



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:26 PM GMT

PDB ID : 1FMW  
Title : CRYSTAL STRUCTURE OF THE MGATP COMPLEX FOR THE MOTOR  
DOMAIN OF DICTYOSTELIUM MYOSIN II  
Authors : Bauer, C.B.; Holden, H.M.; Thoden, J.B.; Smith, R.; Rayment, I.  
Deposited on : 2000-08-18  
Resolution : 2.15 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

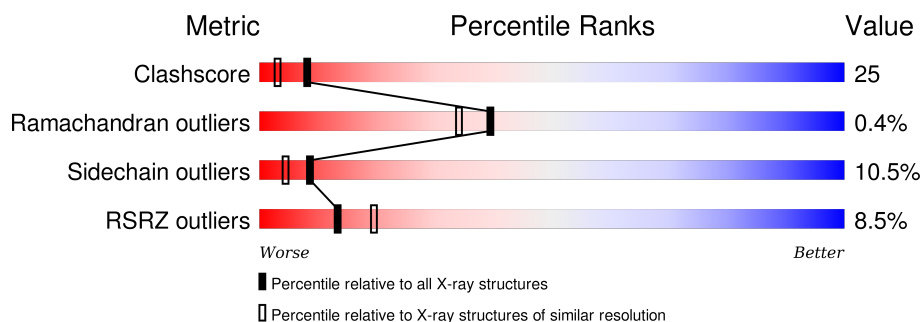
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	761	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6368 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 II HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	2	0
			5864	3726	1012	1110	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	CONFLICT	UNP P08799
A	489	VAL	LEU	CONFLICT	UNP P08799
A	760	PRO	-	CLONING ARTIFACT	UNP P08799
A	761	ASN	-	CLONING ARTIFACT	UNP P08799

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

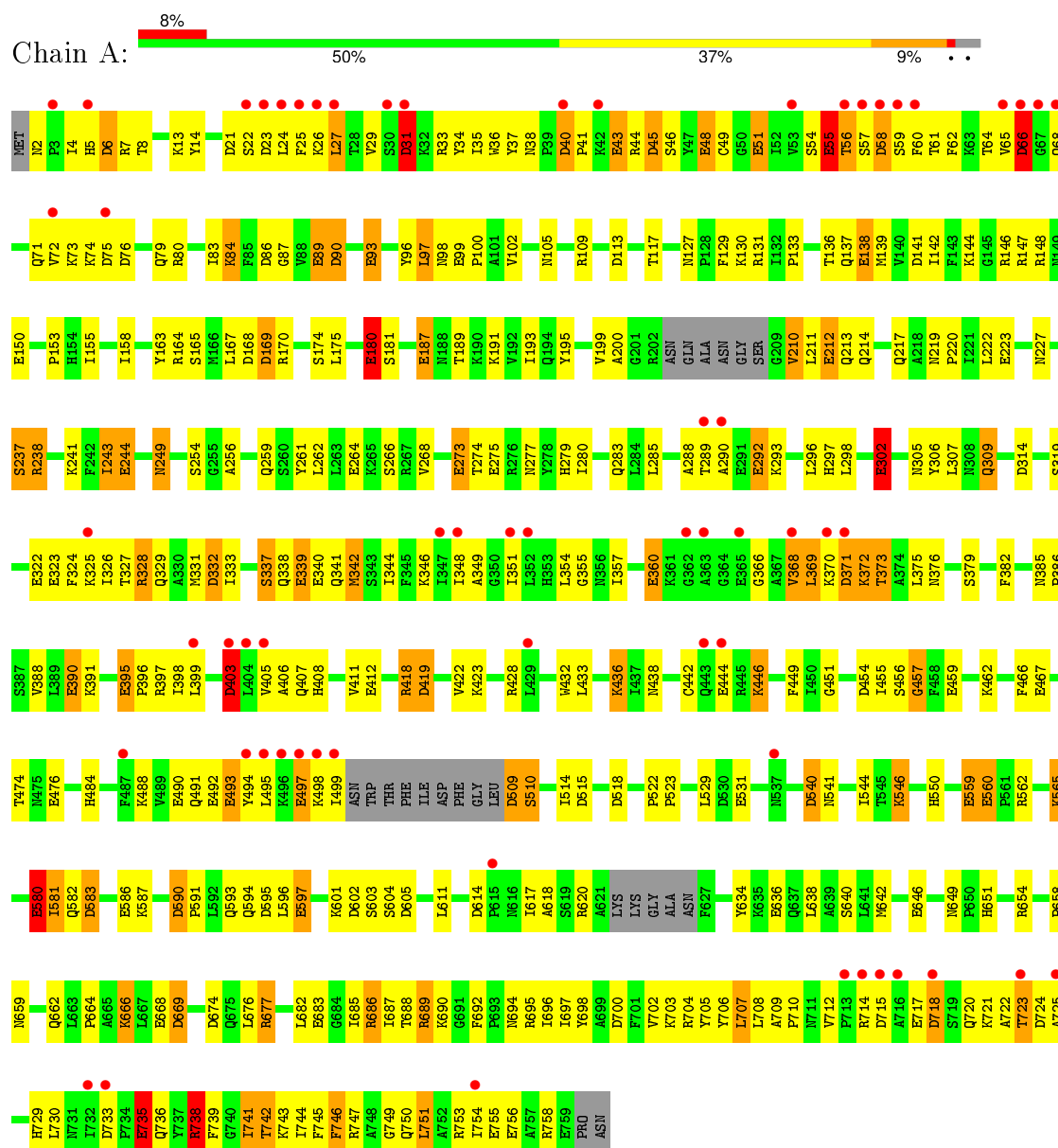
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	472	Total O 472 472	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

#### • Molecule 1: MYOSIN II HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.10 Å   180.40 Å   54.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	100.00 – 2.15 25.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.0 (100.00-2.15) 92.7 (25.49-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.90 (at 2.15 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.206 ,   0.286 0.201 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 117.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52350 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	1.05	43/5985 (0.7%)	1.47	90/8088 (1.1%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	GLU	CD-OE2	6.84	1.33	1.25
1	A	339	GLU	CD-OE2	6.74	1.33	1.25
1	A	467	GLU	CD-OE2	6.73	1.33	1.25
1	A	444	GLU	CD-OE2	6.58	1.32	1.25
1	A	275	GLU	CD-OE2	6.50	1.32	1.25
1	A	412	GLU	CD-OE2	6.41	1.32	1.25
1	A	244	GLU	CD-OE2	6.25	1.32	1.25
1	A	390	GLU	CD-OE2	6.24	1.32	1.25
1	A	735	GLU	CD-OE2	6.19	1.32	1.25
1	A	89	GLU	CD-OE2	6.17	1.32	1.25
1	A	459	GLU	CD-OE2	6.15	1.32	1.25
1	A	48	GLU	CD-OE2	6.07	1.32	1.25
1	A	668	GLU	CD-OE2	6.05	1.32	1.25
1	A	490	GLU	CD-OE2	5.97	1.32	1.25
1	A	340	GLU	CD-OE2	5.92	1.32	1.25
1	A	756	GLU	CD-OE2	5.91	1.32	1.25
1	A	212	GLU	CD-OE2	5.89	1.32	1.25
1	A	360	GLU	CD-OE2	5.85	1.32	1.25
1	A	646	GLU	CD-OE2	5.84	1.32	1.25
1	A	93	GLU	CD-OE2	5.83	1.32	1.25
1	A	683	GLU	CD-OE2	5.80	1.32	1.25
1	A	273	GLU	CD-OE2	5.76	1.31	1.25
1	A	187	GLU	CD-OE2	5.73	1.31	1.25
1	A	559	GLU	CD-OE2	5.72	1.31	1.25
1	A	55	GLU	CD-OE2	5.60	1.31	1.25
1	A	476	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	138	GLU	CD-OE2	5.59	1.31	1.25
1	A	180	GLU	CD-OE2	5.59	1.31	1.25
1	A	717	GLU	CD-OE2	5.55	1.31	1.25
1	A	302	GLU	CD-OE2	5.48	1.31	1.25
1	A	395	GLU	CD-OE2	5.43	1.31	1.25
1	A	323	GLU	CD-OE2	5.41	1.31	1.25
1	A	580	GLU	CD-OE2	5.35	1.31	1.25
1	A	51	GLU	CD-OE2	5.32	1.31	1.25
1	A	597	GLU	CD-OE2	5.31	1.31	1.25
1	A	292	GLU	CD-OE2	5.30	1.31	1.25
1	A	586	GLU	CD-OE2	5.29	1.31	1.25
1	A	492	GLU	CD-OE2	5.29	1.31	1.25
1	A	43	GLU	CD-OE2	5.22	1.31	1.25
1	A	560	GLU	CD-OE2	5.18	1.31	1.25
1	A	497	GLU	CD-OE2	5.15	1.31	1.25
1	A	493	GLU	CD-OE2	5.13	1.31	1.25
1	A	636	GLU	CD-OE2	5.04	1.31	1.25

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	CB-CG-OD2	-9.32	109.91	118.30
1	A	654	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	A	90	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	A	45	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	A	614	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	A	23	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	753	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	169	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	58	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	238	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	6	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	A	90	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	169	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	A	515	ASP	CB-CG-OD1	7.65	125.19	118.30
1	A	45	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	689	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	31	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	724	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	733	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	669	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	733	ASP	CB-CG-OD1	6.96	124.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	113	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	A	674	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	148	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	724	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	515	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	A	518	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	21	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	602	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	419	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	66	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	518	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	509	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	332	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	700	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	249	ASN	CA-CB-CG	-6.30	99.55	113.40
1	A	602	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	58	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	454	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	23	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	715	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	614	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	620	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	31	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	540	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	371	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	595	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	200	ALA	CB-CA-C	-5.89	101.26	110.10
1	A	540	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	718	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	238	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	76	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	686	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	595	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	758	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	454	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	164	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	590	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	562	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	403	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	605	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	677	ARG	NE-CZ-NH2	-5.52	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	40	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	40	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	715	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	674	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	683	GLU	N-CA-CB	5.41	120.34	110.60
1	A	428	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	146	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	718	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	649	ASN	N-CA-C	-5.35	96.56	111.00
1	A	700	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	109	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	66	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	113	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	746	PHE	CB-CA-C	-5.26	99.88	110.40
1	A	371	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	583	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	457	GLY	N-CA-C	-5.19	100.13	113.10
1	A	168	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	148	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	314	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	262	LEU	N-CA-CB	-5.10	100.20	110.40
1	A	418	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	23	ASP	CB-CA-C	-5.06	100.27	110.40
1	A	738	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	332	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	168	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5864	0	5751	286	3
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	11	3	0
4	A	472	0	0	12	3
All	All	6368	0	5762	286	3

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 25.

All (286) 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:398:ILE:HD13	1:A:407:GLN:HG3	1.32	1.05
1:A:61:THR:HG23	1:A:71:GLN:HG3	1.41	1.02
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.41	1.02
1:A:293:LYS:HA	1:A:298:LEU:HD12	1.50	0.93
1:A:369:LEU:HD23	1:A:375:LEU:HD12	1.52	0.92
1:A:397:ARG:HA	1:A:406:ALA:HA	1.54	0.89
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.04	0.87
1:A:217:GLN:HG3	1:A:333:ILE:HD12	1.57	0.85
1:A:703:LYS:HG2	1:A:714:ARG:HE	1.42	0.83
1:A:97:LEU:HB2	1:A:689:ARG:HD2	1.59	0.82
1:A:369:LEU:CD2	1:A:375:LEU:HD12	2.10	0.81
1:A:698:TYR:CZ	1:A:720:GLN:HG3	2.16	0.81
1:A:342:MET:HA	1:A:342:MET:CE	2.11	0.79
1:A:322:GLU:HA	1:A:325:LYS:HD2	1.65	0.79
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.14	0.77
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.20	0.77
1:A:48:GLU:HG2	1:A:65:VAL:CG2	2.16	0.76
1:A:289:THR:HG22	1:A:292:GLU:OE1	1.85	0.75
1:A:499:ILE:HD13	1:A:738:ARG:HB3	1.68	0.75
1:A:61:THR:HG23	1:A:71:GLN:CG	2.16	0.75
1:A:217:GLN:HG3	1:A:333:ILE:CD1	2.16	0.75
1:A:342:MET:HE1	1:A:342:MET:HA	1.67	0.74
1:A:2:ASN:ND2	1:A:5:HIS:ND1	2.34	0.74
1:A:499:ILE:HD11	1:A:738:ARG:O	1.87	0.74
1:A:494:TYR:OH	1:A:692:PHE:HB2	1.88	0.73
1:A:546:LYS:HE2	1:A:550:HIS:HE1	1.52	0.73
1:A:366:GLY:HA3	1:A:408:HIS:CD2	2.23	0.72
1:A:141:ASP:HB3	1:A:144:LYS:HE3	1.72	0.72
1:A:62:PHE:HE2	1:A:72:VAL:HG23	1.53	0.72
1:A:48:GLU:HG3	4:A:1564:HOH:O	1.88	0.72
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:O	1:A:227:ASN:HB2	1.90	0.71
1:A:97:LEU:N	1:A:689:ARG:NH1	2.38	0.71
1:A:703:LYS:HA	1:A:714:ARG:HG3	1.70	0.71
1:A:97:LEU:H	1:A:689:ARG:NH1	1.88	0.71
1:A:395:GLU:HA	1:A:407:GLN:O	1.91	0.70
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.72	0.70
1:A:704:ARG:O	1:A:707:LEU:HD21	1.91	0.70
1:A:698:TYR:O	1:A:702:VAL:HG23	1.91	0.70
1:A:580:GLU:HG3	1:A:582:GLN:OE1	1.91	0.70
1:A:396:PRO:O	1:A:398:ILE:HD12	1.92	0.69
1:A:709:ALA:HB1	1:A:710:PRO:HD2	1.74	0.69
1:A:259:GLN:HG2	1:A:261:TYR:OH	1.93	0.69
1:A:84:LYS:C	1:A:84:LYS:HD2	2.14	0.68
1:A:289:THR:HG22	1:A:292:GLU:CD	2.15	0.67
1:A:97:LEU:H	1:A:689:ARG:CZ	2.07	0.67
1:A:62:PHE:HE2	1:A:72:VAL:CG2	2.07	0.67
1:A:499:ILE:CD1	1:A:738:ARG:HB3	2.24	0.67
1:A:170:ARG:HD3	4:A:1218:HOH:O	1.93	0.67
1:A:219:ASN:N	1:A:220:PRO:HD2	2.10	0.67
1:A:703:LYS:HG2	1:A:714:ARG:NE	2.08	0.66
1:A:687:ILE:HG22	1:A:688:THR:N	2.09	0.66
1:A:66:ASP:OD1	1:A:66:ASP:N	2.29	0.66
1:A:698:TYR:CE1	1:A:720:GLN:HG3	2.30	0.66
1:A:141:ASP:O	1:A:144:LYS:HG2	1.96	0.66
1:A:722:ALA:O	1:A:725:ALA:HB3	1.96	0.66
1:A:597:GLU:O	1:A:601:LYS:HG3	1.96	0.66
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.25	0.65
1:A:31:ASP:OD1	1:A:31:ASP:N	2.29	0.65
1:A:48:GLU:HG2	1:A:65:VAL:HG21	1.76	0.65
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.78	0.65
1:A:35:ILE:HD12	1:A:35:ILE:O	1.96	0.65
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.79	0.65
1:A:499:ILE:HD13	1:A:738:ARG:HG2	1.79	0.65
1:A:158:ILE:HD12	1:A:175:LEU:HD21	1.79	0.65
1:A:677:ARG:HG2	1:A:682:LEU:HD12	1.79	0.65
1:A:38:ASN:ND2	1:A:46:SER:O	2.30	0.64
1:A:87:GLY:H	1:A:105:ASN:ND2	1.95	0.64
1:A:84:LYS:O	1:A:84:LYS:HD2	1.96	0.64
1:A:238:ARG:HD3	1:A:264:GLU:OE1	1.98	0.64
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.80	0.64
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASN:O	1:A:309:GLN:HG2	1.98	0.63
1:A:280:ILE:HG13	1:A:280:ILE:O	1.97	0.62
1:A:147:ARG:HG3	1:A:150:GLU:OE2	2.00	0.62
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.29	0.62
1:A:692:PHE:CE1	1:A:747:ARG:HD3	2.34	0.62
1:A:4:ILE:HD12	1:A:4:ILE:N	2.14	0.62
1:A:546:LYS:HE2	1:A:550:HIS:CE1	2.34	0.62
1:A:372:LYS:HB3	1:A:376:ASN:HD21	1.64	0.62
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.81	0.62
1:A:354:LEU:O	1:A:418:ARG:NH1	2.30	0.62
1:A:289:THR:HG22	1:A:292:GLU:CG	2.30	0.62
1:A:64:THR:HG23	1:A:68:GLN:O	2.00	0.61
1:A:403:ASP:N	1:A:403:ASP:OD1	2.34	0.61
1:A:360:GLU:O	1:A:368:VAL:N	2.32	0.61
1:A:706:TYR:CE1	1:A:714:ARG:HD2	2.36	0.60
1:A:48:GLU:HG2	1:A:65:VAL:HG23	1.82	0.60
1:A:288:ALA:O	1:A:293:LYS:NZ	2.32	0.60
1:A:72:VAL:HG12	1:A:73:LYS:N	2.16	0.60
1:A:703:LYS:HG2	1:A:714:ARG:CG	2.31	0.59
1:A:419:ASP:O	1:A:423:LYS:HG3	2.02	0.59
1:A:56:THR:O	1:A:74:LYS:HE3	2.03	0.59
1:A:187:GLU:HG3	3:A:999:ATP:H2'	1.84	0.59
1:A:59:SER:HB2	1:A:72:VAL:O	2.02	0.59
1:A:735:GLU:HA	1:A:738:ARG:HH22	1.67	0.59
1:A:24:LEU:HD23	1:A:24:LEU:N	2.17	0.58
1:A:692:PHE:CD1	1:A:747:ARG:HD3	2.37	0.58
1:A:26:LYS:O	1:A:29:VAL:HG23	2.04	0.58
1:A:695:ARG:HG2	1:A:745:PHE:CD2	2.39	0.57
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.39	0.57
1:A:689:ARG:NH1	4:A:1599:HOH:O	2.36	0.57
1:A:141:ASP:CB	1:A:144:LYS:HE3	2.34	0.57
1:A:64:THR:OG1	1:A:68:GLN:N	2.38	0.57
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.35	0.56
1:A:329:GLN:O	1:A:332:ASP:HB2	2.05	0.56
1:A:289:THR:O	1:A:293:LYS:HG3	2.06	0.56
1:A:499:ILE:HD13	1:A:738:ARG:CB	2.36	0.56
1:A:25:PHE:HE1	1:A:755:GLU:OE1	1.88	0.56
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.87	0.56
1:A:155:ILE:O	1:A:158:ILE:HG13	2.05	0.56
1:A:34:TYR:CD1	1:A:51:GLU:HB2	2.40	0.55
1:A:662:GLN:NE2	4:A:1273:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.88	0.55
1:A:289:THR:HG23	1:A:292:GLU:N	2.21	0.55
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.26	0.55
1:A:723:THR:HG22	1:A:739:PHE:CZ	2.41	0.55
1:A:62:PHE:CE2	1:A:72:VAL:HG23	2.40	0.54
1:A:98:ASN:O	1:A:102:VAL:HG23	2.07	0.54
1:A:754:ILE:HG22	1:A:755:GLU:N	2.23	0.54
1:A:495:LEU:O	1:A:495:LEU:HD12	2.07	0.54
1:A:279:HIS:O	1:A:283:GLN:HG3	2.07	0.54
1:A:277:ASN:HD22	1:A:307:LEU:HD23	1.73	0.54
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.42	0.54
1:A:290:ALA:HA	1:A:293:LYS:HZ2	1.72	0.54
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.43	0.54
1:A:736:GLN:O	1:A:747:ARG:HG2	2.07	0.54
1:A:676:LEU:HB3	1:A:682:LEU:HG	1.91	0.53
1:A:372:LYS:HB3	1:A:376:ASN:ND2	2.24	0.53
1:A:327:THR:HG22	1:A:331:MET:HE2	1.89	0.53
1:A:219:ASN:HB3	1:A:220:PRO:CD	2.38	0.53
1:A:289:THR:CG2	1:A:292:GLU:HB2	2.39	0.52
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.49	0.52
1:A:696:ILE:O	1:A:743:LYS:HB3	2.08	0.52
1:A:326:ILE:HG22	1:A:327:THR:N	2.21	0.52
1:A:155:ILE:HD12	1:A:158:ILE:HD11	1.92	0.52
1:A:399:LEU:HD12	1:A:403:ASP:O	2.09	0.52
1:A:580:GLU:HG2	1:A:580:GLU:O	2.10	0.52
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.39	0.52
1:A:87:GLY:H	1:A:105:ASN:HD21	1.57	0.52
1:A:83:ILE:HD12	1:A:86:ASP:OD2	2.09	0.52
1:A:273:GLU:C	1:A:274:THR:HG23	2.31	0.52
1:A:83:ILE:HD11	4:A:1129:HOH:O	2.09	0.51
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.45	0.51
1:A:60:PHE:O	1:A:71:GLN:HA	2.10	0.51
1:A:35:ILE:HD13	1:A:37:TYR:HB3	1.91	0.51
1:A:707:LEU:HD23	1:A:707:LEU:H	1.75	0.51
1:A:158:ILE:HD12	1:A:175:LEU:CD2	2.41	0.51
1:A:289:THR:HG22	1:A:292:GLU:HB2	1.93	0.51
1:A:2:ASN:O	1:A:5:HIS:N	2.40	0.51
1:A:706:TYR:HD2	1:A:712:VAL:O	1.94	0.50
1:A:97:LEU:C	1:A:689:ARG:HH11	2.13	0.50
1:A:24:LEU:O	1:A:27:LEU:HG	2.12	0.50
1:A:98:ASN:OD1	1:A:100:PRO:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HD13	1:A:738:ARG:CG	2.41	0.50
1:A:48:GLU:CG	1:A:65:VAL:HG21	2.42	0.49
1:A:324:PHE:HE2	1:A:328:ARG:NH2	2.09	0.49
1:A:219:ASN:HB2	4:A:1309:HOH:O	2.13	0.49
1:A:174:SER:O	1:A:651:HIS:N	2.44	0.49
1:A:386:PRO:O	1:A:390:GLU:HB2	2.13	0.49
1:A:138:GLU:O	1:A:142:ILE:HG13	2.12	0.49
1:A:97:LEU:HD22	1:A:685:ILE:HG23	1.94	0.49
1:A:499:ILE:HD11	1:A:738:ARG:C	2.33	0.48
1:A:141:ASP:CA	1:A:144:LYS:HE3	2.43	0.48
1:A:611:LEU:O	1:A:618:ALA:HB2	2.12	0.48
1:A:306:TYR:CE2	1:A:355:GLY:HA3	2.48	0.48
1:A:565:LYS:NZ	4:A:1442:HOH:O	2.46	0.48
1:A:56:THR:HG23	1:A:59:SER:OG	2.14	0.48
1:A:696:ILE:O	1:A:744:ILE:N	2.40	0.48
1:A:165:SER:O	1:A:169:ASP:HB2	2.13	0.48
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.63	0.48
1:A:397:ARG:HA	1:A:406:ALA:CA	2.34	0.48
1:A:396:PRO:HG2	1:A:398:ILE:HD11	1.95	0.48
1:A:6:ASP:O	1:A:8:THR:N	2.46	0.48
1:A:446:LYS:HE3	1:A:449:PHE:HB3	1.95	0.48
1:A:195:TYR:O	1:A:199:VAL:HG12	2.14	0.48
1:A:137:GLN:O	1:A:137:GLN:HG3	2.14	0.48
1:A:99:GLU:N	1:A:100:PRO:HD2	2.29	0.47
1:A:474:THR:HG1	1:A:634:TYR:HH	1.61	0.47
1:A:96:TYR:CE1	1:A:749:GLY:HA2	2.49	0.47
1:A:35:ILE:HD12	1:A:35:ILE:C	2.34	0.47
1:A:210:VAL:O	1:A:214:GLN:HG3	2.14	0.47
1:A:559:GLU:HG3	1:A:560:GLU:N	2.29	0.47
1:A:337:SER:O	1:A:341:GLN:HG3	2.14	0.47
1:A:90:ASP:O	1:A:93:GLU:HB2	2.14	0.47
1:A:369:LEU:HD23	1:A:375:LEU:CD1	2.34	0.47
1:A:344:ILE:O	1:A:348:ILE:HG12	2.15	0.47
1:A:217:GLN:CG	1:A:333:ILE:HD12	2.36	0.47
1:A:55:GLU:HG3	1:A:56:THR:O	2.15	0.47
1:A:98:ASN:OD1	1:A:100:PRO:HD2	2.16	0.46
1:A:187:GLU:O	1:A:191:LYS:HG2	2.16	0.46
1:A:344:ILE:HD13	1:A:433:LEU:HD21	1.97	0.46
1:A:692:PHE:CE1	1:A:747:ARG:CD	2.98	0.46
1:A:611:LEU:HA	1:A:617:ILE:HG21	1.96	0.46
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:O	1:A:139:MET:N	2.49	0.46
1:A:302:GLU:H	1:A:302:GLU:CD	2.19	0.46
1:A:375:LEU:HD23	1:A:375:LEU:C	2.36	0.46
1:A:706:TYR:HB2	1:A:712:VAL:O	2.16	0.46
1:A:99:GLU:N	1:A:100:PRO:CD	2.78	0.46
1:A:189:THR:O	1:A:193:ILE:HG13	2.16	0.46
1:A:268:VAL:O	1:A:268:VAL:HG12	2.16	0.45
1:A:710:PRO:CD	1:A:729:HIS:CD2	3.00	0.45
1:A:735:GLU:HA	1:A:738:ARG:NH2	2.31	0.45
1:A:40:ASP:OD1	1:A:41:PRO:HD2	2.16	0.45
1:A:219:ASN:N	1:A:220:PRO:CD	2.79	0.45
1:A:72:VAL:CG1	1:A:73:LYS:N	2.80	0.45
1:A:494:TYR:HE1	1:A:695:ARG:CZ	2.30	0.45
1:A:25:PHE:CD2	1:A:707:LEU:HD11	2.52	0.45
1:A:259:GLN:CG	1:A:261:TYR:CZ	3.00	0.45
1:A:750:GLN:NE2	1:A:750:GLN:HA	2.30	0.45
1:A:181:SER:OG	3:A:999:ATP:O2G	2.28	0.45
1:A:51:GLU:O	1:A:62:PHE:HB2	2.17	0.45
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.32	0.44
1:A:6:ASP:C	1:A:8:THR:H	2.20	0.44
1:A:130:LYS:HE2	4:A:1427:HOH:O	2.16	0.44
1:A:328:ARG:O	1:A:332:ASP:OD2	2.35	0.44
1:A:718:ASP:OD2	1:A:721:LYS:HB2	2.17	0.44
1:A:723:THR:HG22	1:A:739:PHE:CE1	2.53	0.44
1:A:705:TYR:OH	1:A:755:GLU:OE1	2.29	0.44
1:A:89:GLU:HB3	1:A:153:PRO:CG	2.47	0.44
1:A:371:ASP:OD1	1:A:373:THR:OG1	2.35	0.44
1:A:37:TYR:O	1:A:48:GLU:N	2.40	0.44
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.53	0.44
1:A:80:ARG:HG3	4:A:1191:HOH:O	2.18	0.44
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.52	0.44
1:A:698:TYR:CD1	1:A:720:GLN:HA	2.53	0.43
1:A:129:PHE:CE2	1:A:662:GLN:HA	2.52	0.43
1:A:583:ASP:O	1:A:587:LYS:HG3	2.18	0.43
1:A:4:ILE:CD1	1:A:4:ILE:N	2.81	0.43
1:A:210:VAL:O	1:A:213:GLN:HB2	2.19	0.43
1:A:79:GLN:HB2	4:A:1262:HOH:O	2.17	0.43
1:A:638:LEU:O	1:A:642:MET:HG2	2.18	0.43
1:A:366:GLY:CA	1:A:408:HIS:CD2	2.95	0.43
1:A:289:THR:HG22	1:A:292:GLU:CB	2.48	0.43
1:A:676:LEU:CB	1:A:682:LEU:HG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASN:O	1:A:442:CYS:HB3	2.18	0.43
1:A:127:ASN:O	1:A:658:PRO:HG3	2.17	0.43
1:A:704:ARG:O	1:A:704:ARG:HG2	2.19	0.43
1:A:522:PRO:CB	1:A:523:PRO:HD2	2.48	0.43
1:A:456:SER:OG	1:A:457:GLY:O	2.30	0.43
1:A:181:SER:HA	3:A:999:ATP:O3G	2.18	0.43
1:A:285:LEU:HA	1:A:285:LEU:HD23	1.70	0.43
1:A:659:ASN:ND2	1:A:666:LYS:HB3	2.34	0.43
1:A:484[B]:HIS:ND1	1:A:488:LYS:HE3	2.34	0.43
1:A:510:SER:O	1:A:514:ILE:HG13	2.18	0.43
1:A:244:GLU:O	1:A:256:ALA:HA	2.19	0.43
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.79	0.43
1:A:180:GLU:HG3	4:A:1130:HOH:O	2.18	0.42
1:A:369:LEU:HD21	1:A:375:LEU:HD12	1.99	0.42
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.86	0.42
1:A:455:ILE:HG13	1:A:455:ILE:O	2.18	0.42
1:A:466:PHE:HB3	1:A:587:LYS:HD3	2.01	0.42
1:A:368:VAL:HG12	1:A:369:LEU:H	1.85	0.42
1:A:736:GLN:HA	1:A:747:ARG:HG3	2.02	0.42
1:A:590:ASP:N	1:A:591:PRO:CD	2.82	0.42
1:A:289:THR:CG2	1:A:292:GLU:CG	2.98	0.42
1:A:129:PHE:O	1:A:664:PRO:HG3	2.19	0.42
1:A:709:ALA:HB1	1:A:710:PRO:CD	2.44	0.42
1:A:163:TYR:O	1:A:167:LEU:HG	2.18	0.42
1:A:211:LEU:HB3	1:A:212:GLU:OE1	2.20	0.42
1:A:297:HIS:N	1:A:297:HIS:ND1	2.68	0.42
1:A:158:ILE:CD1	1:A:175:LEU:CD2	2.98	0.42
1:A:2:ASN:ND2	1:A:5:HIS:CE1	2.87	0.41
1:A:590:ASP:N	1:A:591:PRO:HD3	2.35	0.41
1:A:237:SER:HB2	4:A:1375:HOH:O	2.20	0.41
1:A:243:ILE:O	1:A:451:GLY:HA2	2.21	0.41
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.81	0.41
1:A:395:GLU:HG2	1:A:408:HIS:HA	2.03	0.41
1:A:499:ILE:HD12	1:A:745:PHE:CG	2.55	0.41
1:A:692:PHE:HB3	1:A:745:PHE:HB3	2.02	0.41
1:A:705:TYR:HD1	1:A:708:LEU:HD11	1.85	0.41
1:A:710:PRO:HD2	1:A:729:HIS:CD2	2.55	0.41
1:A:351:ILE:HG23	1:A:422:VAL:HG13	2.03	0.41
1:A:497:GLU:O	1:A:499:ILE:N	2.54	0.41
1:A:382:PHE:O	1:A:603:SER:OG	2.39	0.41
1:A:219:ASN:CB	1:A:220:PRO:CD	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:O	1:A:349:ALA:HB3	2.21	0.40
1:A:99:GLU:HG2	1:A:682:LEU:HD13	2.02	0.40
1:A:22:SER:OG	1:A:24:LEU:HG	2.21	0.40
1:A:338:GLN:HA	1:A:341:GLN:HG3	2.04	0.40
1:A:61:THR:CG2	1:A:71:GLN:HG3	2.30	0.40
1:A:705:TYR:HB3	1:A:708:LEU:HD12	2.02	0.40
1:A:432:TRP:HZ2	1:A:436:LYS:HZ2	1.70	0.40
1:A:541:ASN:HA	1:A:544:ILE:HG22	2.03	0.40

All (3) 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:391[A]:LYS:NZ	4:A:1622:HOH:O[2_565]	1.39	0.81
1:A:391[A]:LYS:CE	4:A:1622:HOH:O[2_565]	2.09	0.11
1:A:391[A]:LYS:CD	4:A:1622:HOH:O[2_565]	2.12	0.08

## 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	732/761 (96%)	688 (94%)	41 (6%)	3 (0%)	<div>39</div> <div>34</div>

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	LYS
1	A	7	ARG
1	A	373	THR

### 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	630/665 (95%)	564 (90%)	66 (10%)	<b>8</b> <b>4</b>

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	27	LEU
1	A	31	ASP
1	A	33	ARG
1	A	43	GLU
1	A	44	ARG
1	A	54	SER
1	A	55	GLU
1	A	56	THR
1	A	57	SER
1	A	58	ASP
1	A	66	ASP
1	A	75	ASP
1	A	84	LYS
1	A	97	LEU
1	A	117	THR
1	A	131	ARG
1	A	180	GLU
1	A	210	VAL
1	A	237	SER
1	A	241	LYS
1	A	243	ILE
1	A	249	ASN
1	A	254	SER
1	A	266	SER
1	A	302	GLU
1	A	309	GLN
1	A	319	SER
1	A	328	ARG
1	A	337	SER

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Mol	Chain	Res	Type
1	A	339	GLU
1	A	342	MET
1	A	368	VAL
1	A	369	LEU
1	A	370	LYS
1	A	372	LYS
1	A	379	SER
1	A	403	ASP
1	A	405	VAL
1	A	411	VAL
1	A	436	LYS
1	A	446	LYS
1	A	462	LYS
1	A	491	GLN
1	A	493	GLU
1	A	509	ASP
1	A	510	SER
1	A	529	LEU
1	A	546	LYS
1	A	565	LYS
1	A	580	GLU
1	A	581	ILE
1	A	594	GLN
1	A	604	SER
1	A	640	SER
1	A	666	LYS
1	A	669	ASP
1	A	686	ARG
1	A	690	LYS
1	A	707	LEU
1	A	723	THR
1	A	735	GLU
1	A	738	ARG
1	A	741	ILE
1	A	742	THR
1	A	751	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	194	GLN
1	A	234	ASN
1	A	235	ASN
1	A	283	GLN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN
1	A	479	GLN
1	A	550	HIS
1	A	594	GLN
1	A	662	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	ATP	A	999	2	24,33,33	1.96	1 (4%)	31,52,52	1.39	4 (12%)

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	ATP	A	999	2	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ATP	C2'-C3'	-8.59	1.30	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ATP	C1'-N9-C4	-2.63	122.97	126.94
3	A	999	ATP	O2B-PB-O3B	2.07	114.50	105.09
3	A	999	ATP	O3'-C3'-C2'	2.21	119.02	111.83
3	A	999	ATP	C2'-C3'-C4'	4.42	111.70	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ATP	3	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	738/761 (96%)	0.37	63 (8%) 13 19	13, 38, 80, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	VAL	6.3
1	A	65	VAL	6.1
1	A	444	GLU	4.5
1	A	405	VAL	4.5
1	A	23	ASP	4.5
1	A	56	THR	4.4
1	A	362	GLY	4.2
1	A	58	ASP	4.2
1	A	67	GLY	4.1
1	A	443	GLN	4.0
1	A	347	ILE	4.0
1	A	24	LEU	4.0
1	A	66	ASP	3.9
1	A	31	ASP	3.8
1	A	348	ILE	3.7
1	A	429	LEU	3.7
1	A	5	HIS	3.6
1	A	68	GLN	3.6
1	A	494	TYR	3.5
1	A	27	LEU	3.4
1	A	57	SER	3.4
1	A	290	ALA	3.2
1	A	25	PHE	3.1
1	A	498	LYS	3.1
1	A	72	VAL	3.0
1	A	725	ALA	3.0
1	A	715	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	22	SER	2.9
1	A	42	LYS	2.7
1	A	495	LEU	2.7
1	A	487	PHE	2.7
1	A	403	ASP	2.6
1	A	351	ILE	2.6
1	A	499	ILE	2.6
1	A	496	LYS	2.6
1	A	30	SER	2.6
1	A	40	ASP	2.5
1	A	59	SER	2.5
1	A	289	THR	2.5
1	A	404	LEU	2.5
1	A	615	PRO	2.5
1	A	399	LEU	2.5
1	A	714	ARG	2.4
1	A	716	ALA	2.4
1	A	370	LYS	2.4
1	A	537	ASN	2.4
1	A	60	PHE	2.3
1	A	3	PRO	2.3
1	A	365	GLU	2.3
1	A	75	ASP	2.2
1	A	732	ILE	2.2
1	A	352	LEU	2.1
1	A	733	ASP	2.1
1	A	363	ALA	2.1
1	A	368	VAL	2.1
1	A	723	THR	2.1
1	A	371	ASP	2.1
1	A	497	GLU	2.0
1	A	754	ILE	2.0
1	A	26	LYS	2.0
1	A	718	ASP	2.0
1	A	713	PRO	2.0
1	A	325	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	A	999	31/31	0.97	0.11	-0.03	6,28,52,100	0
2	MG	A	800	1/1	0.94	0.06	-2.34	26,26,26,26	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.