25
1	A	717	GLU	CD-OE2	5.44	1.31	1.25
1	A	138	GLU	CD-OE2	5.43	1.31	1.25
1	A	323	GLU	CD-OE2	5.35	1.31	1.25
1	A	459	GLU	CD-OE2	5.33	1.31	1.25
1	A	560	GLU	CD-OE2	5.33	1.31	1.25
1	A	646	GLU	CD-OE2	5.32	1.31	1.25
1	A	51	GLU	CD-OE2	5.27	1.31	1.25
1	A	597	GLU	CD-OE2	5.23	1.31	1.25
1	A	490	GLU	CD-OE2	5.19	1.31	1.25
1	A	559	GLU	CD-OE2	5.14	1.31	1.25
1	A	567	GLU	CD-OE2	5.07	1.31	1.25
1	A	244	GLU	CD-OE2	5.07	1.31	1.25

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	HIS	CA-CB-CG	-8.03	99.95	113.60
1	A	202	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	605	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	A	66	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	45	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	A	276	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	A	168	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	168	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	21	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	332	ASP	CB-CG-OD2	-6.95	112.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	614	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	A	605	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	76	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	A	729	HIS	CA-CB-CG	-6.59	102.39	113.60
1	A	141	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	314	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	371	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	322	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	58	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	23	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	328	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	10	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	711	ASN	CB-CA-C	-6.25	97.89	110.40
1	A	169	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	614	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	169	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	345	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	A	58	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	674	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	530	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	A	602	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	724	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	75	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	6	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	45	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	332	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	23	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	711	ASN	O-C-N	5.96	132.24	122.70
1	A	320	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	76	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	113	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	345	PHE	CB-CG-CD2	5.86	124.90	120.80
1	A	718	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	86	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	403	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	21	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	718	ASP	CB-CG-OD2	-5.82	113.07	118.30
1	A	322	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	261	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	A	419	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	509	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	160	ASP	CB-CG-OD2	-5.72	113.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	700	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	509	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	66	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	371	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	595	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	606	ASN	CB-CA-C	5.62	121.65	110.40
1	A	44	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	674	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	669	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	314	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	75	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	602	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	530	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	713	PRO	N-CA-CB	5.45	109.84	103.30
1	A	320	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	518	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	494	TYR	CB-CG-CD2	5.37	124.22	121.00
1	A	146	ARG	N-CA-CB	5.36	120.25	110.60
1	A	724	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	733	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	30	SER	N-CA-CB	5.28	118.42	110.50
1	A	86	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	160	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	583	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	90	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	706	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	10	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	419	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	6	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	148	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	66	ASP	CB-CA-C	-5.07	100.26	110.40
1	A	620	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	677	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	80	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	355	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	355	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 (355) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:397:ARG:HD2	1:A:404:LEU:HD21	1.68	0.75
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:45:ASP:CG	1:A:677:ARG:HH22	1.96	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:91:MET:HE1	1:A:106:LEU:HD13	1.76	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:MET:HE2	1:A:106:LEU:HD13	1.82	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:698:TYR:OH	1:A:740:GLY:O	2.20	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: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:296:LEU:HD21	1:A:342:MET:CE	2.36	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: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:385:ASN:OD1	1:A:386:PRO:HD2	2.07	0.54
1:A:90:ASP:HA	1:A:118:TYR:O	2.08	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:84:LYS:HD3	1:A:755:GLU:CD	2.29	0.53
1:A:576:GLN:HG3	1:A:577:VAL:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:LEU:HB2	1:A:732:ILE:HD11	1.89	0.53
1:A:296:LEU:HD21	1:A:342:MET:HE1	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: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:302:GLU:H	1:A:302:GLU:CD	2.14	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
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:718:ASP:CG	1:A:721:LYS:HB2	2.32	0.50
1:A:562:ARG:NH1	1:A:563:PHE:CZ	2.80	0.50
1:A:418:ARG:C	1:A:418:ARG:HD2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:ASP:C	1:A:170:ARG:HG2	2.31	0.49
1:A:510:SER:C	1:A:514:ILE:HD12	2.32	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:241:LYS:O	1:A:453:LEU:HD12	2.14	0.48
1:A:369:LEU:HB2	1:A:394:MET:HE1	1.96	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: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:321:GLU:CD	1:A:321:GLU:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:LEU:HD12	1:A:106:LEU:HA	1.72	0.45
1:A:397:ARG:HG3	1:A:406:ALA:HB2	1.99	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:C	1:A:142:ILE:HD12	2.37	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: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: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
1:A:497:GLU:CD	1:A:742:THR:HB	2.38	0.43
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:91:MET:HE2	1:A:106:LEU:CD1	2.48	0.42
1:A:142:ILE:HG22	1:A:142:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:694:ASN:C	1:A:695:ARG:HG2	2.39	0.42
1:A:326:ILE:HG22	1:A:327:THR:N	2.33	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:192:VAL:HG12	1:A:193:ILE:N	2.32	0.41
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: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:376:ASN:O	1:A:380:THR:OG1	2.35	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: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: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
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.46	0.41
1:A:64:THR:HG23	1:A:68:GLN:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:459:GLU:C	1:A:460:ILE:HG12	2.42	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/762 (96%)	675 (92%)	49 (7%)	10 (1%)	11	28

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

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	650	PRO
1	A	734	PRO
1	A	83	ILE

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	625/665 (94%)	527 (84%)	98 (16%)	2	6

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
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
1	A	64	THR
1	A	71	GLN
1	A	73	LYS
1	A	83	ILE
1	A	92	SER
1	A	94	LEU
1	A	138	GLU
1	A	148	ARG

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Mol	Chain	Res	Type
1	A	150	GLU
1	A	158	ILE
1	A	159	SER
1	A	213	GLN
1	A	234	ASN
1	A	236	SER
1	A	237	SER
1	A	249	ASN
1	A	265	LYS
1	A	267	ARG
1	A	272	SER
1	A	280	ILE
1	A	283	GLN
1	A	291	GLU
1	A	294	LYS
1	A	302	GLU
1	A	316	LYS
1	A	321	GLU
1	A	328	ARG
1	A	337	SER
1	A	339	GLU
1	A	342	MET
1	A	360	GLU
1	A	368	VAL
1	A	369	LEU
1	A	375	LEU
1	A	380	THR
1	A	381	VAL
1	A	387	SER
1	A	394	MET
1	A	399	LEU
1	A	407	GLN
1	A	412	GLU
1	A	417	SER
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

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Mol	Chain	Res	Type
1	A	486	MET
1	A	487	PHE
1	A	491	GLN
1	A	495	LEU
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	657	ILE
1	A	661	LYS
1	A	666	LYS
1	A	690	LYS
1	A	695	ARG
1	A	697	ILE
1	A	703	LYS
1	A	717	GLU
1	A	727	LEU
1	A	728	LYS
1	A	731	ASN
1	A	733	ASP
1	A	738	ARG
1	A	741	ILE
1	A	744	ILE
1	A	747	ARG
1	A	753	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	137	GLN
1	A	219	ASN
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	283	GLN
1	A	376	ASN
1	A	408	HIS
1	A	439	ASN
1	A	485	HIS
1	A	541	ASN
1	A	550	HIS
1	A	594	GLN
1	A	633	GLN
1	A	729	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.29	0	13,13,13	1.00	1 (7%)

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(^{o})	Ideal(^{o})
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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.