



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 10:06 AM EDT

PDB ID : 3M3N  
Title : Structure of a Longitudinal Actin Dimer Assembled by Tandem W Domains  
Authors : Rebowski, G.; Namgoong, S.; Dominguez, R.  
Deposited on : 2010-03-09  
Resolution : 7.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

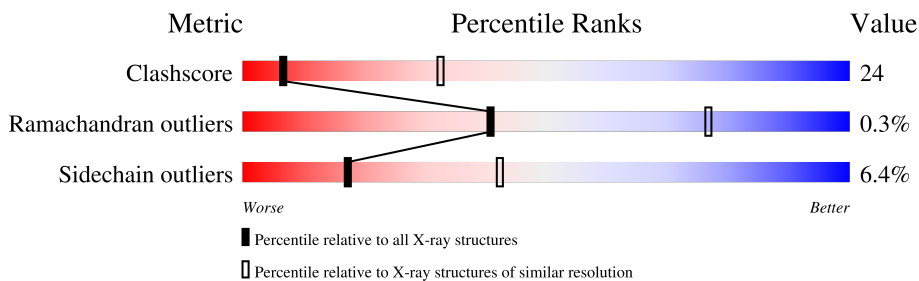
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.00 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	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	375	65% 29% . . .
1	B	375	66% 26% . .
2	W	101	14% 23% . 60%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6032 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2854	1806	481	548	19			
1	B	359	Total	C	N	O	S	0	0	0
			2811	1780	470	543	18			

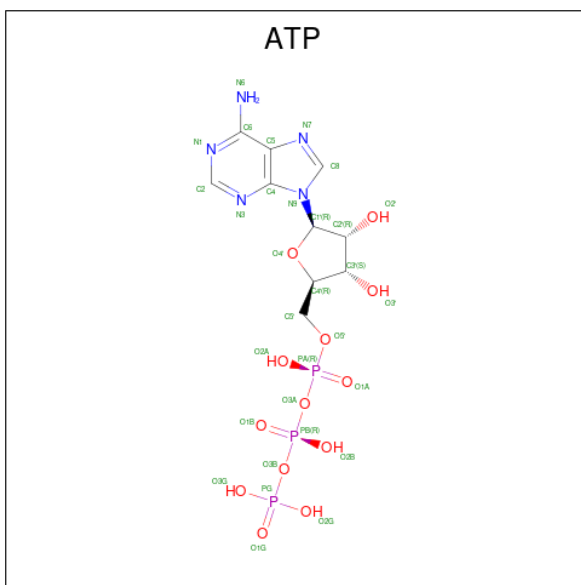
- Molecule 2 is a protein called Neural Wiskott-Aldrich syndrome protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	40	Total	C	N	O	S	0	0	0
			303	187	60	55	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	2	CYS	PRO	engineered mutation	UNP Q91YD9
W	31	ALA	CYS	engineered mutation	UNP Q91YD9
W	59	ALA	CYS	engineered mutation	UNP Q91YD9

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

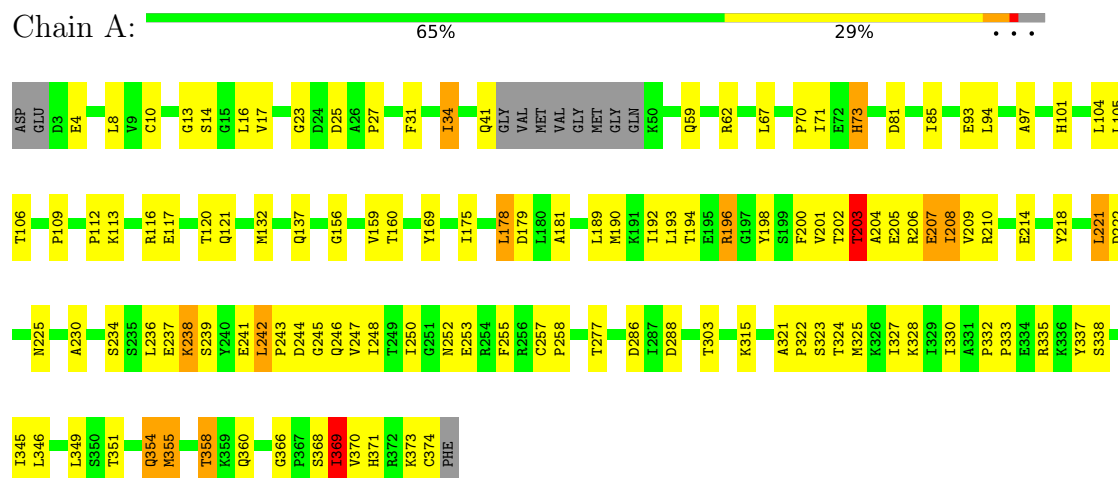
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

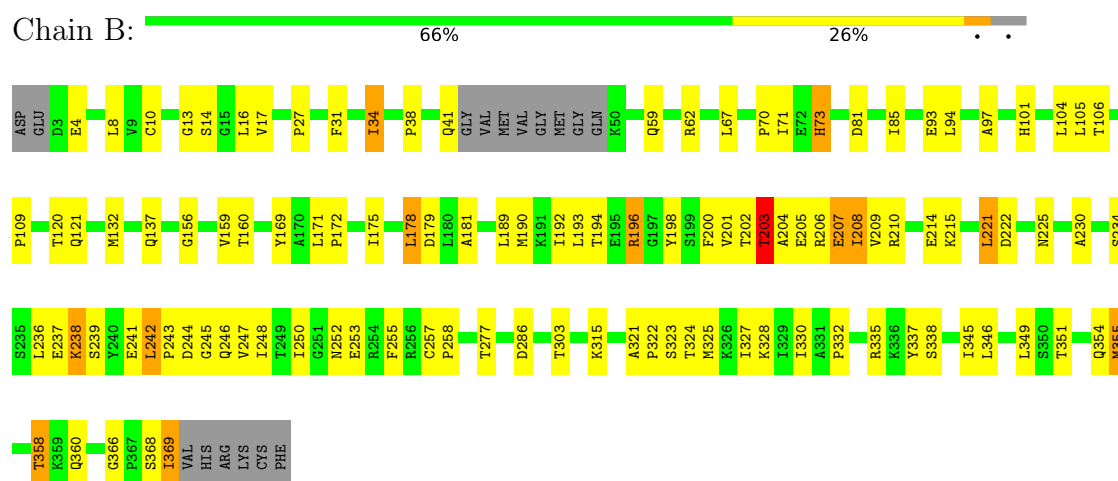
### 3 Residue-property plots

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.

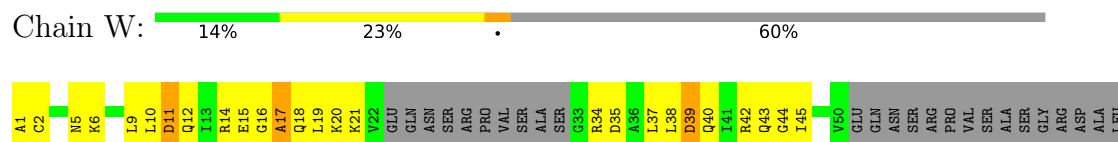
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Neural Wiskott-Aldrich syndrome protein



LEU	ASP	GLN	ILE	ARG	GLN	GLY	ILE	GLN	LEU	LYS	LYS	THR	GLU	THR	GLN	GLU	LYS	ASN	PRO	LEU	PRO	PRO	SER	LYS	GLU	THR	ILE	GLU	GLN	GLU	LYS	GLN	ALA	GLY	GLU	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.74Å 100.74Å 458.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 7.00 33.15 – 6.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-7.00) 74.9 (33.15-6.98)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 7.27Å)	Xtriage
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available) 0.340 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	361.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.66	EDS
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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, 0.333 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: HIC, CA, 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	0.33	0/2902	0.53	2/3931 (0.1%)
1	B	0.34	0/2858	0.53	2/3873 (0.1%)
2	W	0.28	0/301	0.66	3/397 (0.8%)
All	All	0.33	0/6061	0.54	7/8201 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ARG	CB-CA-C	-5.48	99.44	110.40
1	B	196	ARG	CB-CA-C	-5.46	99.48	110.40
1	B	203	THR	N-CA-CB	-5.23	100.37	110.30
2	W	35	ASP	CB-CG-OD2	5.22	123.00	118.30
2	W	11	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	203	THR	N-CA-CB	-5.20	100.43	110.30
2	W	39	ASP	CB-CG-OD2	5.17	122.96	118.30

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	2854	0	2818	134	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2811	0	2772	130	3
2	W	303	0	332	63	1
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	6032	0	5946	282	7

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 24.

All (282) 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:B:169:TYR:CE1	2:W:34:ARG:CZ	2.13	1.30
1:B:349:LEU:HD21	2:W:45:ILE:CD1	1.63	1.28
2:W:44:GLY:O	2:W:45:ILE:HG13	1.10	1.27
2:W:44:GLY:O	2:W:45:ILE:CG1	1.86	1.21
1:A:169:TYR:CE1	2:W:6:LYS:NZ	2.10	1.20
1:B:169:TYR:CD1	2:W:34:ARG:NH2	2.11	1.18
1:B:349:LEU:HD21	2:W:45:ILE:HD13	1.21	1.14
1:A:201:VAL:HG12	1:A:202:THR:N	1.56	1.14
1:B:201:VAL:HG12	1:B:202:THR:N	1.56	1.14
1:A:242:LEU:N	1:A:242:LEU:HD23	1.50	1.14
1:A:116:ARG:HH21	1:A:371:HIS:CE1	1.63	1.13
1:A:201:VAL:CG1	1:A:202:THR:H	1.63	1.12
1:B:242:LEU:HD23	1:B:242:LEU:N	1.50	1.10
1:A:203:THR:HG22	1:A:204:ALA:N	1.66	1.09
1:B:201:VAL:CG1	1:B:202:THR:H	1.63	1.09
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.33	1.08
2:W:44:GLY:C	2:W:45:ILE:HG13	1.65	1.06
2:W:34:ARG:O	2:W:38:LEU:HD13	1.53	1.06
1:B:203:THR:HG22	1:B:204:ALA:N	1.66	1.05
1:A:366:GLY:O	1:A:369:ILE:HG22	1.58	1.04
1:A:189:LEU:HD12	1:A:192:ILE:HD11	1.33	1.03
1:B:366:GLY:O	1:B:369:ILE:HG22	1.58	1.03
1:B:169:TYR:CD1	2:W:34:ARG:CZ	2.40	1.01
1:A:201:VAL:HG12	1:A:202:THR:H	0.86	1.00
1:B:201:VAL:HG12	1:B:202:THR:H	0.86	0.99
1:B:369:ILE:O	1:B:369:ILE:HG13	1.63	0.96
1:B:169:TYR:HE1	2:W:34:ARG:CZ	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:HG13	1:A:369:ILE:O	1.63	0.95
1:A:202:THR:OG1	1:A:206:ARG:HD3	1.67	0.95
1:B:349:LEU:HD21	2:W:45:ILE:HD11	1.46	0.94
1:B:202:THR:OG1	1:B:206:ARG:HD3	1.67	0.94
1:A:349:LEU:HB3	2:W:12:GLN:NE2	1.82	0.94
1:A:242:LEU:N	1:A:242:LEU:CD2	2.30	0.94
1:A:169:TYR:HE1	2:W:6:LYS:NZ	1.64	0.93
1:A:370:VAL:HG13	1:A:370:VAL:O	1.66	0.93
1:B:349:LEU:HB3	2:W:40:GLN:NE2	1.82	0.92
1:A:349:LEU:HB3	2:W:12:GLN:HE21	1.35	0.92
1:A:373:LYS:O	2:W:2:CYS:SG	2.28	0.92
1:A:242:LEU:HD23	1:A:242:LEU:H	1.32	0.89
1:B:242:LEU:HD23	1:B:242:LEU:H	1.32	0.89
1:B:349:LEU:HB3	2:W:40:GLN:HE21	1.35	0.89
1:B:38:PRO:HB2	1:B:41:GLN:HE21	1.38	0.89
1:B:349:LEU:CD2	2:W:45:ILE:HD13	2.02	0.88
1:A:116:ARG:HD2	1:A:371:HIS:CE1	2.09	0.88
1:A:203:THR:CG2	1:A:204:ALA:N	2.37	0.88
1:B:169:TYR:CE1	2:W:34:ARG:NH1	2.43	0.87
1:B:242:LEU:N	1:B:242:LEU:CD2	2.30	0.86
1:B:203:THR:CG2	1:B:204:ALA:N	2.37	0.85
1:A:203:THR:HG22	1:A:204:ALA:H	1.42	0.83
1:A:116:ARG:NH2	1:A:371:HIS:CE1	2.47	0.83
1:B:62:ARG:HG2	1:B:62:ARG:HH21	1.45	0.82
1:B:202:THR:HA	1:B:206:ARG:HG3	1.60	0.82
1:A:62:ARG:HG2	1:A:62:ARG:HH21	1.45	0.81
1:B:345:ILE:HG23	2:W:45:ILE:HD12	1.63	0.81
1:B:203:THR:HG22	1:B:204:ALA:H	1.42	0.81
1:A:202:THR:HA	1:A:206:ARG:HG3	1.60	0.80
1:B:202:THR:OG1	1:B:206:ARG:CD	2.30	0.79
1:A:202:THR:OG1	1:A:206:ARG:CD	2.30	0.78
1:B:349:LEU:CD2	2:W:45:ILE:CD1	2.55	0.78
1:B:189:LEU:CD1	1:B:192:ILE:HD11	2.14	0.77
1:A:244:ASP:OD1	1:A:245:GLY:N	2.18	0.76
1:B:244:ASP:OD1	1:B:245:GLY:N	2.18	0.76
1:A:189:LEU:CD1	1:A:192:ILE:HD11	2.14	0.75
2:W:18:GLN:O	2:W:19:LEU:HD23	1.86	0.74
1:A:116:ARG:HD2	1:A:371:HIS:HE1	1.52	0.73
1:B:169:TYR:CE1	2:W:34:ARG:NE	2.57	0.73
1:A:169:TYR:HE1	2:W:6:LYS:HZ3	1.25	0.73
1:B:242:LEU:HB2	1:B:244:ASP:OD1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:O	1:B:205:GLU:HB2	1.89	0.73
1:A:201:VAL:O	1:A:205:GLU:HB2	1.89	0.72
2:W:34:ARG:O	2:W:38:LEU:CD1	2.35	0.72
1:A:242:LEU:HB2	1:A:244:ASP:OD1	1.89	0.72
1:A:169:TYR:CD1	2:W:6:LYS:NZ	2.46	0.70
1:B:38:PRO:CB	1:B:41:GLN:NE2	2.55	0.70
1:A:169:TYR:CE1	2:W:6:LYS:CE	2.75	0.69
2:W:16:GLY:O	2:W:17:ALA:HB2	1.91	0.69
1:B:169:TYR:HE1	2:W:34:ARG:NE	1.92	0.68
1:A:200:PHE:HD2	1:A:205:GLU:HB3	1.59	0.67
1:A:370:VAL:O	1:A:370:VAL:CG1	2.40	0.67
1:B:38:PRO:CB	1:B:41:GLN:HE21	2.07	0.67
1:A:238:LYS:HE2	1:A:239:SER:H	1.60	0.67
1:A:192:ILE:HG13	1:A:193:LEU:N	2.10	0.66
1:B:200:PHE:HD2	1:B:205:GLU:HB3	1.59	0.66
1:B:238:LYS:HE2	1:B:239:SER:H	1.60	0.66
1:B:335:ARG:HA	1:B:338:SER:OG	1.96	0.66
1:B:62:ARG:HG2	1:B:62:ARG:NH2	2.10	0.66
1:B:192:ILE:HG13	1:B:193:LEU:N	2.10	0.66
1:A:335:ARG:HA	1:A:338:SER:OG	1.96	0.66
1:B:200:PHE:CD2	1:B:205:GLU:HB3	2.31	0.66
1:A:200:PHE:CD2	1:A:205:GLU:HB3	2.31	0.65
1:A:242:LEU:HG	1:A:246:GLN:O	1.97	0.65
1:B:242:LEU:HG	1:B:246:GLN:O	1.97	0.65
1:B:38:PRO:HB2	1:B:41:GLN:NE2	2.10	0.64
1:A:354:GLN:HE22	2:W:5:ASN:ND2	1.98	0.62
2:W:44:GLY:O	2:W:45:ILE:HG12	1.96	0.62
1:A:192:ILE:CG1	1:A:193:LEU:N	2.63	0.62
1:B:192:ILE:CG1	1:B:193:LEU:N	2.63	0.62
1:B:207:GLU:OE2	1:B:207:GLU:HA	1.99	0.61
1:A:207:GLU:HA	1:A:207:GLU:OE2	1.99	0.61
1:A:373:LYS:O	1:A:374:CYS:HB2	2.01	0.60
2:W:39:ASP:OD1	2:W:42:ARG:NH2	2.35	0.60
1:A:198:TYR:CZ	1:A:248:ILE:HB	2.37	0.60
1:B:349:LEU:CD2	2:W:45:ILE:HD11	2.27	0.60
1:B:198:TYR:CZ	1:B:248:ILE:HB	2.37	0.60
1:A:370:VAL:O	1:A:371:HIS:ND1	2.35	0.60
1:A:373:LYS:O	1:A:374:CYS:CB	2.48	0.59
1:B:192:ILE:CG1	1:B:193:LEU:H	2.15	0.59
1:B:369:ILE:O	1:B:369:ILE:CG1	2.42	0.59
1:A:169:TYR:CD1	2:W:6:LYS:HE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TYR:HD1	2:W:34:ARG:NH2	1.92	0.59
2:W:11:ASP:OD1	2:W:14:ARG:NH2	2.35	0.59
1:A:62:ARG:HG2	1:A:62:ARG:NH2	2.09	0.58
2:W:11:ASP:O	2:W:15:GLU:HG3	2.03	0.58
1:A:192:ILE:CG1	1:A:193:LEU:H	2.15	0.58
1:A:330:ILE:HD12	1:A:330:ILE:N	2.19	0.58
1:A:169:TYR:CD1	2:W:6:LYS:CE	2.87	0.58
1:A:116:ARG:NH2	1:A:371:HIS:ND1	2.51	0.58
2:W:6:LYS:O	2:W:10:LEU:HG	2.04	0.57
1:A:169:TYR:HE1	2:W:6:LYS:CE	2.13	0.57
1:B:330:ILE:N	1:B:330:ILE:HD12	2.19	0.57
1:A:189:LEU:HD12	1:A:192:ILE:CD1	2.23	0.57
1:A:25:ASP:HA	2:W:19:LEU:HB2	1.87	0.57
1:B:345:ILE:CG2	2:W:45:ILE:HD12	2.34	0.56
1:A:202:THR:CB	1:A:206:ARG:HD2	2.36	0.56
1:A:189:LEU:O	1:A:192:ILE:HG12	2.05	0.56
1:A:369:ILE:O	1:A:369:ILE:CG1	2.42	0.56
1:B:189:LEU:O	1:B:192:ILE:HG12	2.05	0.56
1:A:23:GLY:O	2:W:20:LYS:N	2.37	0.55
1:B:358:THR:HB	1:B:360:GLN:HE21	1.71	0.55
1:B:202:THR:CB	1:B:206:ARG:HD2	2.36	0.55
1:A:358:THR:HB	1:A:360:GLN:HE21	1.71	0.55
1:B:70:PRO:HG3	1:B:81:ASP:HB3	1.89	0.55
2:W:16:GLY:O	2:W:17:ALA:CB	2.54	0.55
1:A:360:GLN:H	1:A:360:GLN:NE2	2.05	0.54
1:B:169:TYR:CE1	2:W:34:ARG:NH2	2.53	0.54
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.89	0.54
1:A:202:THR:CB	1:A:206:ARG:CD	2.85	0.54
1:A:116:ARG:HH21	1:A:371:HIS:HE1	1.46	0.54
1:A:238:LYS:HE2	1:A:238:LYS:CA	2.37	0.54
1:B:202:THR:CB	1:B:206:ARG:CD	2.85	0.54
2:W:1:ALA:O	2:W:2:CYS:HB2	2.08	0.54
1:B:238:LYS:HE2	1:B:238:LYS:CA	2.37	0.54
1:B:360:GLN:H	1:B:360:GLN:NE2	2.05	0.53
1:A:23:GLY:O	2:W:19:LEU:HA	2.09	0.53
1:B:345:ILE:HG23	2:W:45:ILE:CD1	2.34	0.52
1:B:201:VAL:CG1	1:B:202:THR:N	2.30	0.52
1:B:106:THR:HB	1:B:137:GLN:HG3	1.91	0.52
1:A:106:THR:HB	1:A:137:GLN:HG3	1.91	0.52
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.91	0.52
1:B:202:THR:HA	1:B:206:ARG:CG	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:CYS:HB3	1:B:105:LEU:HD23	1.91	0.51
1:A:25:ASP:CA	2:W:19:LEU:HB2	2.41	0.51
1:A:202:THR:HA	1:A:206:ARG:CG	2.35	0.51
1:A:14:SER:HA	1:A:71:ILE:CG2	2.40	0.51
1:B:14:SER:HA	1:B:71:ILE:CG2	2.40	0.51
1:B:210:ARG:O	1:B:214:GLU:HG3	2.11	0.51
1:B:189:LEU:HD12	1:B:192:ILE:CD1	2.23	0.51
1:A:31:PHE:CE1	1:A:93:GLU:HG3	2.45	0.51
1:A:207:GLU:OE2	1:A:207:GLU:CA	2.59	0.51
1:A:358:THR:HB	1:A:360:GLN:NE2	2.26	0.50
1:B:207:GLU:OE2	1:B:207:GLU:CA	2.59	0.50
1:B:358:THR:HB	1:B:360:GLN:NE2	2.26	0.50
1:A:210:ARG:O	1:A:214:GLU:HG3	2.11	0.50
1:A:97:ALA:O	1:A:101:HIS:HD2	1.95	0.50
1:B:31:PHE:CE1	1:B:93:GLU:HG3	2.45	0.50
1:A:27:PRO:HG2	1:A:337:TYR:CD1	2.47	0.50
1:B:97:ALA:O	1:B:101:HIS:HD2	1.95	0.50
1:B:27:PRO:HG2	1:B:337:TYR:CD1	2.47	0.49
1:B:230:ALA:HB2	1:B:236:LEU:HD12	1.94	0.49
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.95	0.49
1:B:205:GLU:O	1:B:208:ILE:N	2.47	0.48
1:B:252:ASN:HA	1:B:255:PHE:CE2	2.48	0.48
1:A:194:THR:C	1:A:196:ARG:H	2.16	0.48
1:B:200:PHE:HD2	1:B:205:GLU:CB	2.25	0.48
1:A:200:PHE:HD2	1:A:205:GLU:CB	2.25	0.48
1:A:205:GLU:O	1:A:208:ILE:N	2.46	0.48
1:B:194:THR:C	1:B:196:ARG:H	2.16	0.48
1:B:355:MET:HE3	1:B:355:MET:HA	1.95	0.48
1:B:169:TYR:CD1	2:W:34:ARG:NE	2.79	0.48
1:B:241:GLU:HG3	1:B:247:VAL:HG22	1.95	0.48
2:W:18:GLN:O	2:W:19:LEU:CD2	2.59	0.48
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.94	0.48
1:A:73:HIC:CE1	1:A:179:ASP:CG	2.82	0.48
1:A:241:GLU:HG3	1:A:247:VAL:HG22	1.94	0.48
1:B:192:ILE:HG13	1:B:193:LEU:H	1.76	0.48
1:B:330:ILE:HG22	1:B:332:PRO:HD3	1.95	0.47
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.49	0.47
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.96	0.47
1:B:321:ALA:HB1	1:B:322:PRO:HD2	1.96	0.47
1:A:238:LYS:HE2	1:A:239:SER:N	2.27	0.47
1:B:73:HIC:CE1	1:B:179:ASP:CG	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG22	1:A:160:THR:N	2.30	0.47
1:A:355:MET:HE3	1:A:355:MET:HA	1.96	0.47
1:B:303:THR:HG22	1:B:303:THR:O	2.15	0.47
1:B:159:VAL:HG22	1:B:160:THR:N	2.29	0.47
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.96	0.47
1:A:178:LEU:HD12	1:A:277:THR:HG21	1.96	0.46
1:A:321:ALA:HB1	1:A:322:PRO:HD2	1.96	0.46
2:W:18:GLN:C	2:W:19:LEU:HG	2.36	0.46
1:A:169:TYR:HD1	2:W:6:LYS:HE2	1.80	0.46
1:B:109:PRO:HB3	1:B:175:ILE:HD13	1.98	0.46
1:A:201:VAL:CG1	1:A:202:THR:N	2.30	0.46
1:A:238:LYS:HE2	1:A:238:LYS:HA	1.98	0.46
1:B:222:ASP:HB3	1:B:225:ASN:HB3	1.98	0.46
1:A:200:PHE:HD2	1:A:205:GLU:CG	2.29	0.46
1:A:303:THR:O	1:A:303:THR:HG22	2.15	0.46
1:B:34:ILE:HD12	1:B:67:LEU:HD13	1.98	0.46
1:B:200:PHE:HD2	1:B:205:GLU:CG	2.29	0.46
1:A:250:ILE:CG2	1:A:253:GLU:HB2	2.47	0.45
1:B:17:VAL:HG11	1:B:31:PHE:CZ	2.52	0.45
1:B:178:LEU:HD12	1:B:277:THR:HG21	1.96	0.45
1:B:238:LYS:HE2	1:B:239:SER:N	2.27	0.45
1:A:17:VAL:HG11	1:A:31:PHE:CZ	2.52	0.45
1:A:222:ASP:HB3	1:A:225:ASN:HB3	1.98	0.45
1:B:250:ILE:CG2	1:B:253:GLU:HB2	2.47	0.45
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.98	0.45
1:A:34:ILE:HD12	1:A:67:LEU:HD13	1.97	0.44
1:B:105:LEU:HD12	1:B:132:MET:CE	2.47	0.44
1:B:204:ALA:O	1:B:207:GLU:HB2	2.16	0.44
1:B:234:SER:HB2	1:B:237:GLU:HG3	1.99	0.44
1:B:238:LYS:HE2	1:B:238:LYS:HA	1.98	0.44
1:A:202:THR:HB	1:A:206:ARG:HD2	1.99	0.44
1:A:204:ALA:O	1:A:207:GLU:HB2	2.16	0.44
1:B:8:LEU:HD22	1:B:94:LEU:HD13	1.99	0.44
1:B:70:PRO:HG2	1:B:85:ILE:HD12	1.98	0.44
1:A:8:LEU:HD22	1:A:94:LEU:HD13	1.99	0.44
1:B:59:GLN:O	1:B:62:ARG:NH2	2.51	0.44
1:A:105:LEU:HD12	1:A:132:MET:CE	2.47	0.44
1:A:120:THR:HA	1:A:132:MET:SD	2.58	0.44
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.98	0.44
1:A:221:LEU:CD2	1:A:315:LYS:HD2	2.48	0.44
2:W:12:GLN:O	2:W:15:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:HB2	1:A:237:GLU:HG3	1.99	0.43
1:A:156:GLY:O	1:A:181:ALA:HB1	2.18	0.43
1:B:156:GLY:O	1:B:181:ALA:HB1	2.18	0.43
1:B:202:THR:O	1:B:203:THR:C	2.56	0.43
1:B:221:LEU:CD2	1:B:315:LYS:HD2	2.48	0.43
1:A:202:THR:O	1:A:203:THR:C	2.56	0.43
1:A:117:GLU:HG3	1:A:371:HIS:NE2	2.34	0.43
1:A:243:PRO:O	1:A:244:ASP:C	2.56	0.43
1:B:243:PRO:O	1:B:244:ASP:C	2.56	0.43
1:B:120:THR:HA	1:B:132:MET:SD	2.58	0.43
1:B:351:THR:OG1	2:W:37:LEU:HA	2.19	0.43
1:B:351:THR:H	2:W:40:GLN:HE22	1.65	0.43
1:B:202:THR:HB	1:B:206:ARG:HD2	1.99	0.42
2:W:1:ALA:O	2:W:2:CYS:CB	2.66	0.42
1:B:104:LEU:HD23	1:B:104:LEU:C	2.40	0.42
1:A:198:TYR:OH	1:A:248:ILE:HB	2.19	0.42
1:A:104:LEU:C	1:A:104:LEU:HD23	2.40	0.42
1:A:192:ILE:HG13	1:A:193:LEU:H	1.76	0.42
1:B:105:LEU:HD12	1:B:132:MET:HE3	2.00	0.42
1:B:205:GLU:O	1:B:206:ARG:C	2.58	0.42
1:A:345:ILE:O	1:A:346:LEU:C	2.57	0.42
1:B:200:PHE:HA	1:B:205:GLU:HG2	2.02	0.42
1:B:202:THR:OG1	1:B:206:ARG:HD2	2.13	0.42
1:A:351:THR:H	2:W:12:GLN:HE22	1.66	0.42
1:B:345:ILE:O	1:B:346:LEU:C	2.57	0.42
1:B:190:MET:HB2	1:B:209:VAL:HG11	2.02	0.42
1:B:241:GLU:C	1:B:242:LEU:HD23	2.30	0.42
1:B:171:LEU:HA	1:B:172:PRO:HD3	1.88	0.42
1:A:59:GLN:O	1:A:62:ARG:NH2	2.51	0.41
1:A:351:THR:OG1	2:W:9:LEU:HA	2.20	0.41
1:A:190:MET:HB2	1:A:209:VAL:HG11	2.02	0.41
1:A:202:THR:OG1	1:A:206:ARG:HD2	2.13	0.41
1:A:205:GLU:O	1:A:206:ARG:C	2.58	0.41
1:A:332:PRO:HA	1:A:333:PRO:HD3	1.95	0.41
1:A:13:GLY:HA3	3:A:400:ATP:PB	2.60	0.41
1:A:200:PHE:HA	1:A:205:GLU:HG2	2.02	0.41
1:B:327:ILE:CG2	1:B:328:LYS:N	2.84	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.85	0.41
1:A:218:TYR:O	1:A:255:PHE:HA	2.21	0.41
1:B:13:GLY:HA3	3:B:400:ATP:PB	2.60	0.41
1:B:169:TYR:HE1	2:W:34:ARG:NH1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PHE:HD2	1:B:205:GLU:HG2	1.86	0.41
1:A:160:THR:HB	1:A:178:LEU:HB3	2.03	0.41
1:B:198:TYR:OH	1:B:248:ILE:HB	2.19	0.41
1:A:200:PHE:HD2	1:A:205:GLU:HG2	1.86	0.40
1:A:169:TYR:CE1	2:W:6:LYS:HE2	2.51	0.40
1:A:327:ILE:CG2	1:A:328:LYS:N	2.84	0.40
1:A:345:ILE:HG12	2:W:19:LEU:HD21	2.04	0.40
1:B:160:THR:HB	1:B:178:LEU:HB3	2.03	0.40
1:B:201:VAL:HG12	1:B:202:THR:HG22	2.04	0.40

All (7) 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:288:ASP:OD1	1:B:203:THR:OG1[5_455]	1.18	1.02
1:A:41:GLN:NE2	1:A:113:LYS:N[10_665]	1.81	0.39
1:A:41:GLN:OE1	1:A:113:LYS:N[10_665]	1.86	0.34
1:B:215:LYS:O	2:W:21:LYS:NZ[8_665]	1.94	0.26
1:A:41:GLN:OE1	1:A:112:PRO:CA[10_665]	1.99	0.21
1:A:41:GLN:CD	1:A:113:LYS:N[10_665]	2.07	0.13
1:A:288:ASP:OD1	1:B:203:THR:CB[5_455]	2.11	0.09

## 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	359/375 (96%)	331 (92%)	27 (8%)	1 (0%)	41	77
1	B	354/375 (94%)	329 (93%)	25 (7%)	0	100	100
2	W	36/101 (36%)	32 (89%)	3 (8%)	1 (3%)	5	30
All	All	749/851 (88%)	692 (92%)	55 (7%)	2 (0%)	41	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	W	17	ALA
1	A	369	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	309/317 (98%)	289 (94%)	20 (6%)	17	42
1	B	304/317 (96%)	284 (93%)	20 (7%)	16	41
2	W	31/85 (36%)	30 (97%)	1 (3%)	39	61
All	All	644/719 (90%)	603 (94%)	41 (6%)	17	42

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	16	LEU
1	A	34	ILE
1	A	121	GLN
1	A	178	LEU
1	A	203	THR
1	A	207	GLU
1	A	208	ILE
1	A	221	LEU
1	A	238	LYS
1	A	242	LEU
1	A	286	ASP
1	A	323	SER
1	A	324	THR
1	A	325	MET
1	A	354	GLN
1	A	355	MET
1	A	358	THR
1	A	368	SER

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Mol	Chain	Res	Type
1	A	369	ILE
1	B	4	GLU
1	B	16	LEU
1	B	34	ILE
1	B	121	GLN
1	B	178	LEU
1	B	203	THR
1	B	207	GLU
1	B	208	ILE
1	B	221	LEU
1	B	238	LYS
1	B	242	LEU
1	B	286	ASP
1	B	323	SER
1	B	324	THR
1	B	325	MET
1	B	354	GLN
1	B	355	MET
1	B	358	THR
1	B	368	SER
1	B	369	ILE
2	W	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	101	HIS
1	A	121	GLN
1	A	280	ASN
1	A	354	GLN
1	A	360	GLN
1	B	41	GLN
1	B	92	ASN
1	B	101	HIS
1	B	121	GLN
1	B	280	ASN
1	B	360	GLN
2	W	12	GLN
2	W	40	GLN
2	W	43	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	HIC	A	73	1	8,11,12	2.89	3 (37%)	6,14,16	0.86	0
1	HIC	B	73	1	8,11,12	2.90	3 (37%)	6,14,16	0.87	0

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
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1
1	HIC	B	73	1	-	0/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIC	CD2-CG	6.88	1.46	1.36
1	A	73	HIC	CD2-CG	6.85	1.46	1.36
1	A	73	HIC	CE1-ND1	3.61	1.41	1.35
1	B	73	HIC	CE1-ND1	3.59	1.41	1.35
1	A	73	HIC	CZ-NE2	-2.51	1.41	1.48
1	B	73	HIC	CZ-NE2	-2.49	1.41	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	1	0
1	B	73	HIC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	400	4	26,33,33	0.96	1 (3%)	31,52,52	1.33	5 (16%)
3	ATP	B	400	4	26,33,33	0.96	1 (3%)	31,52,52	1.33	5 (16%)

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	400	4	-	2/18/38/38	0/3/3/3
3	ATP	B	400	4	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ATP	C5-C4	2.48	1.47	1.40
3	B	400	ATP	C5-C4	2.45	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ATP	N3-C2-N1	-3.38	123.39	128.68
3	B	400	ATP	N3-C2-N1	-3.36	123.43	128.68
3	B	400	ATP	C4-C5-N7	-2.50	106.79	109.40
3	A	400	ATP	C4-C5-N7	-2.50	106.80	109.40
3	B	400	ATP	PB-O3B-PG	-2.35	124.78	132.83
3	A	400	ATP	PB-O3B-PG	-2.35	124.78	132.83
3	A	400	ATP	PA-O3A-PB	-2.09	125.66	132.83
3	B	400	ATP	PA-O3A-PB	-2.09	125.67	132.83
3	A	400	ATP	O3G-PG-O2G	2.03	115.41	107.64
3	B	400	ATP	O3G-PG-O2G	2.03	115.40	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

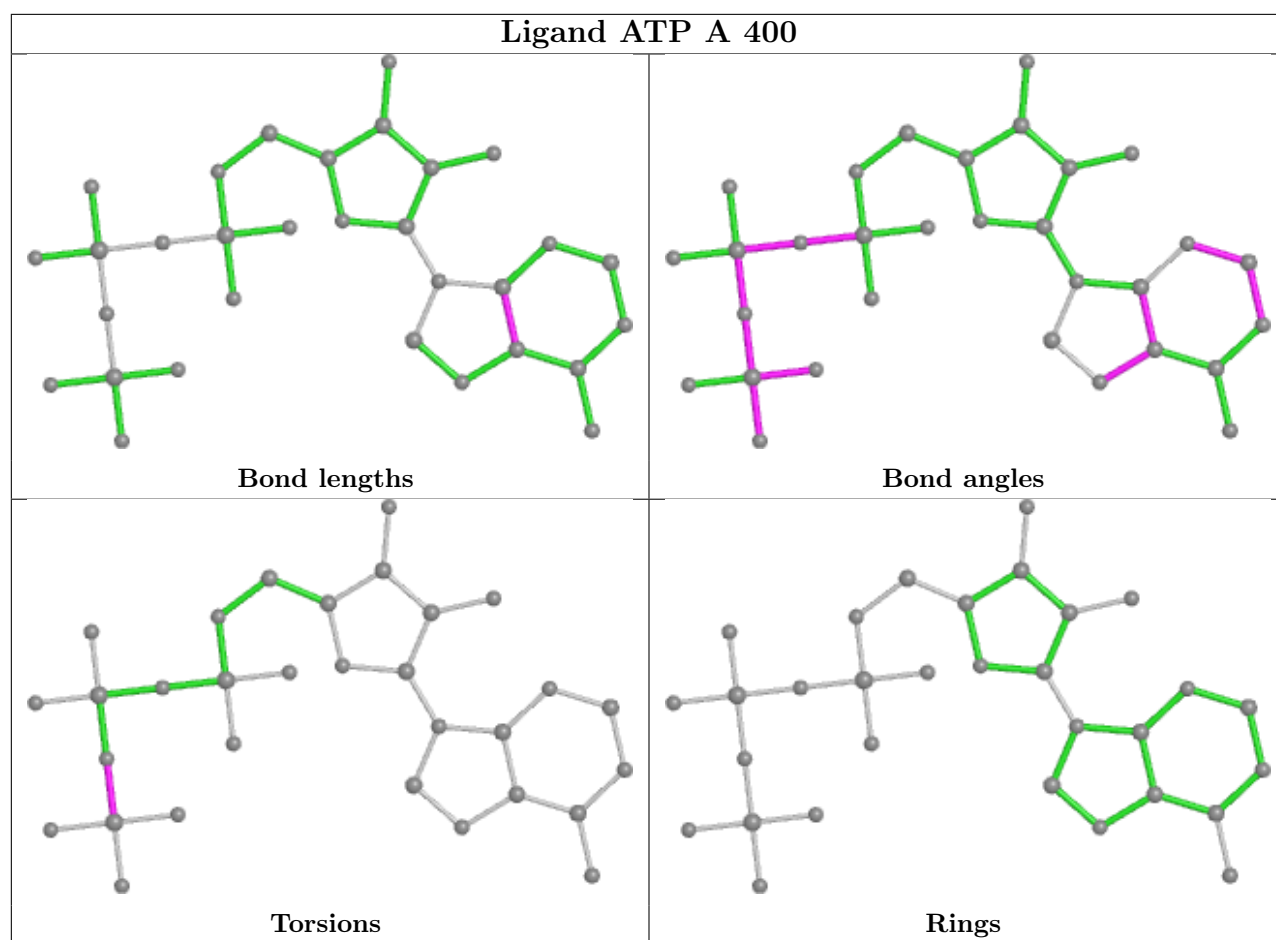
Mol	Chain	Res	Type	Atoms
3	A	400	ATP	PB-O3B-PG-O2G
3	B	400	ATP	PB-O3B-PG-O2G
3	A	400	ATP	PB-O3B-PG-O1G
3	B	400	ATP	PB-O3B-PG-O1G

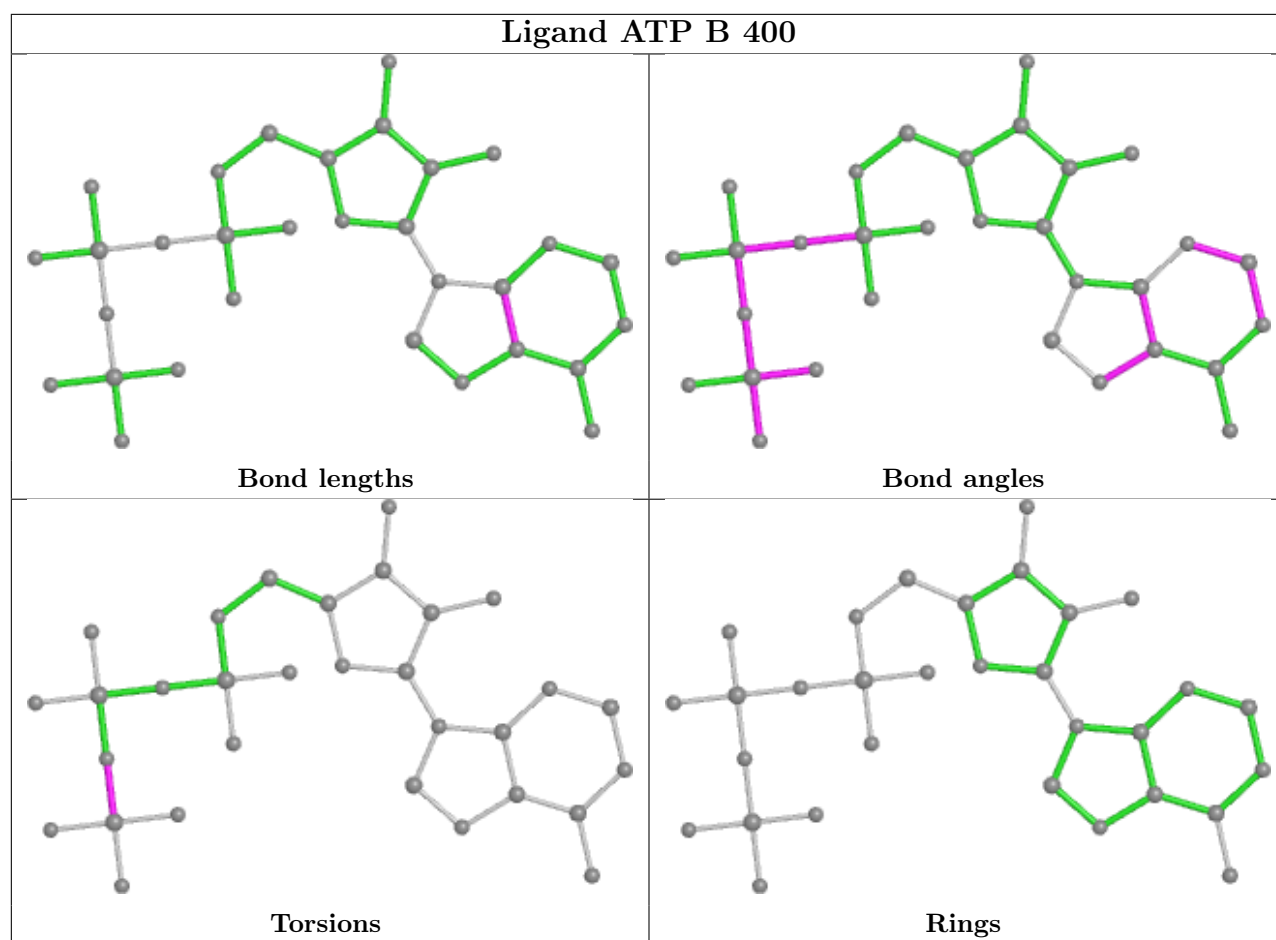
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	ATP	1	0
3	B	400	ATP	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

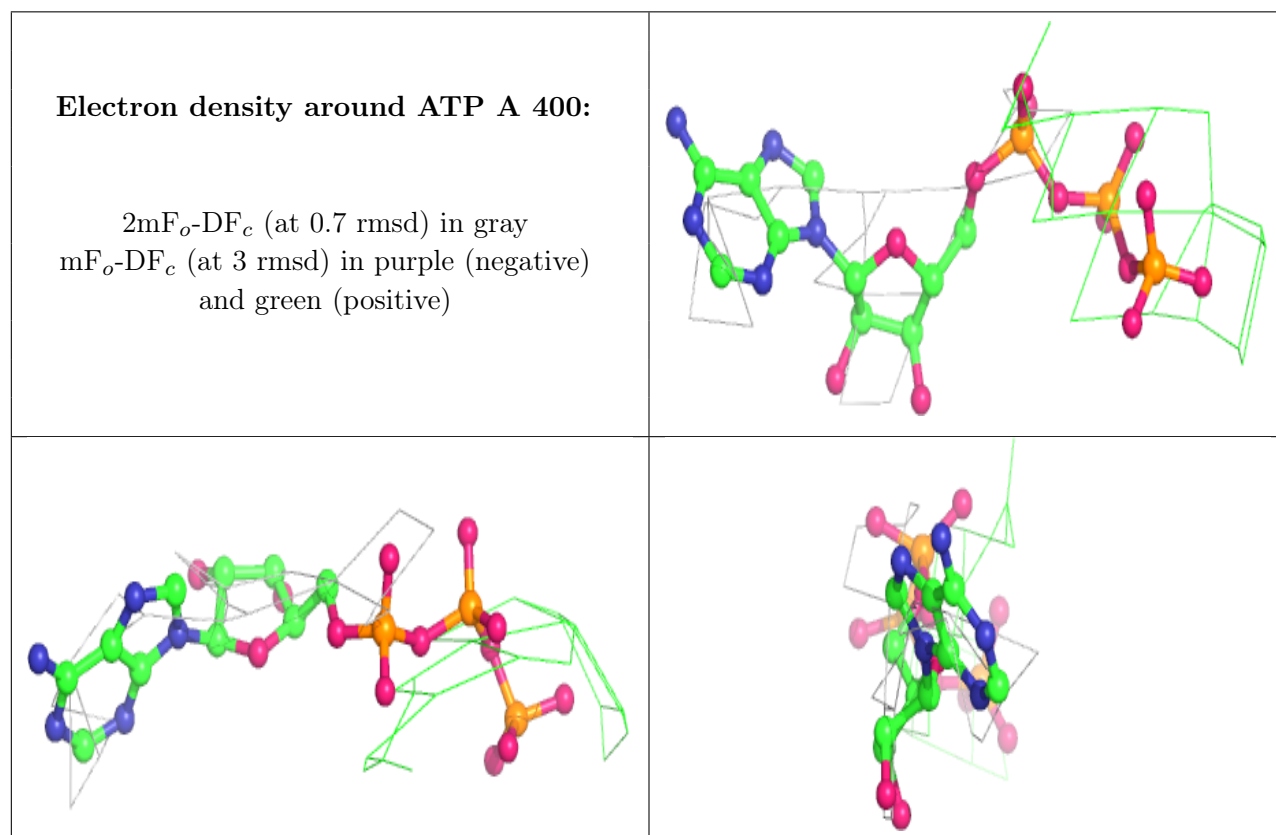
### 6.3 Carbohydrates [i](#)

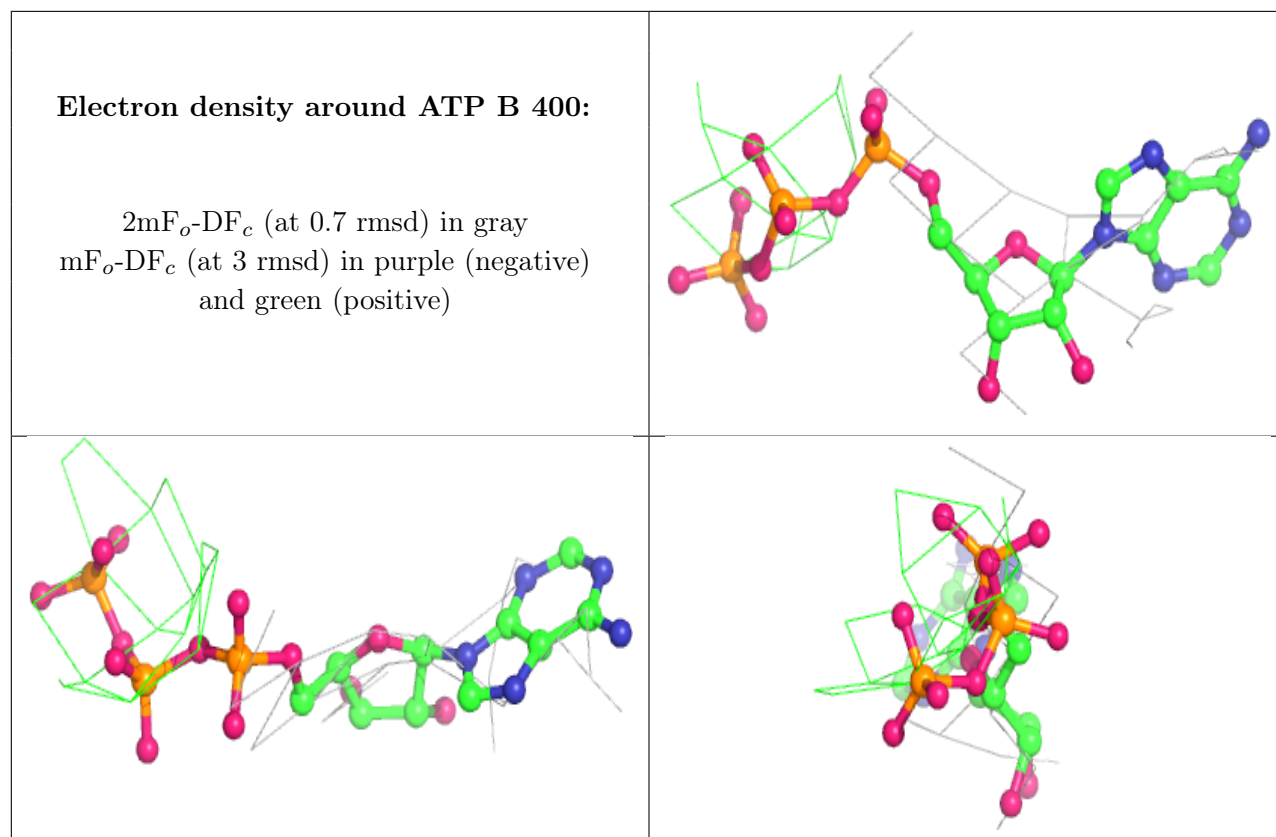
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.