



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 AM UTC

PDB ID : 7Y77 / pdb_00007y77
Title : Crystal structure of rice NAL1
Authors : Yan, J.J.; Guan, Z.Y.; Yin, P.; Xiong, L.Z.
Deposited on : 2022-06-21
Resolution : 2.60 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

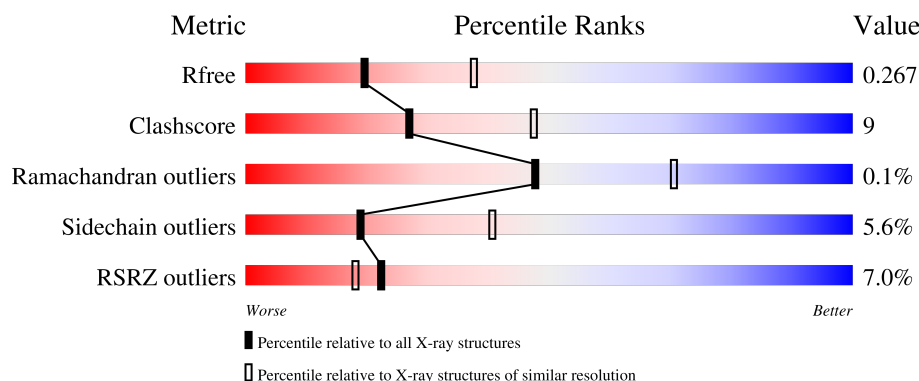
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	435	5% 68% 20% 11%
1	B	435	6% 68% 18% 11%
1	C	435	8% 67% 19% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9030 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 Protein NARROW LEAF 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2988	1895	522	565	6			
1	B	386	Total	C	N	O	S	0	0	0
			2978	1890	519	563	6			
1	C	382	Total	C	N	O	S	0	0	0
			2945	1866	514	559	6			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP B4XT64
A	32	GLY	-	expression tag	UNP B4XT64
A	33	SER	-	expression tag	UNP B4XT64
A	34	SER	-	expression tag	UNP B4XT64
A	35	HIS	-	expression tag	UNP B4XT64
A	36	HIS	-	expression tag	UNP B4XT64
A	37	HIS	-	expression tag	UNP B4XT64
A	38	HIS	-	expression tag	UNP B4XT64
A	39	HIS	-	expression tag	UNP B4XT64
A	40	HIS	-	expression tag	UNP B4XT64
A	41	SER	-	expression tag	UNP B4XT64
A	42	SER	-	expression tag	UNP B4XT64
A	43	GLY	-	expression tag	UNP B4XT64
A	44	LEU	-	expression tag	UNP B4XT64
A	45	VAL	-	expression tag	UNP B4XT64
A	46	PRO	-	expression tag	UNP B4XT64
A	47	ARG	-	expression tag	UNP B4XT64
A	48	GLY	-	expression tag	UNP B4XT64
A	49	SER	-	expression tag	UNP B4XT64
A	50	HIS	-	expression tag	UNP B4XT64
A	51	SER	-	expression tag	UNP B4XT64
A	52	ASP	-	expression tag	UNP B4XT64
A	53	GLU	-	expression tag	UNP B4XT64

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Chain	Residue	Modelled	Actual	Comment	Reference
A	54	VAL	-	expression tag	UNP B4XT64
A	55	ASP	-	expression tag	UNP B4XT64
A	56	ALA	-	expression tag	UNP B4XT64
A	57	HIS	-	expression tag	UNP B4XT64
A	58	MET	-	expression tag	UNP B4XT64
A	61	SER	CYS	engineered mutation	UNP B4XT64
A	193	SER	CYS	engineered mutation	UNP B4XT64
A	198	SER	CYS	engineered mutation	UNP B4XT64
A	326	SER	CYS	engineered mutation	UNP B4XT64
A	337	SER	CYS	engineered mutation	UNP B4XT64
A	364	SER	CYS	engineered mutation	UNP B4XT64
A	470	ARG	-	expression tag	UNP B4XT64
A	471	PHE	-	expression tag	UNP B4XT64
B	31	MET	-	initiating methionine	UNP B4XT64
B	32	GLY	-	expression tag	UNP B4XT64
B	33	SER	-	expression tag	UNP B4XT64
B	34	SER	-	expression tag	UNP B4XT64
B	35	HIS	-	expression tag	UNP B4XT64
B	36	HIS	-	expression tag	UNP B4XT64
B	37	HIS	-	expression tag	UNP B4XT64
B	38	HIS	-	expression tag	UNP B4XT64
B	39	HIS	-	expression tag	UNP B4XT64
B	40	HIS	-	expression tag	UNP B4XT64
B	41	SER	-	expression tag	UNP B4XT64
B	42	SER	-	expression tag	UNP B4XT64
B	43	GLY	-	expression tag	UNP B4XT64
B	44	LEU	-	expression tag	UNP B4XT64
B	45	VAL	-	expression tag	UNP B4XT64
B	46	PRO	-	expression tag	UNP B4XT64
B	47	ARG	-	expression tag	UNP B4XT64
B	48	GLY	-	expression tag	UNP B4XT64
B	49	SER	-	expression tag	UNP B4XT64
B	50	HIS	-	expression tag	UNP B4XT64
B	51	SER	-	expression tag	UNP B4XT64
B	52	ASP	-	expression tag	UNP B4XT64
B	53	GLU	-	expression tag	UNP B4XT64
B	54	VAL	-	expression tag	UNP B4XT64
B	55	ASP	-	expression tag	UNP B4XT64
B	56	ALA	-	expression tag	UNP B4XT64
B	57	HIS	-	expression tag	UNP B4XT64
B	58	MET	-	expression tag	UNP B4XT64
B	61	SER	CYS	engineered mutation	UNP B4XT64

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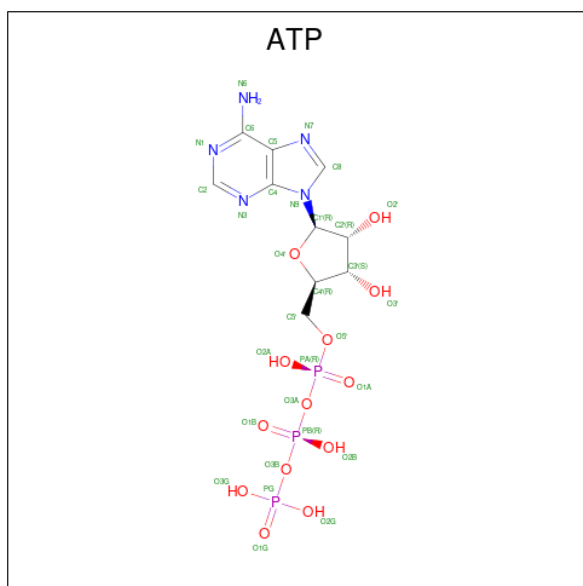
Chain	Residue	Modelled	Actual	Comment	Reference
B	193	SER	CYS	engineered mutation	UNP B4XT64
B	198	SER	CYS	engineered mutation	UNP B4XT64
B	326	SER	CYS	engineered mutation	UNP B4XT64
B	337	SER	CYS	engineered mutation	UNP B4XT64
B	364	SER	CYS	engineered mutation	UNP B4XT64
B	464	ARG	-	expression tag	UNP B4XT64
B	465	PHE	-	expression tag	UNP B4XT64
C	31	MET	-	initiating methionine	UNP B4XT64
C	32	GLY	-	expression tag	UNP B4XT64
C	33	SER	-	expression tag	UNP B4XT64
C	34	SER	-	expression tag	UNP B4XT64
C	35	HIS	-	expression tag	UNP B4XT64
C	36	HIS	-	expression tag	UNP B4XT64
C	37	HIS	-	expression tag	UNP B4XT64
C	38	HIS	-	expression tag	UNP B4XT64
C	39	HIS	-	expression tag	UNP B4XT64
C	40	HIS	-	expression tag	UNP B4XT64
C	41	SER	-	expression tag	UNP B4XT64
C	42	SER	-	expression tag	UNP B4XT64
C	43	GLY	-	expression tag	UNP B4XT64
C	44	LEU	-	expression tag	UNP B4XT64
C	45	VAL	-	expression tag	UNP B4XT64
C	46	PRO	-	expression tag	UNP B4XT64
C	47	ARG	-	expression tag	UNP B4XT64
C	48	GLY	-	expression tag	UNP B4XT64
C	49	SER	-	expression tag	UNP B4XT64
C	50	HIS	-	expression tag	UNP B4XT64
C	51	SER	-	expression tag	UNP B4XT64
C	52	ASP	-	expression tag	UNP B4XT64
C	53	GLU	-	expression tag	UNP B4XT64
C	54	VAL	-	expression tag	UNP B4XT64
C	55	ASP	-	expression tag	UNP B4XT64
C	56	ALA	-	expression tag	UNP B4XT64
C	57	HIS	-	expression tag	UNP B4XT64
C	58	MET	-	expression tag	UNP B4XT64
C	61	SER	CYS	engineered mutation	UNP B4XT64
C	193	SER	CYS	engineered mutation	UNP B4XT64
C	198	SER	CYS	engineered mutation	UNP B4XT64
C	326	SER	CYS	engineered mutation	UNP B4XT64
C	337	SER	CYS	engineered mutation	UNP B4XT64
C	364	SER	CYS	engineered mutation	UNP B4XT64
C	464	ARG	-	expression tag	UNP B4XT64

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Chain	Residue	Modelled	Actual	Comment	Reference
C	465	PHE	-	expression tag	UNP B4XT64

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

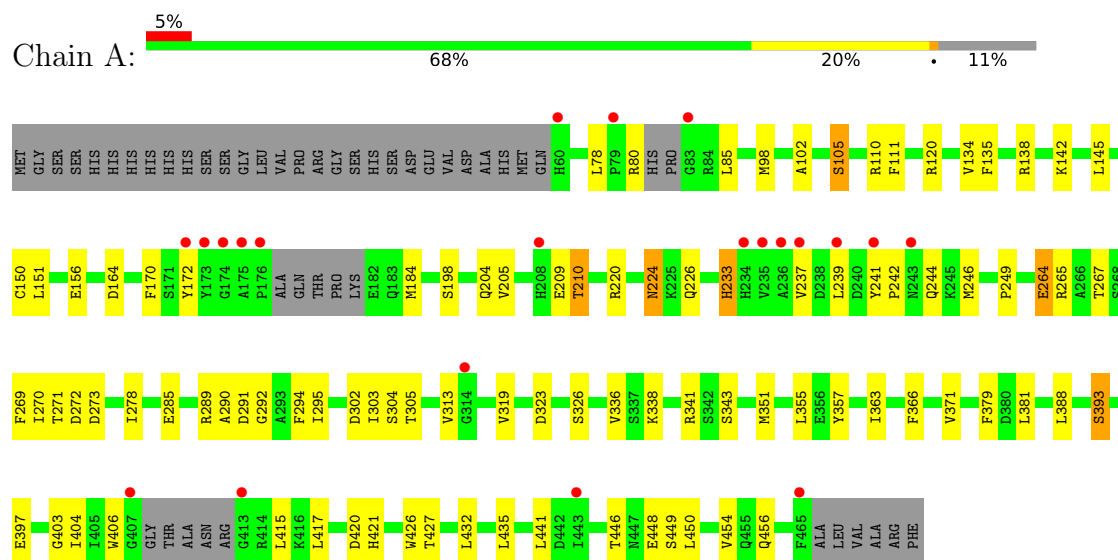
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	11	Total O 11 11	0	0
3	C	8	Total O 8 8	0	0

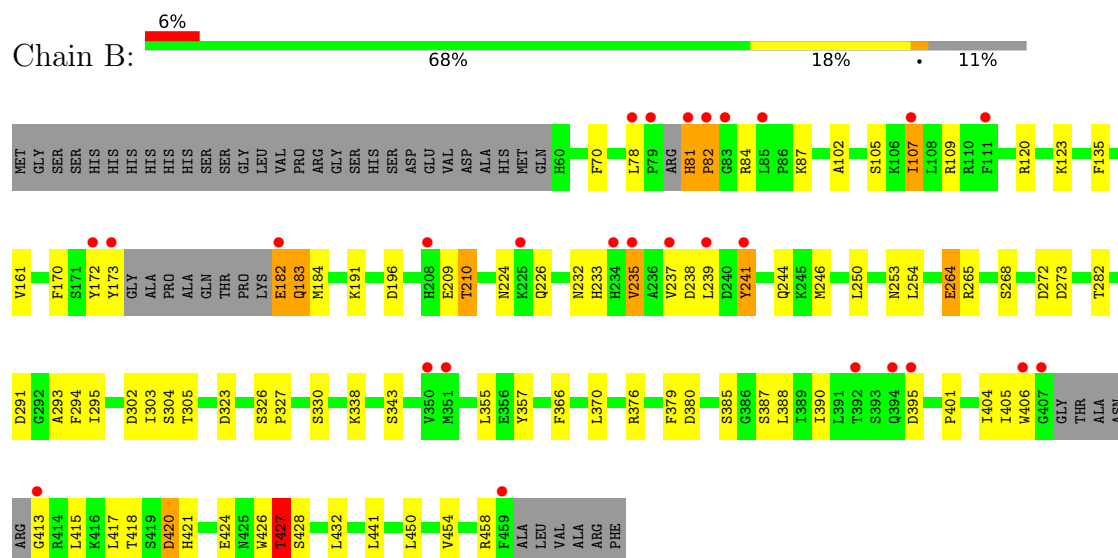
3 Residue-property plots [i](#)

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: Protein NARROW LEAF 1

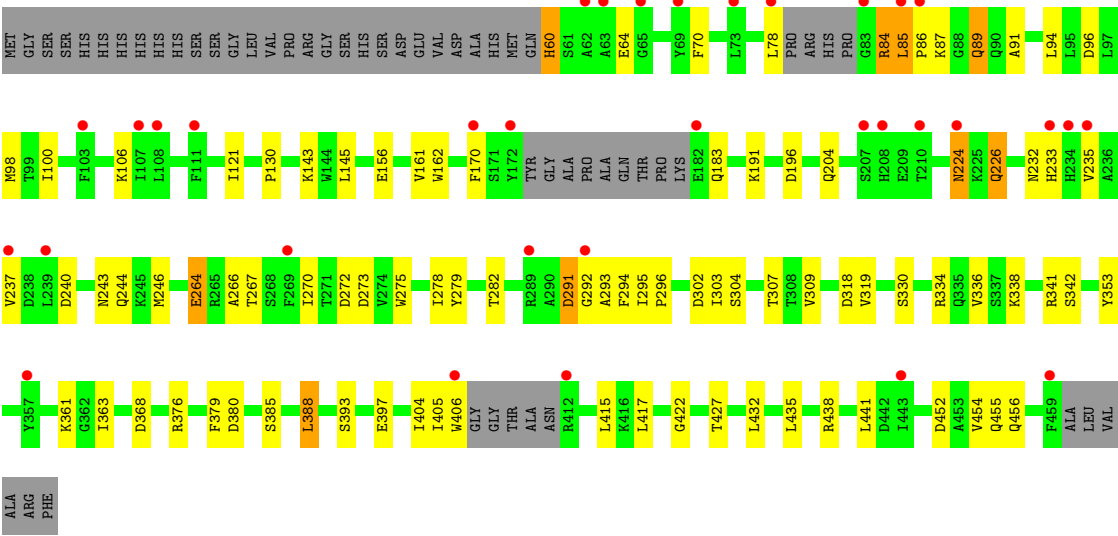


• Molecule 1: Protein NARROW LEAF 1



• Molecule 1: Protein NARROW LEAF 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.41Å 194.40Å 173.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 2.60 49.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.67-2.60) 99.9 (49.67-2.60)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.268 0.224 , 0.267	Depositor DCC
R_{free} test set	2280 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: 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	0.18	0/3049	0.37	0/4131
1	B	0.39	0/3040	0.63	2/4120 (0.0%)
1	C	0.31	0/3003	0.52	3/4067 (0.1%)
All	All	0.31	0/9092	0.52	5/12318 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	PHE	CA-CB-CG	7.62	121.42	113.80
1	B	427	THR	OG1-CB-CG2	6.71	122.73	109.30
1	C	89	GLN	N-CA-C	-6.22	105.45	113.16
1	C	240	ASP	N-CA-C	-5.72	106.27	113.20
1	B	241	TYR	CB-CA-C	5.03	116.86	109.22

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	2988	0	2956	58	1
1	B	2978	0	2942	52	0
1	C	2945	0	2914	55	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	12	2	0
2	B	31	0	12	0	0
2	C	31	0	12	2	0
3	A	7	0	0	2	0
3	B	11	0	0	0	0
3	C	8	0	0	2	0
All	All	9030	0	8848	165	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (165) 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:406:TRP:HE3	1:B:428:SER:HG	1.11	0.98
1:A:420:ASP:OD1	1:A:421:HIS:ND1	2.06	0.88
1:A:237:VAL:HA	1:A:244:GLN:HG2	1.60	0.84
1:C:237:VAL:HA	1:C:244:GLN:HG2	1.61	0.82
1:C:60:HIS:CE1	1:C:64:GLU:OE1	2.37	0.78
1:B:237:VAL:HA	1:B:244:GLN:HG2	1.64	0.78
1:A:291:ASP:HB2	1:A:406:TRP:CD1	2.21	0.76
1:A:291:ASP:HB2	1:A:406:TRP:HD1	1.50	0.73
1:A:204:GLN:OE1	1:A:341:ARG:NH1	2.24	0.70
1:A:110:ARG:O	3:A:601:HOH:O	2.07	0.70
2:C:501:ATP:O1G	3:C:601:HOH:O	2.08	0.70
1:B:184:MET:HG3	1:B:343:SER:HA	1.76	0.67
1:B:173:TYR:O	1:B:413:GLY:N	2.28	0.67
1:C:267:THR:HG21	1:C:438:ARG:HG3	1.77	0.67
1:B:253:ASN:OD1	1:B:254:LEU:HD12	1.95	0.66
1:B:82:PRO:HD2	1:B:84:ARG:HB2	1.78	0.65
1:A:246:MET:HG3	1:A:295:ILE:HG12	1.78	0.65
1:B:380:ASP:OD2	1:B:427:THR:OG1	2.15	0.64
1:B:418:THR:HG23	1:B:421:HIS:H	1.62	0.63
1:C:224:ASN:HB2	1:C:226:GLN:HG2	1.81	0.63
1:A:102:ALA:O	1:A:105:SER:OG	2.17	0.62
1:B:224:ASN:HB2	1:B:226:GLN:HG2	1.83	0.61
1:C:60:HIS:HE1	1:C:64:GLU:OE1	1.82	0.60
1:A:142:LYS:HE2	1:A:150:CYS:SG	2.42	0.60
1:C:204:GLN:HG3	1:C:341:ARG:HD2	1.83	0.59
1:C:303:ILE:HG21	1:C:454:VAL:HG21	1.83	0.59
1:C:121:ILE:O	3:C:601:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:PHE:HB2	1:B:441:LEU:HD11	1.84	0.59
1:C:96:ASP:O	1:C:100:ILE:HG13	2.03	0.59
1:B:232:ASN:ND2	1:B:235:VAL:H	2.01	0.57
1:A:305:THR:HG22	1:C:143:LYS:HD3	1.85	0.57
1:A:446:THR:HG23	1:A:449:SER:H	1.70	0.57
1:A:388:LEU:HD12	1:A:404:ILE:HG22	1.87	0.56
1:C:338:LYS:HD2	1:C:405:ILE:HD11	1.86	0.56
1:A:204:GLN:NE2	1:A:249:PRO:O	2.38	0.56
1:A:184:MET:HG3	1:A:343:SER:HA	1.87	0.56
1:A:450:LEU:O	1:A:454:VAL:HG23	2.06	0.56
1:B:323:ASP:HB3	1:B:326:SER:OG	2.04	0.56
1:A:267:THR:OG1	1:A:290:ALA:O	2.24	0.56
1:A:85:LEU:HD13	1:A:156:GLU:HG2	1.89	0.54
1:B:291:ASP:HB2	1:B:406:TRP:HD1	1.74	0.53
1:C:388:LEU:HD12	1:C:404:ILE:HG22	1.92	0.52
1:A:420:ASP:OD1	1:A:421:HIS:CE1	2.63	0.52
1:B:70:PHE:HE2	1:B:282:THR:HA	1.75	0.52
1:B:102:ALA:O	1:B:105:SER:OG	2.26	0.52
1:A:302:ASP:OD1	1:A:304:SER:OG	2.23	0.52
1:A:138:ARG:NH1	1:B:250:LEU:HD11	2.25	0.52
1:A:448:GLU:OE1	1:A:448:GLU:N	2.27	0.52
1:A:415:LEU:CD2	1:A:426:TRP:HB3	2.41	0.51
1:C:380:ASP:OD2	1:C:427:THR:OG1	2.26	0.51
1:C:379:PHE:HD2	1:C:427:THR:HG21	1.75	0.51
1:C:415:LEU:HD13	1:C:417:LEU:HG	1.92	0.50
1:C:294:PHE:HB2	1:C:441:LEU:HD11	1.94	0.50
1:A:393:SER:HB2	1:A:397:GLU:O	2.12	0.50
1:B:302:ASP:OD1	1:B:304:SER:OG	2.24	0.50
1:C:404:ILE:HG23	1:C:432:LEU:HD13	1.94	0.50
1:A:134:VAL:HG11	1:A:151:LEU:HD21	1.94	0.49
1:B:370:LEU:HD21	1:B:426:TRP:HB2	1.94	0.49
1:A:371:VAL:HB	1:A:427:THR:HG22	1.95	0.49
1:A:273:ASP:N	1:A:273:ASP:OD1	2.44	0.49
1:A:379:PHE:HD2	1:A:427:THR:HG21	1.77	0.49
1:C:70:PHE:HE2	1:C:282:THR:HA	1.77	0.49
1:C:302:ASP:OD1	1:C:304:SER:OG	2.23	0.49
1:B:246:MET:HG3	1:B:295:ILE:HG12	1.95	0.49
1:A:404:ILE:HG23	1:A:432:LEU:HD13	1.94	0.49
1:A:292:GLY:HA3	1:A:435:LEU:HD11	1.95	0.48
1:B:182:GLU:OE1	1:B:183:GLN:N	2.45	0.48
1:B:327:PRO:O	1:B:330:SER:OG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:HB2	1:C:406:TRP:HD1	1.77	0.48
1:A:209:GLU:OE1	1:A:209:GLU:N	2.46	0.48
1:B:302:ASP:O	1:B:305:THR:OG1	2.31	0.48
1:B:450:LEU:O	1:B:454:VAL:HG23	2.14	0.48
1:B:388:LEU:HD12	1:B:404:ILE:HG22	1.94	0.48
1:C:438:ARG:O	1:C:438:ARG:HD3	2.14	0.48
1:A:241:TYR:HE1	1:A:244:GLN:HA	1.77	0.47
1:A:241:TYR:CE1	1:A:244:GLN:HG3	2.49	0.47
1:C:246:MET:HG3	1:C:295:ILE:HG12	1.96	0.47
1:B:191:LYS:HB3	1:B:196:ASP:HB2	1.97	0.47
1:A:241:TYR:HB2	1:A:242:PRO:HD2	1.97	0.47
1:B:379:PHE:HD2	1:B:427:THR:HG21	1.80	0.47
1:A:145:LEU:HD11	2:A:501:ATP:C4	2.50	0.47
1:C:84:ARG:HA	1:C:84:ARG:HD2	1.66	0.47
1:C:145:LEU:HD11	2:C:501:ATP:C4	2.50	0.46
1:C:338:LYS:HD2	1:C:405:ILE:CD1	2.46	0.46
1:A:205:VAL:HB	1:A:246:MET:HE3	1.98	0.46
1:B:209:GLU:N	1:B:209:GLU:OE1	2.49	0.46
1:C:233:HIS:ND1	1:C:266:ALA:HB1	2.30	0.46
1:C:397:GLU:H	1:C:397:GLU:CD	2.24	0.46
1:C:78:LEU:HA	1:C:78:LEU:HD23	1.79	0.46
1:C:94:LEU:O	1:C:98:MET:HG3	2.16	0.46
1:C:270:ILE:HD11	1:C:438:ARG:CZ	2.46	0.45
1:A:110:ARG:HG2	1:A:111:PHE:CE2	2.51	0.45
1:A:323:ASP:HB3	1:A:326:SER:OG	2.16	0.45
1:B:233:HIS:HA	1:B:293:ALA:HB2	1.98	0.45
1:C:278:ILE:HD12	1:C:279:TYR:C	2.41	0.45
1:A:184:MET:HE2	1:A:381:LEU:HD11	1.99	0.45
1:B:107:ILE:H	1:B:107:ILE:HG13	1.54	0.45
1:B:380:ASP:CG	1:B:427:THR:OG1	2.60	0.45
1:B:238:ASP:HB3	1:B:241:TYR:HE1	1.81	0.45
1:A:98:MET:HE2	1:A:278:ILE:HD11	1.99	0.45
1:B:81:HIS:O	1:B:81:HIS:CG	2.70	0.45
1:B:415:LEU:HD13	1:B:417:LEU:HG	1.98	0.45
1:C:233:HIS:HA	1:C:293:ALA:HB2	1.98	0.45
1:C:452:ASP:O	1:C:456:GLN:HG2	2.17	0.44
1:A:135:PHE:HB3	1:A:170:PHE:HB3	1.98	0.44
1:A:233:HIS:CE1	1:A:237:VAL:HB	2.53	0.44
1:C:264:GLU:HG2	1:C:296:PRO:HG3	1.99	0.44
1:C:307:THR:OG1	1:C:309:VAL:HG12	2.17	0.44
1:B:264:GLU:HG3	1:B:265:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:HB2	1:C:406:TRP:CD1	2.52	0.44
1:B:135:PHE:HB3	1:B:170:PHE:HB3	2.00	0.44
1:C:338:LYS:HG2	1:C:379:PHE:CZ	2.53	0.44
1:C:318:ASP:OD1	1:C:319:VAL:N	2.48	0.44
1:A:294:PHE:HB2	1:A:441:LEU:HD11	1.99	0.44
1:C:330:SER:O	1:C:334:ARG:NH1	2.51	0.43
1:A:85:LEU:H	1:A:85:LEU:HD23	1.84	0.43
1:B:387:SER:HB2	1:B:405:ILE:HD12	2.01	0.43
1:C:156:GLU:HA	1:C:162:TRP:HA	1.99	0.43
1:B:172:TYR:CE2	1:B:357:TYR:HD1	2.37	0.43
1:A:355:LEU:O	1:A:366:PHE:HA	2.19	0.43
1:A:351:MET:CE	1:A:417:LEU:HD11	2.48	0.42
1:B:272:ASP:OD1	1:B:272:ASP:N	2.50	0.42
1:C:270:ILE:HG22	1:C:275:TRP:HB2	2.01	0.42
1:A:264:GLU:OE2	1:A:265:ARG:NE	2.47	0.42
1:B:303:ILE:HD12	1:B:304:SER:N	2.34	0.42
1:C:183:GLN:HE22	1:C:342:SER:HA	1.85	0.42
1:B:376:ARG:NH1	1:B:424:GLU:OE2	2.51	0.42
1:A:209:GLU:HG2	1:A:210:THR:HG22	2.02	0.42
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.76	0.42
1:B:238:ASP:HB3	1:B:241:TYR:CE1	2.55	0.42
1:C:272:ASP:OD1	1:C:272:ASP:N	2.52	0.42
1:A:289:ARG:HD3	1:A:406:TRP:CZ2	2.55	0.42
1:A:403:GLY:HA2	1:A:432:LEU:HB2	2.01	0.42
1:C:70:PHE:CE2	1:C:282:THR:HA	2.54	0.42
1:A:241:TYR:HE1	1:A:244:GLN:HG3	1.85	0.42
1:B:233:HIS:HB3	1:B:291:ASP:OD1	2.20	0.42
1:B:404:ILE:HG23	1:B:432:LEU:HD13	2.02	0.42
1:B:420:ASP:HB2	1:B:421:HIS:ND1	2.35	0.42
1:C:191:LYS:HB3	1:C:196:ASP:HB2	2.00	0.42
1:C:270:ILE:HD11	1:C:438:ARG:NH1	2.35	0.42
1:A:120:ARG:NH1	1:A:164:ASP:OD2	2.53	0.41
1:A:272:ASP:OD1	1:A:272:ASP:N	2.51	0.41
1:A:80:ARG:CZ	1:A:80:ARG:HB2	2.50	0.41
1:C:393:SER:HB2	1:C:397:GLU:O	2.20	0.41
1:C:376:ARG:HH22	1:C:422:GLY:C	2.28	0.41
1:B:454:VAL:HG12	1:B:458:ARG:HE	1.86	0.41
1:B:355:LEU:O	1:B:366:PHE:HA	2.20	0.41
1:C:70:PHE:CD2	1:C:282:THR:HG22	2.55	0.41
1:C:292:GLY:HA3	1:C:435:LEU:HD11	2.01	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CZ	1:A:357:TYR:HB2	2.56	0.41
1:A:269:PHE:C	1:A:270:ILE:HD13	2.46	0.41
1:B:390:ILE:HA	1:B:401:PRO:HA	2.02	0.41
1:B:232:ASN:HD21	1:B:235:VAL:H	1.68	0.41
1:B:70:PHE:CE2	1:B:282:THR:HA	2.55	0.40
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.93	0.40
1:A:220:ARG:NH2	1:A:224:ASN:OD1	2.54	0.40
1:A:303:ILE:HG21	1:A:454:VAL:HG21	2.03	0.40
1:B:209:GLU:HG2	1:B:210:THR:N	2.37	0.40
1:C:85:LEU:HG	1:C:86:PRO:HD2	2.03	0.40
2:A:501:ATP:O1G	3:A:602:HOH:O	2.22	0.40
1:B:105:SER:O	1:B:109:ARG:HG3	2.20	0.40
1:C:91:ALA:O	1:C:130:PRO:HG2	2.21	0.40
1:C:89:GLN:O	1:C:161:VAL:HA	2.21	0.40
1:C:353:TYR:HA	1:C:368:ASP:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:OE2	1:C:243:ASN:ND2[3_455]	2.08	0.12

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	380/435 (87%)	364 (96%)	16 (4%)	0	100	100
1	B	378/435 (87%)	365 (97%)	12 (3%)	1 (0%)	36	58
1	C	374/435 (86%)	362 (97%)	12 (3%)	0	100	100
All	All	1132/1305 (87%)	1091 (96%)	40 (4%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	PRO

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	321/360 (89%)	305 (95%)	16 (5%)	22	46
1	B	321/360 (89%)	301 (94%)	20 (6%)	16	36
1	C	318/360 (88%)	300 (94%)	18 (6%)	18	40
All	All	960/1080 (89%)	906 (94%)	54 (6%)	19	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	SER
1	A	198	SER
1	A	210	THR
1	A	224	ASN
1	A	226	GLN
1	A	233	HIS
1	A	239	LEU
1	A	264	GLU
1	A	271	THR
1	A	313	VAL
1	A	319	VAL
1	A	336	VAL
1	A	338	LYS
1	A	363	ILE
1	A	393	SER
1	A	456	GLN
1	B	78	LEU
1	B	81	HIS
1	B	87	LYS
1	B	107	ILE

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Mol	Chain	Res	Type
1	B	120	ARG
1	B	123	LYS
1	B	161	VAL
1	B	182	GLU
1	B	183	GLN
1	B	210	THR
1	B	235	VAL
1	B	239	LEU
1	B	264	GLU
1	B	268	SER
1	B	273	ASP
1	B	338	LYS
1	B	385	SER
1	B	395	ASP
1	B	420	ASP
1	B	427	THR
1	C	60	HIS
1	C	84	ARG
1	C	85	LEU
1	C	87	LYS
1	C	106	LYS
1	C	224	ASN
1	C	226	GLN
1	C	232	ASN
1	C	235	VAL
1	C	264	GLU
1	C	273	ASP
1	C	291	ASP
1	C	336	VAL
1	C	361	LYS
1	C	363	ILE
1	C	385	SER
1	C	388	LEU
1	C	455	GLN

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	68	ASN
1	A	74	GLN
1	A	183	GLN
1	A	345	HIS

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Mol	Chain	Res	Type
1	A	358	ASN
1	A	455	GLN
1	B	90	GLN
1	B	243	ASN
1	B	345	HIS
1	C	60	HIS
1	C	74	GLN
1	C	89	GLN
1	C	104	HIS
1	C	208	HIS
1	C	232	ASN
1	C	345	HIS
1	C	375	ASN

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](#)

3 ligands 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	$\# Z > 2$
2	ATP	A	501	-	32,33,33	0.28	0	48,52,52	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	C	501	-	32,33,33	0.27	0	48,52,52	0.30	0
2	ATP	B	501	-	32,33,33	0.56	0	48,52,52	0.53	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
2	ATP	A	501	-	-	0/22/38/38	0/3/3/3
2	ATP	C	501	-	-	0/22/38/38	0/3/3/3
2	ATP	B	501	-	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

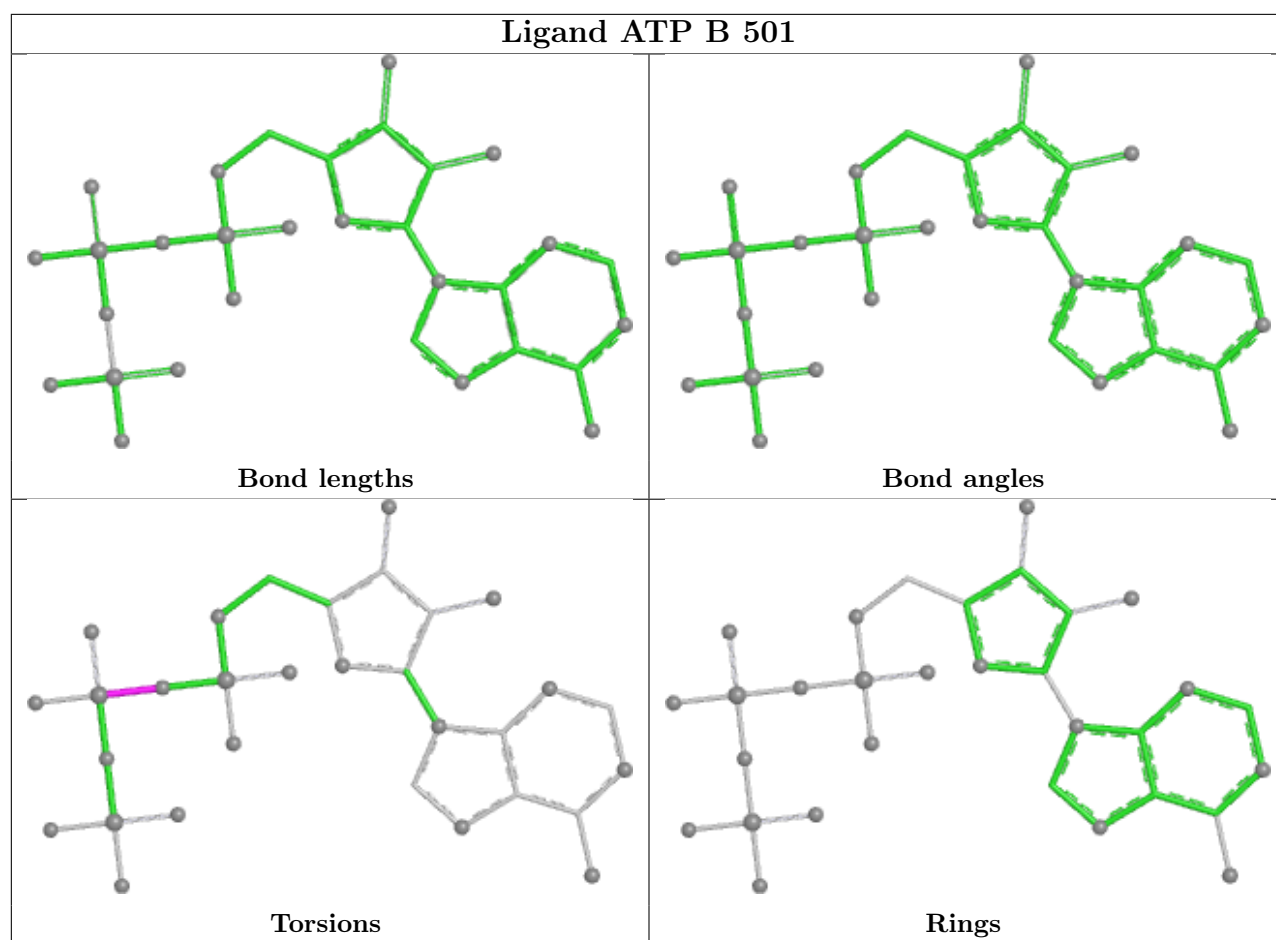
Mol	Chain	Res	Type	Atoms
2	B	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ATP	2	0
2	C	501	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	388/435 (89%)	0.26	21 (5%)	31 26	48, 70, 118, 147	0
1	B	386/435 (88%)	0.49	27 (6%)	22 18	52, 72, 137, 198	0
1	C	382/435 (87%)	0.59	33 (8%)	16 12	56, 80, 135, 185	0
All	All	1156/1305 (88%)	0.45	81 (7%)	22 18	48, 74, 130, 198	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	459	PHE	5.3
1	B	407	GLY	5.2
1	B	83	GLY	4.7
1	B	79	PRO	4.5
1	C	85	LEU	4.2
1	B	82	PRO	4.2
1	C	78	LEU	4.2
1	A	235	VAL	4.1
1	A	237	VAL	4.1
1	A	176	PRO	3.9
1	B	208	HIS	3.8
1	C	86	PRO	3.8
1	A	236	ALA	3.7
1	B	239	LEU	3.7
1	C	208	HIS	3.5
1	A	407	GLY	3.5
1	C	234	HIS	3.4
1	B	172	TYR	3.4
1	B	351	MET	3.3
1	A	173	TYR	3.3
1	C	83	GLY	3.3
1	A	175	ALA	3.3
1	A	241	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	85	LEU	3.1
1	C	172	TYR	3.0
1	C	239	LEU	3.0
1	A	172	TYR	3.0
1	B	241	TYR	3.0
1	B	234	HIS	2.9
1	B	107	ILE	2.9
1	C	412	ARG	2.9
1	B	173	TYR	2.9
1	C	63	ALA	2.9
1	C	65	GLY	2.8
1	B	235	VAL	2.8
1	A	79	PRO	2.7
1	A	60	HIS	2.7
1	A	465	PHE	2.7
1	C	235	VAL	2.7
1	B	394	GLN	2.7
1	B	392	THR	2.7
1	A	413	GLY	2.6
1	A	208	HIS	2.6
1	C	108	LEU	2.6
1	C	62	ALA	2.5
1	C	237	VAL	2.5
1	A	234	HIS	2.5
1	A	239	LEU	2.5
1	B	406	TRP	2.4
1	C	233	HIS	2.4
1	C	406	TRP	2.4
1	C	69	TYR	2.4
1	B	459	PHE	2.4
1	C	170	PHE	2.4
1	B	413	GLY	2.4
1	B	78	LEU	2.4
1	C	443	ILE	2.4
1	A	83	GLY	2.3
1	B	237	VAL	2.3
1	B	350	VAL	2.3
1	B	182	GLU	2.3
1	C	269	PHE	2.3
1	C	357	TYR	2.2
1	A	314	GLY	2.2
1	C	182	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	210	THR	2.2
1	A	243	ASN	2.2
1	C	224	ASN	2.1
1	C	292	GLY	2.1
1	C	103	PHE	2.1
1	C	207	SER	2.1
1	C	289	ARG	2.1
1	B	225	LYS	2.1
1	B	111	PHE	2.1
1	A	443	ILE	2.1
1	B	395	ASP	2.0
1	C	111	PHE	2.1
1	C	107	ILE	2.0
1	C	73	LEU	2.0
1	B	81	HIS	2.0
1	A	174	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](#)

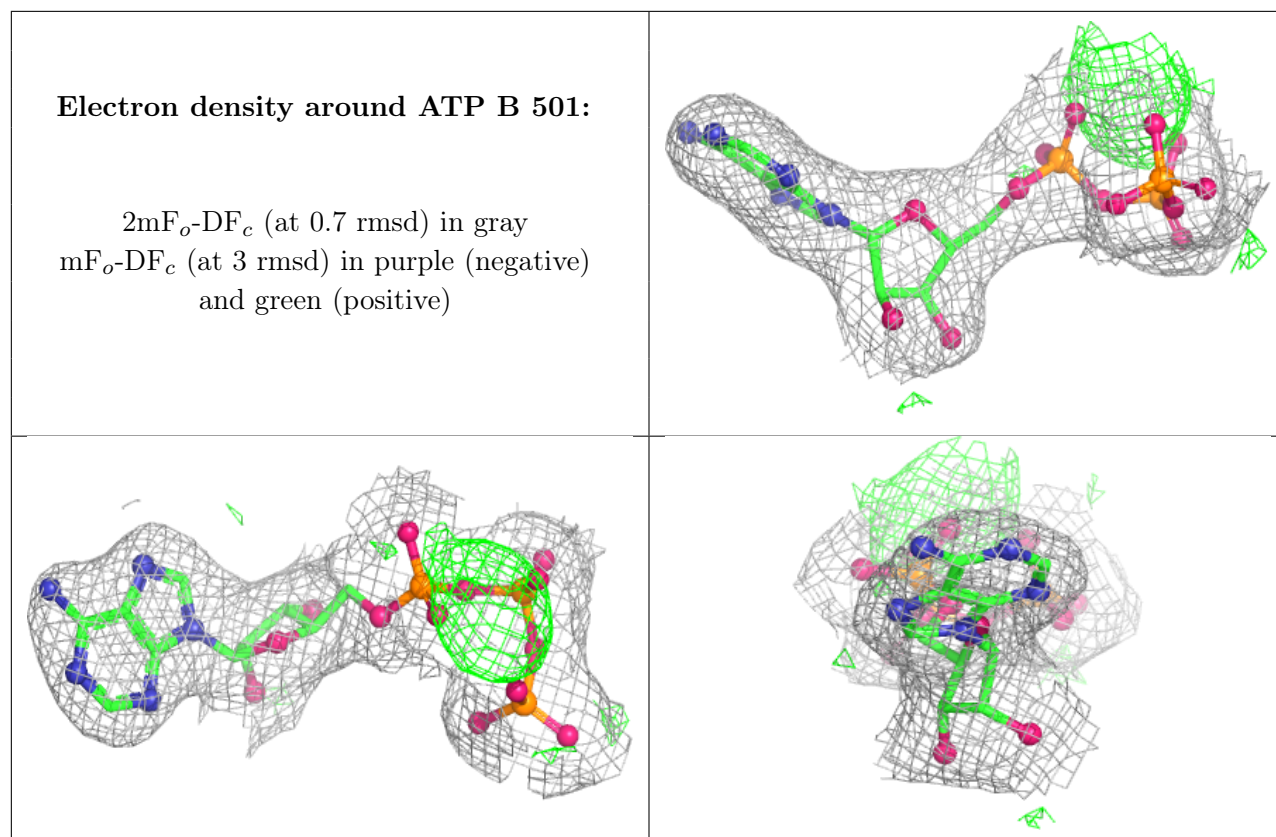
There are no oligosaccharides in this entry.

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	ATP	A	501	31/31	0.94	0.09	45,64,79,133	0
2	ATP	B	501	31/31	0.94	0.08	49,60,70,74	0
2	ATP	C	501	31/31	0.96	0.08	64,74,85,88	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.