



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 AM UTC

PDB ID : 1FMW / pdb_00001fmw
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

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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

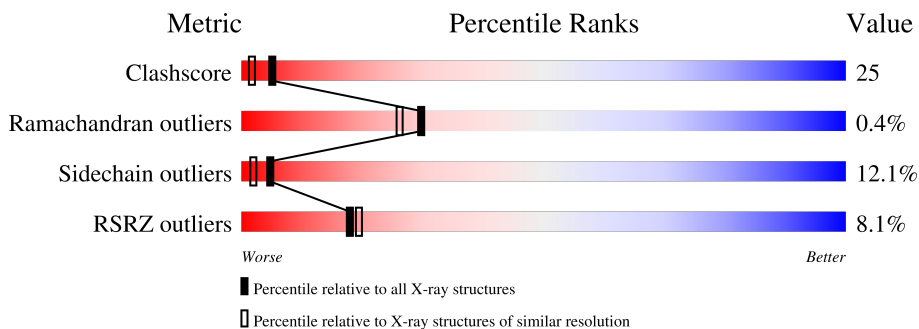
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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 $\leq 5\%$. 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

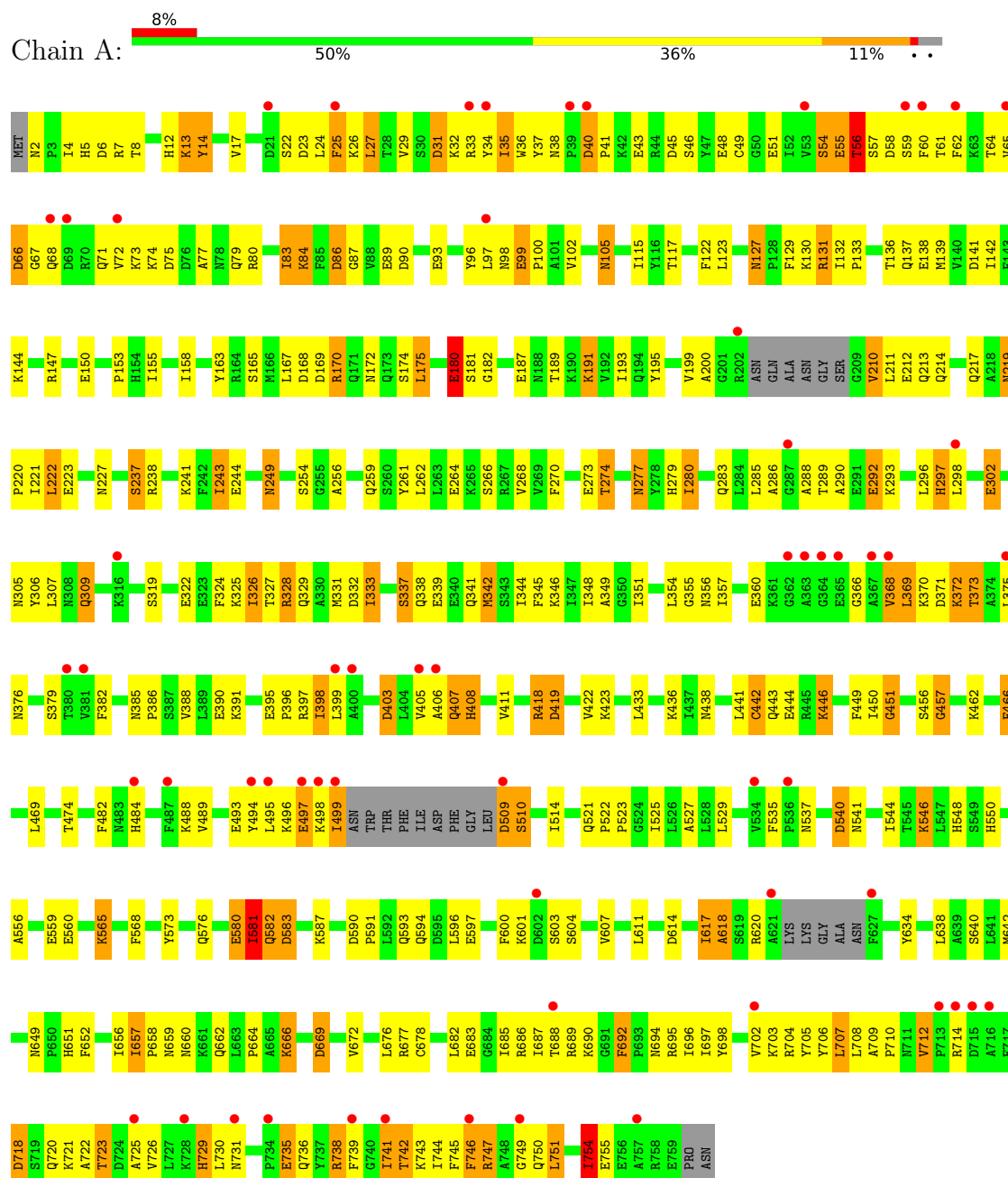
- Molecule 4 is water.

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

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 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, α , β , γ	104.10Å 180.40Å 54.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.15 90.20 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.0 (100.00-2.15) 92.6 (90.20-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.15Å)	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.	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 134.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

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: 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	1.29	8/5985 (0.1%)	1.77	102/8088 (1.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ILE	CA-CB	-6.60	1.49	1.54
1	A	326	ILE	CA-CB	-5.67	1.48	1.54
1	A	200	ALA	CA-C	-5.60	1.45	1.52
1	A	657	ILE	CA-C	5.50	1.57	1.53
1	A	678	CYS	CA-C	-5.47	1.45	1.52
1	A	451	GLY	CA-C	-5.29	1.48	1.52
1	A	13	LYS	N-CA	-5.08	1.40	1.46
1	A	222	LEU	N-CA	-5.07	1.39	1.46

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	CA-CB-CG	-13.05	99.55	112.60
1	A	657	ILE	CB-CA-C	8.27	118.63	110.94
1	A	262	LEU	N-CA-CB	-7.99	100.20	111.62
1	A	731	ASN	CA-CB-CG	7.93	120.53	112.60
1	A	67	GLY	N-CA-C	-7.79	103.96	115.72
1	A	442	CYS	N-CA-C	7.61	121.37	109.96
1	A	729	HIS	CA-CB-CG	-7.47	106.33	113.80
1	A	482	PHE	CA-CB-CG	-7.25	106.55	113.80
1	A	297	HIS	CA-CB-CG	-7.23	106.57	113.80
1	A	131	ARG	CA-C-N	7.16	129.08	122.85
1	A	131	ARG	C-N-CA	7.16	129.08	122.85
1	A	683	GLU	N-CA-CB	7.13	120.34	110.01
1	A	292	GLU	N-CA-C	-7.06	105.20	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	GLY	N-CA-C	-7.05	100.13	112.55
1	A	286	ALA	N-CA-C	7.04	119.99	111.40
1	A	652	PHE	N-CA-C	7.01	119.94	108.52
1	A	535	PHE	CA-CB-CG	-7.00	106.80	113.80
1	A	556	ALA	N-CA-C	6.97	120.88	112.38
1	A	573	TYR	CA-C-N	6.93	130.27	120.28
1	A	573	TYR	C-N-CA	6.93	130.27	120.28
1	A	180	GLU	N-CA-C	6.80	119.10	110.33
1	A	649	ASN	N-CA-C	-6.74	96.56	108.69
1	A	581	ILE	N-CA-C	6.71	122.20	113.07
1	A	40	ASP	CA-C-N	6.65	128.15	119.84
1	A	40	ASP	C-N-CA	6.65	128.15	119.84
1	A	450	ILE	CA-C-N	-6.61	116.39	122.80
1	A	450	ILE	C-N-CA	-6.61	116.39	122.80
1	A	277	ASN	N-CA-C	-6.59	101.25	110.35
1	A	614	ASP	CB-CA-C	6.42	116.53	110.17
1	A	418	ARG	N-CA-C	-6.42	104.28	111.28
1	A	122	PHE	CA-CB-CG	6.21	120.00	113.80
1	A	280	ILE	N-CA-C	6.16	118.75	111.05
1	A	692	PHE	CA-C-N	6.12	125.68	119.19
1	A	692	PHE	C-N-CA	6.12	125.68	119.19
1	A	657	ILE	N-CA-C	-6.12	103.37	108.63
1	A	600	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	356	ASN	CA-CB-CG	-6.09	106.51	112.60
1	A	583	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	617	ILE	N-CA-CB	-5.88	104.94	111.41
1	A	618	ALA	N-CA-C	5.87	120.06	113.01
1	A	175	LEU	N-CA-CB	5.83	119.75	110.65
1	A	56	THR	N-CA-C	-5.83	101.55	109.95
1	A	568	PHE	CA-C-N	-5.80	118.10	122.33
1	A	568	PHE	C-N-CA	-5.80	118.10	122.33
1	A	509	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	123	LEU	N-CA-CB	5.76	120.04	110.47
1	A	535	PHE	O-C-N	5.75	125.89	121.23
1	A	219	ASN	CA-CB-CG	-5.72	106.88	112.60
1	A	25	PHE	CA-C-N	5.72	128.22	120.38
1	A	25	PHE	C-N-CA	5.72	128.22	120.38
1	A	12	HIS	CA-CB-CG	-5.71	108.09	113.80
1	A	443	GLN	N-CA-C	5.69	118.23	109.07
1	A	333	ILE	CB-CA-C	-5.67	104.39	112.22
1	A	540	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	747	ARG	N-CA-C	-5.67	102.90	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	VAL	N-CA-C	-5.63	106.97	111.81
1	A	469	LEU	N-CA-C	-5.55	105.13	111.07
1	A	419	ASP	CB-CA-C	-5.54	101.42	110.85
1	A	746	PHE	CA-CB-CG	-5.54	108.26	113.80
1	A	54	SER	CB-CA-C	-5.52	101.01	110.95
1	A	86	ASP	CA-CB-CG	-5.52	107.08	112.60
1	A	525	ILE	N-CA-C	5.49	115.69	110.42
1	A	660	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	712	VAL	N-CA-C	5.43	113.92	107.73
1	A	537	ASN	N-CA-C	5.42	119.88	113.16
1	A	77	ALA	N-CA-C	5.41	118.29	110.28
1	A	14	TYR	N-CA-C	5.38	119.90	113.23
1	A	127	ASN	O-C-N	5.38	125.99	121.31
1	A	105	ASN	CA-C-O	5.38	126.25	120.55
1	A	718	ASP	N-CA-CB	5.37	116.36	110.35
1	A	99	GLU	CB-CA-C	-5.37	104.29	113.04
1	A	122	PHE	N-CA-C	5.35	118.44	110.52
1	A	620	ARG	N-CA-C	5.35	117.19	111.36
1	A	131	ARG	CB-CA-C	5.33	118.53	109.53
1	A	172	ASN	CA-C-N	-5.32	114.25	122.59
1	A	172	ASN	C-N-CA	-5.32	114.25	122.59
1	A	548	HIS	CA-C-N	5.31	127.34	120.44
1	A	548	HIS	C-N-CA	5.31	127.34	120.44
1	A	17	VAL	N-CA-C	-5.31	101.89	108.89
1	A	656	ILE	N-CA-C	5.23	115.49	108.17
1	A	466	PHE	N-CA-C	5.20	116.63	111.07
1	A	35	ILE	CB-CA-C	-5.17	102.69	110.55
1	A	754	ILE	O-C-N	5.17	126.98	121.91
1	A	262	LEU	N-CA-C	5.16	118.32	111.30
1	A	168	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	525	ILE	CB-CA-C	-5.15	105.38	111.97
1	A	170	ARG	CD-NE-CZ	-5.15	117.20	124.40
1	A	489	VAL	N-CA-CB	5.13	119.42	110.65
1	A	23	ASP	CB-CA-C	-5.12	100.27	109.24
1	A	40	ASP	O-C-N	5.11	125.68	121.44
1	A	527	ALA	N-CA-C	-5.11	105.71	111.28
1	A	115	ILE	N-CA-C	5.10	119.18	112.04
1	A	669	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	576	GLN	N-CA-C	5.05	117.75	110.28
1	A	649	ASN	CB-CA-C	5.04	115.17	110.17
1	A	582	GLN	CB-CG-CD	5.04	121.16	112.60
1	A	200	ALA	CB-CA-C	-5.02	101.26	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	HIS	CA-CB-CG	-5.01	108.79	113.80
1	A	672	VAL	N-CA-C	5.01	115.23	110.42
1	A	496	LYS	N-CA-CB	5.00	118.05	110.14
1	A	172	ASN	CA-CB-CG	-5.00	107.60	112.60
1	A	600	PHE	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5864	0	5751	289	3
2	A	1	0	0	0	0
3	A	31	0	11	2	0
4	A	472	0	0	12	3
All	All	6368	0	5762	289	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 (289) 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:342:MET:HE2	1:A:342:MET:HA	1.33	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:84:LYS:HD2	1:A:84:LYS:C	2.14	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:289:THR:HG22	1:A:292:GLU:CD	2.15	0.72
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.72	0.72
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: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:687:ILE:HG22	1:A:688:THR:N	2.09	0.66
1:A:703:LYS:HG2	1:A:714:ARG:NE	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:ASP:N	1:A:31:ASP:OD1	2.29	0.65
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.25	0.65
1:A:48:GLU:HG2	1:A:65:VAL:HG21	1.76	0.65
1:A:35:ILE:HD12	1:A:35:ILE:O	1.96	0.65
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.78	0.65
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.79	0.65
1:A:158:ILE:HD12	1:A:175:LEU:HD21	1.79	0.65
1:A:499:ILE:HD13	1:A:738:ARG:HG2	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:HD2	1:A:84:LYS:O	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
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:N	1:A:4:ILE:HD12	2.14	0.62
1:A:372:LYS:HB3	1:A:376:ASN:HD21	1.64	0.62
1:A:546:LYS:HE2	1:A:550:HIS:CE1	2.34	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:331:MET:HE1	1:A:345:PHE:CZ	2.33	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:OD1	1:A:403:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:24:LEU:HD23	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:64:THR:OG1	1:A:68:GLN:N	2.38	0.57
1:A:141:ASP:CB	1:A:144:LYS:HE3	2.34	0.57
1:A:273:GLU:C	1:A:274:THR:HG23	2.31	0.56
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:25:PHE:HE1	1:A:755:GLU:OE1	1.88	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: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
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:97:LEU:C	1:A:689:ARG:HH11	2.13	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:495:LEU:O	1:A:495:LEU:HD12	2.07	0.54
1:A:754:ILE:HG22	1:A:755:GLU:N	2.23	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: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:499:ILE:HD11	1:A:738:ARG:C	2.33	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:ILE:HD12	1:A:35:ILE:C	2.34	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:87:GLY:H	1:A:105:ASN:HD21	1.57	0.52
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.39	0.52
1:A:83:ILE:HD12	1:A:86:ASP:OD2	2.09	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:35:ILE:HD13	1:A:37:TYR:HB3	1.91	0.51
1:A:60:PHE:O	1:A:71:GLN:HA	2.10	0.51
1:A:158:ILE:HD12	1:A:175:LEU:CD2	2.41	0.51
1:A:707:LEU:HD23	1:A:707:LEU:H	1.75	0.51
1:A:2:ASN:O	1:A:5:HIS:N	2.40	0.51
1:A:289:THR:HG22	1:A:292:GLU:HB2	1.93	0.51
1:A:302:GLU:H	1:A:302:GLU:CD	2.19	0.50
1:A:24:LEU:O	1:A:27:LEU:HG	2.12	0.50
1:A:375:LEU:HD23	1:A:375:LEU:C	2.36	0.50
1:A:706:TYR:HD2	1:A:712:VAL:O	1.94	0.50
1:A:98:ASN:OD1	1:A:100:PRO:HG2	2.12	0.50
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:6:ASP:C	1:A:8:THR:H	2.20	0.49
1:A:174:SER:O	1:A:651:HIS:N	2.44	0.49
1:A:219:ASN:HB2	4:A:1309:HOH:O	2.13	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:290:ALA:HA	1:A:293:LYS:HZ2	1.78	0.49
1:A:97:LEU:HD22	1:A:685:ILE:HG23	1.94	0.49
1:A:141:ASP:CA	1:A:144:LYS:HE3	2.43	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:611:LEU:O	1:A:618:ALA:HB2	2.12	0.48
1:A:64:THR:HG1	1:A:68:GLN:H	1.62	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:HD12	1:A:369:LEU:HA	1.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:HA	1:A:406:ALA:CA	2.34	0.48
1:A:6:ASP:O	1:A:8:THR:N	2.46	0.48
1:A:396:PRO:HG2	1:A:398:ILE:HD11	1.95	0.48
1:A:195:TYR:O	1:A:199:VAL:HG12	2.14	0.48
1:A:446:LYS:HE3	1:A:449:PHE:HB3	1.95	0.48
1:A:137:GLN:O	1:A:137:GLN:HG3	2.14	0.48
1:A:96:TYR:CE1	1:A:749:GLY:HA2	2.49	0.47
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:210:VAL:O	1:A:214:GLN:HG3	2.14	0.47
1:A:337:SER:O	1:A:341:GLN:HG3	2.14	0.47
1:A:580:GLU:O	1:A:580:GLU:HG2	2.10	0.47
1:A:90:ASP:O	1:A:93:GLU:HB2	2.14	0.47
1:A:344:ILE:O	1:A:348:ILE:HG12	2.15	0.47
1:A:369:LEU:HD23	1:A:375:LEU:CD1	2.34	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:6:ASP:OD1	1:A:8:THR:OG1	2.30	0.46
1:A:136:THR:O	1:A:139:MET:N	2.49	0.46
1:A:559:GLU:HG3	1:A:560:GLU:N	2.29	0.46
1:A:611:LEU:HA	1:A:617:ILE:HG21	1.96	0.46
1:A:692:PHE:CE1	1:A:747:ARG:CD	2.98	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:40:ASP:OD1	1:A:41:PRO:HD2	2.16	0.45
1:A:735:GLU:HA	1:A:738:ARG:NH2	2.31	0.45
1:A:219:ASN:N	1:A:220:PRO:CD	2.79	0.45
1:A:25:PHE:CD2	1:A:707:LEU:HD11	2.52	0.45
1:A:72:VAL:CG1	1:A:73:LYS:N	2.80	0.45
1:A:259:GLN:CG	1:A:261:TYR:CZ	3.00	0.45
1:A:494:TYR:HE1	1:A:695:ARG:CZ	2.30	0.45
1:A:750:GLN:NE2	1:A:750:GLN:HA	2.30	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:130:LYS:HE2	4:A:1427:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:C	1:A:657:ILE:HD12	2.42	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: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:80:ARG:HG3	4:A:1191:HOH:O	2.18	0.44
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.53	0.44
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.52	0.44
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:698:TYR:CD1	1:A:720:GLN:HA	2.53	0.43
1:A:4:ILE:N	1:A:4:ILE:CD1	2.81	0.43
1:A:79:GLN:HB2	4:A:1262:HOH:O	2.17	0.43
1:A:210:VAL:O	1:A:213:GLN:HB2	2.19	0.43
1:A:638:LEU:O	1:A:642:MET:HG2	2.18	0.43
1:A:127:ASN:O	1:A:658:PRO:HG3	2.17	0.43
1:A:289:THR:HG22	1:A:292:GLU:CB	2.48	0.43
1:A:366:GLY:CA	1:A:408:HIS:CD2	2.95	0.43
1:A:438:ASN:O	1:A:442:CYS:HB3	2.18	0.43
1:A:676:LEU:CB	1:A:682:LEU:HG	2.48	0.43
1:A:456:SER:OG	1:A:457:GLY:O	2.30	0.43
1:A:522:PRO:CB	1:A:523:PRO:HD2	2.48	0.43
1:A:704:ARG:O	1:A:704:ARG:HG2	2.19	0.43
1:A:181:SER:HA	3:A:999:ATP:O3G	2.18	0.43
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.70	0.43
1:A:659:ASN:ND2	1:A:666:LYS:HB3	2.34	0.43
1:A:244:GLU:O	1:A:256:ALA:HA	2.19	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:521:GLN:HA	1:A:522:PRO:C	2.43	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:222:LEU:HD23	1:A:222:LEU:HA	1.86	0.42
1:A:369:LEU:HD21	1:A:375:LEU:HD12	1.99	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:590:ASP:N	1:A:591:PRO:CD	2.82	0.42
1:A:736:GLN:HA	1:A:747:ARG:HG3	2.02	0.42
1:A:129:PHE:O	1:A:664:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:CG2	1:A:292:GLU:CG	2.98	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:ND1	1:A:297:HIS:N	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:237:SER:HB2	4:A:1375:HOH:O	2.20	0.41
1:A:590:ASP:N	1:A:591:PRO:HD3	2.35	0.41
1:A:418:ARG:C	1:A:418:ARG:HD2	2.45	0.41
1:A:243:ILE:O	1:A:451:GLY:HA2	2.21	0.41
1:A:270:PHE:CD2	1:A:270:PHE:C	2.96	0.41
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.81	0.41
1:A:351:ILE:HG23	1:A:422:VAL:HG13	2.03	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:6:ASP:C	1:A:8:THR:N	2.79	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:169:ASP:C	1:A:170:ARG:HG2	2.46	0.40
1:A:219:ASN:CB	1:A:220:PRO:CD	2.99	0.40
1:A:346:LYS:O	1:A:349:ALA:HB3	2.21	0.40
1:A:22:SER:OG	1:A:24:LEU:HG	2.21	0.40
1:A:99:GLU:HG2	1:A:682:LEU:HD13	2.02	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: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 [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	732/761 (96%)	688 (94%)	41 (6%)	3 (0%)	30	26

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 [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	630/665 (95%)	554 (88%)	76 (12%)	5	2

All (76) 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	32	LYS
1	A	33	ARG
1	A	43	GLU
1	A	54	SER
1	A	55	GLU

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Mol	Chain	Res	Type
1	A	56	THR
1	A	57	SER
1	A	58	ASP
1	A	66	ASP
1	A	75	ASP
1	A	83	ILE
1	A	84	LYS
1	A	117	THR
1	A	131	ARG
1	A	180	GLU
1	A	191	LYS
1	A	210	VAL
1	A	221	ILE
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	274	THR
1	A	302	GLU
1	A	309	GLN
1	A	319	SER
1	A	328	ARG
1	A	337	SER
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	398	ILE
1	A	403	ASP
1	A	405	VAL
1	A	407	GLN
1	A	411	VAL
1	A	436	LYS
1	A	441	LEU
1	A	444	GLU
1	A	446	LYS
1	A	462	LYS

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Mol	Chain	Res	Type
1	A	493	GLU
1	A	497	GLU
1	A	499	ILE
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	726	VAL
1	A	735	GLU
1	A	738	ARG
1	A	741	ILE
1	A	742	THR
1	A	751	LEU
1	A	754	ILE

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	2	ASN
1	A	12	HIS
1	A	105	ASN
1	A	188	ASN
1	A	194	GLN
1	A	219	ASN
1	A	234	ASN
1	A	235	ASN
1	A	283	GLN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN

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Mol	Chain	Res	Type
1	A	479	GLN
1	A	550	HIS
1	A	594	GLN
1	A	649	ASN
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 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	ATP	A	999	2	32,33,33	2.16	5 (15%)	48,52,52	1.43	6 (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	-	1/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ATP	C2'-C3'	-8.62	1.30	1.53
3	A	999	ATP	PB-O3A	6.09	1.66	1.59
3	A	999	ATP	PA-O3A	-2.22	1.57	1.59
3	A	999	ATP	C2-N3	-2.19	1.30	1.33
3	A	999	ATP	C5-C6	2.02	1.46	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ATP	C2'-C3'-C4'	4.70	111.70	102.61
3	A	999	ATP	C3'-C2'-C1'	3.94	108.92	101.46
3	A	999	ATP	C5-C4-N9	2.71	108.77	105.81
3	A	999	ATP	O2B-PB-O3B	2.67	114.50	107.27
3	A	999	ATP	C4-C5-N7	-2.39	107.85	110.58
3	A	999	ATP	O3'-C3'-C2'	2.25	119.02	111.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	ATP	PA-O3A-PB-O2B

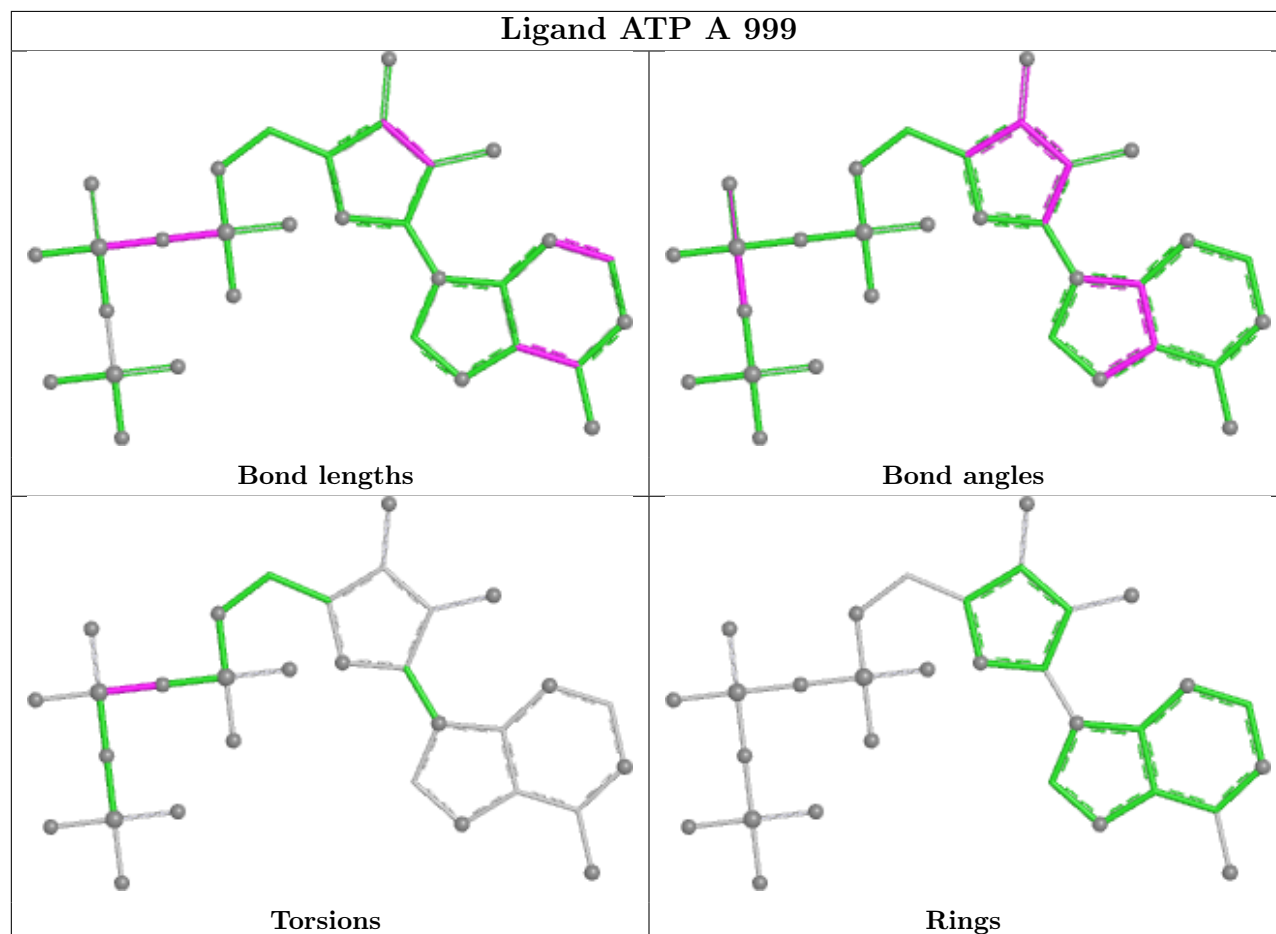
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 ²)	Q<0.9
1	A	738/761 (96%)	0.44	60 (8%) 18 19	13, 38, 80, 100	2 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	VAL	6.8
1	A	367	ALA	4.5
1	A	368	VAL	3.9
1	A	621	ALA	3.8
1	A	65	VAL	3.8
1	A	494	TYR	3.8
1	A	381	VAL	3.6
1	A	60	PHE	3.6
1	A	364	GLY	3.5
1	A	739	PHE	3.4
1	A	536	PRO	3.4
1	A	627	PHE	3.3
1	A	363	ALA	3.1
1	A	400	ALA	3.1
1	A	716	ALA	3.0
1	A	59	SER	3.0
1	A	757	ALA	2.9
1	A	725	ALA	2.9
1	A	741	ILE	2.8
1	A	298	LEU	2.8
1	A	380	THR	2.7
1	A	406	ALA	2.7
1	A	734	PRO	2.7
1	A	25	PHE	2.6
1	A	68	GLN	2.6
1	A	731	ASN	2.6
1	A	375	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLY	2.5
1	A	69	ASP	2.5
1	A	509	ASP	2.4
1	A	316	LYS	2.4
1	A	202	ARG	2.4
1	A	72	VAL	2.4
1	A	33	ARG	2.4
1	A	498	LYS	2.3
1	A	714	ARG	2.3
1	A	688	THR	2.3
1	A	495	LEU	2.3
1	A	702	VAL	2.3
1	A	365	GLU	2.3
1	A	399	LEU	2.3
1	A	487	PHE	2.2
1	A	40	ASP	2.2
1	A	713	PRO	2.2
1	A	34	TYR	2.2
1	A	21	ASP	2.2
1	A	715	ASP	2.2
1	A	602	ASP	2.2
1	A	405	VAL	2.1
1	A	749	GLY	2.1
1	A	746	PHE	2.1
1	A	534	VAL	2.1
1	A	497	GLU	2.1
1	A	39	PRO	2.1
1	A	499	ILE	2.1
1	A	728	LYS	2.1
1	A	97	LEU	2.1
1	A	484[A]	HIS	2.1
1	A	62	PHE	2.1
1	A	287	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

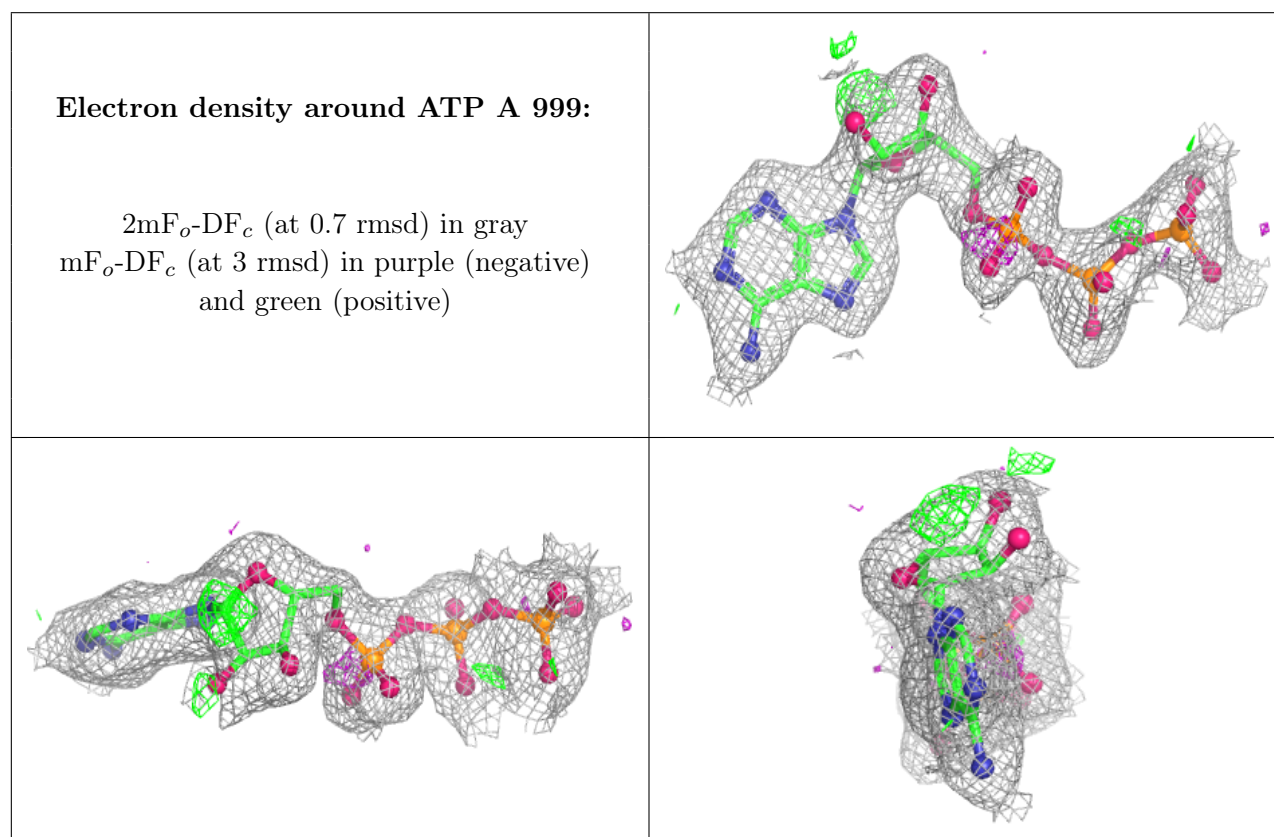
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	800	1/1	0.96	0.05	26,26,26,26	0
3	ATP	A	999	31/31	0.97	0.08	6,28,52,100	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.