



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:26 AM UTC

PDB ID : 2DPY / pdb\_00002dpy  
Title : Crystal structure of the flagellar type III ATPase FliI  
Authors : Imada, K.; Namba, K.; Minamino, T.  
Deposited on : 2006-05-18  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

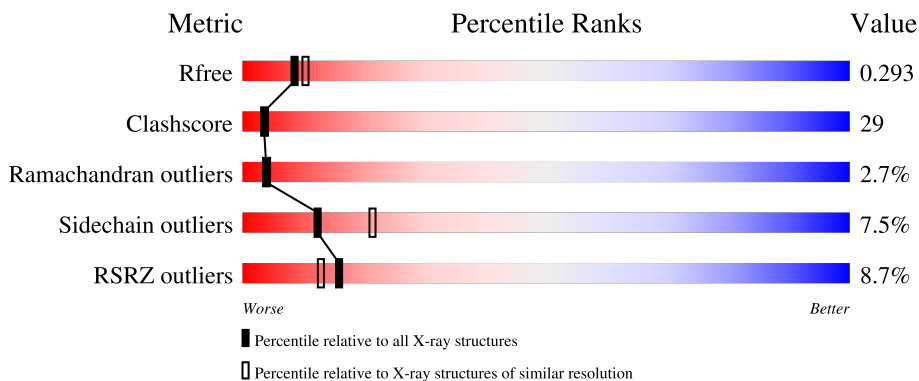
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\leq 5\%$ . 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	438	 9% 52% 37% 6% . .
1	B	438	 8% 54% 35% 8% . .

## 2 Entry composition [i](#)

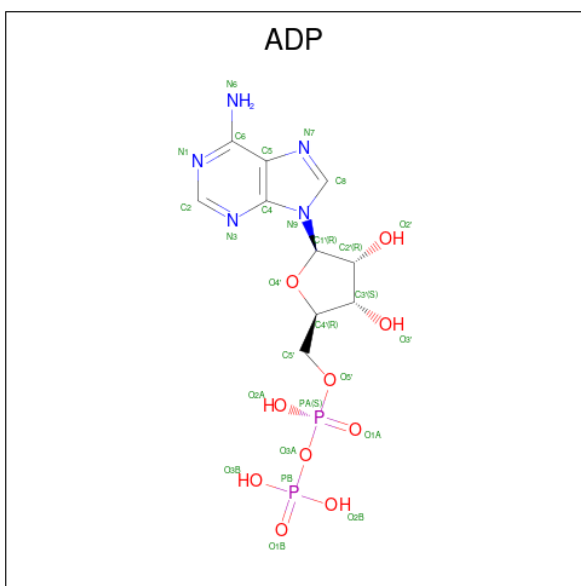
There are 3 unique types of molecules in this entry. The entry contains 6604 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Flagellum-specific ATP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	Total 3211	C 2032	N 575	O 594	S 10	0	0	0
1	B	426	Total 3233	C 2045	N 579	O 599	S 10	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total 71 O 71	0	0

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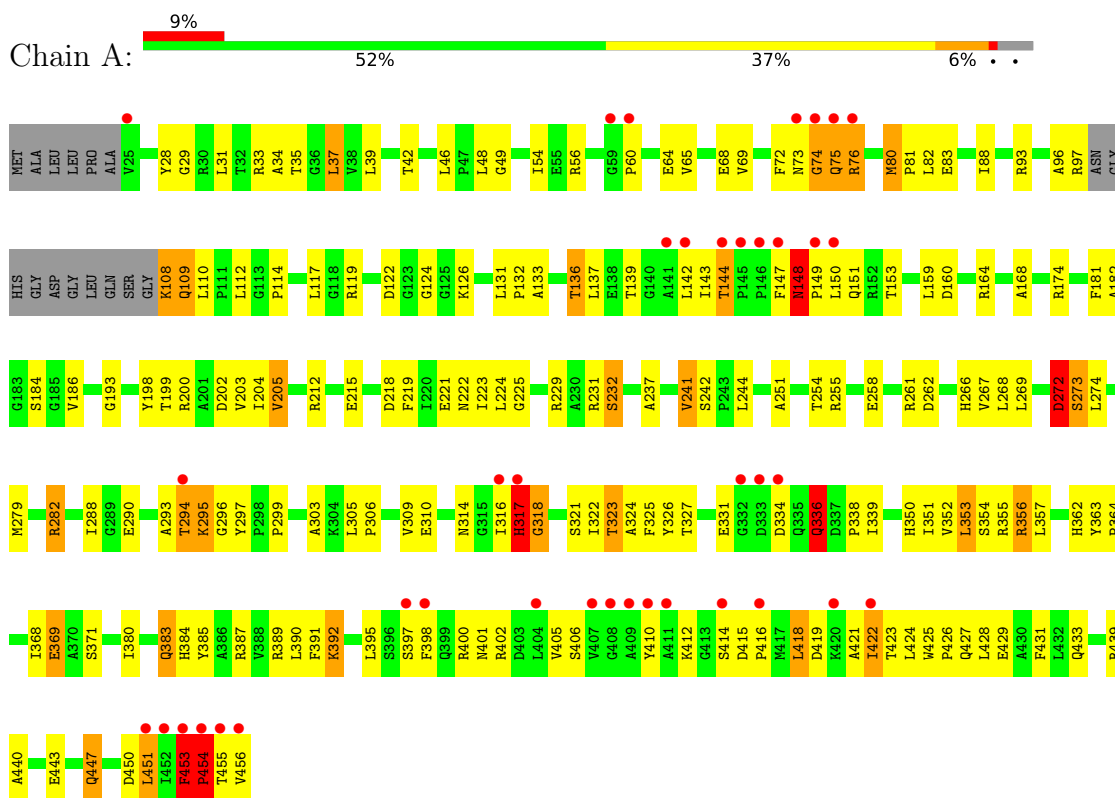
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	62	Total	O	0	0
			62	62		

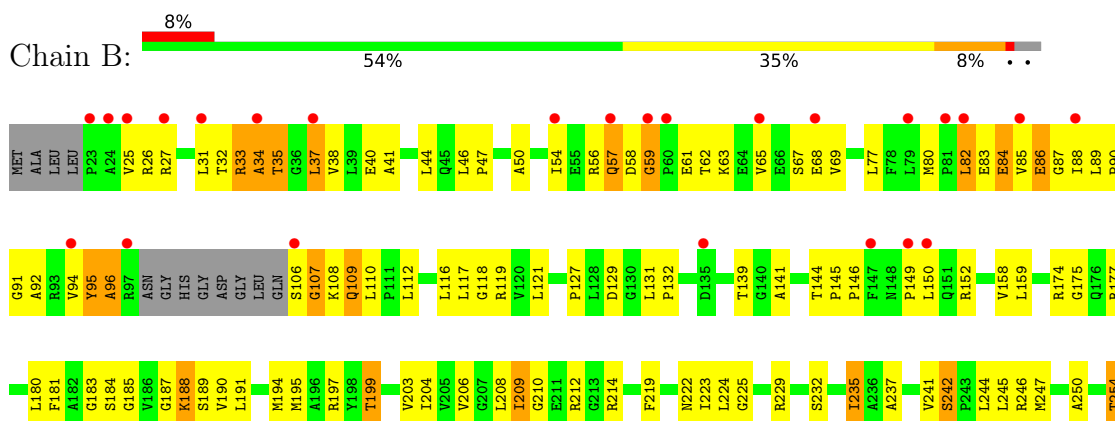
### 3 Residue-property plots i

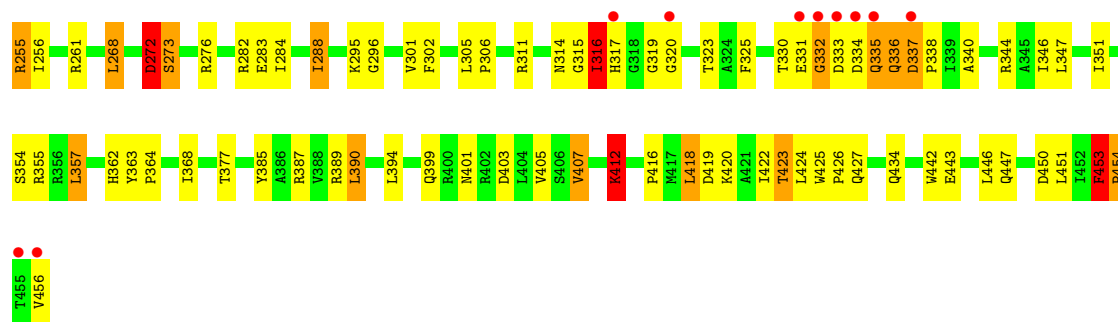
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Flagellum-specific ATP synthase



#### • Molecule 1: Flagellum-specific ATP synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.16Å 72.75Å 125.74Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	45.98 – 2.40 45.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.98-2.40) 99.5 (45.98-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.244 , 0.295 0.243 , 0.293	Depositor DCC
$R_{free}$ test set	1680 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtrriage
Anisotropy	0.407	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: ADP

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	0.51	2/3268 (0.1%)	1.06	23/4431 (0.5%)
1	B	0.51	1/3291 (0.0%)	1.05	23/4462 (0.5%)
All	All	0.51	3/6559 (0.0%)	1.06	46/8893 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	ASP	CA-C	5.27	1.60	1.53
1	B	106	SER	N-CA	-5.11	1.36	1.46
1	A	108	LYS	N-CA	-5.08	1.36	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	GLY	N-CA-C	-9.55	90.53	113.18
1	A	272	ASP	N-CA-C	8.87	121.05	108.54
1	B	337	ASP	CA-C-N	8.59	130.57	119.84
1	B	337	ASP	C-N-CA	8.59	130.57	119.84
1	A	273	SER	N-CA-CB	8.34	124.24	111.56
1	B	82	LEU	N-CA-C	-7.30	103.68	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	TYR	N-CA-C	7.05	117.55	108.24
1	A	303	ALA	N-CA-C	-7.03	104.85	113.50
1	A	380	ILE	N-CA-C	6.97	118.64	108.53
1	A	453	PHE	CA-C-N	-6.84	111.29	119.84
1	A	453	PHE	C-N-CA	-6.84	111.29	119.84
1	A	317	HIS	N-CA-C	6.82	120.37	110.28
1	B	453	PHE	CA-C-N	6.76	128.29	119.84
1	B	453	PHE	C-N-CA	6.76	128.29	119.84
1	B	273	SER	N-CA-CB	6.64	121.81	111.24
1	B	183	GLY	N-CA-C	-6.58	102.55	112.41
1	A	29	GLY	N-CA-C	-6.55	98.28	110.73
1	B	209	ILE	N-CA-C	6.29	118.46	108.89
1	A	237	ALA	CA-C-N	6.20	126.56	119.92
1	A	237	ALA	C-N-CA	6.20	126.56	119.92
1	B	237	ALA	CA-C-N	6.04	126.88	120.11
1	B	237	ALA	C-N-CA	6.04	126.88	120.11
1	B	175	GLY	N-CA-C	-5.99	106.82	114.37
1	A	82	LEU	N-CA-C	-5.95	105.67	113.17
1	A	431	PHE	N-CA-C	-5.92	104.41	111.69
1	A	232	SER	N-CA-C	5.83	117.83	109.14
1	B	59	GLY	N-CA-C	-5.57	100.97	112.34
1	A	168	ALA	N-CA-C	5.56	118.53	111.69
1	A	323	THR	N-CA-C	-5.55	100.65	109.59
1	A	336	GLN	N-CA-C	-5.50	107.11	113.88
1	B	37	LEU	N-CA-C	-5.46	105.41	111.36
1	B	368	ILE	N-CA-C	5.43	115.63	110.42
1	A	453	PHE	N-CA-C	5.34	121.62	109.81
1	A	148	ASN	N-CA-C	-5.33	103.06	109.83
1	B	206	VAL	N-CA-C	5.32	115.52	107.75
1	B	242	SER	CA-C-N	5.31	125.37	119.32
1	B	242	SER	C-N-CA	5.31	125.37	119.32
1	A	294	THR	CB-CA-C	-5.27	108.84	116.54
1	B	222	ASN	N-CA-C	5.22	119.92	113.50
1	B	272	ASP	N-CA-C	5.16	117.50	107.71
1	A	80	MET	CA-C-N	5.15	125.07	119.76
1	A	80	MET	C-N-CA	5.15	125.07	119.76
1	B	272	ASP	CB-CA-C	-5.11	104.24	111.76
1	B	316	ILE	N-CA-C	5.11	119.96	109.34
1	B	84	GLU	N-CA-C	5.07	117.70	109.24
1	A	221	GLU	N-CA-C	5.01	117.85	111.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ASP	Peptide,Mainchain
1	B	272	ASP	Peptide,Mainchain

## 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	3211	0	3277	193	0
1	B	3233	0	3298	193	0
2	B	27	0	12	6	0
3	A	71	0	0	3	0
3	B	62	0	0	17	0
All	All	6604	0	6587	385	0

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 29.

All (385) 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:412:LYS:H	1:B:412:LYS:HD3	1.30	0.97
1:B:450:ASP:HA	1:B:454:PRO:HG3	1.46	0.97
1:A:356:ARG:H	1:A:356:ARG:HD3	1.27	0.96
1:B:54:ILE:HG23	1:B:65:VAL:HB	1.50	0.92
1:A:148:ASN:ND2	1:A:151:GLN:HE21	1.67	0.91
1:A:261:ARG:HG2	1:A:261:ARG:HH11	1.35	0.90
1:B:38:VAL:HG21	1:B:288:ILE:HD11	1.57	0.87
1:A:148:ASN:HD21	1:A:151:GLN:HE21	1.22	0.86
1:B:109:GLN:HG3	1:B:139:THR:HG22	1.55	0.86
1:A:33:ARG:HH11	1:A:35:THR:HG21	1.45	0.82
1:A:142:LEU:HD21	1:A:251:ALA:HB1	1.59	0.82
1:B:450:ASP:HA	1:B:454:PRO:CG	2.10	0.81
1:A:425:TRP:CE3	1:A:428:LEU:HD11	2.16	0.81
1:B:158:VAL:HG12	3:B:656:HOH:O	1.80	0.79
1:B:209:ILE:HG22	1:B:276:ARG:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LYS:HD3	1:B:338:PRO:CD	2.13	0.79
1:B:419:ASP:O	1:B:423:THR:HG23	1.83	0.79
1:A:387:ARG:HD2	1:A:454:PRO:HG3	1.66	0.78
1:B:107:GLY:HA2	3:B:628:HOH:O	1.85	0.77
1:A:153:THR:HG21	1:A:317:HIS:HB2	1.66	0.77
1:B:242:SER:OG	1:B:245:LEU:HD23	1.84	0.77
1:A:279:MET:HG2	1:A:282:ARG:HH22	1.49	0.76
1:B:336:GLN:H	1:B:336:GLN:NE2	1.83	0.76
1:B:27:ARG:HG3	3:B:640:HOH:O	1.86	0.75
1:B:204:ILE:HG23	1:B:268:LEU:HD12	1.69	0.75
1:A:136:THR:O	1:A:137:LEU:HB2	1.84	0.75
1:B:247:MET:HE2	1:B:284:ILE:HD12	1.69	0.75
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.50	0.74
1:A:447:GLN:O	1:A:451:LEU:HG	1.86	0.74
1:A:453:PHE:HB3	1:A:454:PRO:HD3	1.68	0.74
1:A:33:ARG:HD3	1:A:35:THR:OG1	1.87	0.73
1:B:187:GLY:HA2	2:B:600:ADP:H5'1	1.71	0.73
1:B:412:LYS:H	1:B:412:LYS:CD	2.02	0.73
1:B:56:ARG:HD2	1:B:63:LYS:HD2	1.70	0.73
1:B:85:VAL:HG22	1:B:88:ILE:HD12	1.71	0.72
1:B:141:ALA:O	1:B:255:ARG:HD3	1.89	0.72
1:B:447:GLN:O	1:B:451:LEU:HG	1.90	0.72
1:B:412:LYS:HD3	1:B:412:LYS:N	2.04	0.71
1:B:453:PHE:HB2	1:B:454:PRO:CD	2.21	0.71
1:B:85:VAL:HG13	1:B:88:ILE:HD12	1.73	0.71
1:A:182:ALA:HB2	1:A:353:LEU:HB2	1.72	0.71
1:A:314:ASN:HD22	1:A:321:SER:HB2	1.56	0.70
1:A:148:ASN:C	1:A:150:LEU:H	2.00	0.70
1:A:305:LEU:HB2	1:A:306:PRO:HD3	1.74	0.69
1:A:136:THR:HG23	1:A:137:LEU:H	1.57	0.69
1:A:428:LEU:HD12	1:A:429:GLU:N	2.07	0.69
1:B:453:PHE:H	1:B:454:PRO:HD2	1.57	0.69
1:A:33:ARG:NH1	1:A:35:THR:HG21	2.07	0.69
1:A:415:ASP:OD2	1:A:418:LEU:HB2	1.92	0.69
1:A:109:GLN:HG3	1:A:139:THR:HB	1.75	0.69
1:B:174:ARG:HA	1:B:323:THR:OG1	1.93	0.68
1:B:194:MET:HE1	1:B:364:PRO:HG3	1.74	0.67
1:B:295:LYS:HD3	1:B:338:PRO:HD3	1.74	0.67
1:A:279:MET:HG2	1:A:282:ARG:NH2	2.10	0.67
1:A:424:LEU:HD23	1:A:427:GLN:NE2	2.08	0.67
1:B:302:PHE:HZ	1:B:338:PRO:HB3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:PRO:O	1:B:420:LYS:HG3	1.95	0.67
1:B:282:ARG:HH21	1:B:296:GLY:HA3	1.59	0.67
1:A:147:PHE:HE2	1:A:316:ILE:H	1.41	0.67
1:A:401:ASN:CG	1:A:418:LEU:HD11	2.21	0.66
1:A:96:ALA:O	1:A:97:ARG:HB2	1.96	0.66
1:B:302:PHE:CZ	1:B:338:PRO:HB3	2.30	0.66
1:A:383:GLN:HB3	3:A:509:HOH:O	1.95	0.66
1:B:212:ARG:HD3	1:B:214:ARG:NH1	2.10	0.66
1:B:44:LEU:HG	1:B:46:LEU:HD23	1.79	0.65
1:B:316:ILE:HG13	1:B:317:HIS:H	1.60	0.65
1:B:57:GLN:HA	1:B:57:GLN:HE21	1.60	0.65
1:B:225:GLY:O	1:B:229:ARG:HG3	1.96	0.65
1:B:363:TYR:HA	1:B:364:PRO:C	2.21	0.65
1:A:33:ARG:HH11	1:A:35:THR:CG2	2.09	0.65
1:A:200:ARG:HE	1:A:439:ARG:HH21	1.45	0.65
1:A:153:THR:CG2	1:A:317:HIS:HB2	2.27	0.65
1:B:58:ASP:HB2	1:B:63:LYS:HE2	1.78	0.65
1:B:187:GLY:HA2	2:B:600:ADP:H8	1.62	0.64
1:B:31:LEU:HD13	1:B:54:ILE:HD13	1.78	0.64
1:A:261:ARG:HG2	1:A:261:ARG:NH1	2.10	0.64
1:B:121:LEU:HD23	1:B:127:PRO:HA	1.80	0.64
1:A:317:HIS:HD2	1:A:318:GLY:H	1.47	0.63
1:A:453:PHE:CB	1:A:454:PRO:HD3	2.29	0.63
1:A:108:LYS:HE2	1:A:110:LEU:HD21	1.80	0.63
1:B:47:PRO:O	1:B:69:VAL:HG11	1.99	0.63
1:A:148:ASN:HD21	1:A:151:GLN:NE2	1.95	0.62
1:B:25:VAL:HG22	1:B:26:ARG:H	1.63	0.62
1:B:119:ARG:NH1	1:B:119:ARG:HB3	2.15	0.62
1:B:82:LEU:HA	1:B:245:LEU:HD21	1.80	0.62
1:A:425:TRP:HA	1:A:428:LEU:HG	1.81	0.62
1:A:439:ARG:HG3	1:A:439:ARG:HH11	1.64	0.62
1:B:208:LEU:C	1:B:209:ILE:HD12	2.25	0.62
1:B:56:ARG:HD2	1:B:63:LYS:CD	2.30	0.62
1:A:200:ARG:HE	1:A:439:ARG:NH2	1.96	0.61
1:A:114:PRO:O	1:A:117:LEU:HD23	2.01	0.61
1:A:73:ASN:O	1:A:75:GLN:N	2.34	0.61
1:A:288:ILE:HD12	1:A:290:GLU:H	1.65	0.61
1:A:159:LEU:HD22	1:A:323:THR:HG21	1.83	0.61
1:B:56:ARG:HD3	1:B:57:GLN:N	2.16	0.60
1:B:84:GLU:HG3	3:B:611:HOH:O	2.00	0.60
1:A:387:ARG:HD2	1:A:454:PRO:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:HB3	1:B:119:ARG:HH11	1.65	0.60
1:B:57:GLN:HA	1:B:61:GLU:O	2.02	0.60
1:B:184:SER:O	1:B:355:ARG:NH2	2.34	0.60
1:A:142:LEU:HD21	1:A:251:ALA:CB	2.30	0.60
1:B:50:ALA:H	1:B:69:VAL:CG1	2.14	0.60
1:B:250:ALA:O	1:B:254:THR:HG22	2.00	0.60
1:A:42:THR:OG1	1:A:76:ARG:NE	2.36	0.59
1:A:261:ARG:HH11	1:A:261:ARG:CG	2.13	0.59
1:A:148:ASN:O	1:A:150:LEU:N	2.34	0.59
1:A:200:ARG:NE	1:A:439:ARG:HH21	2.00	0.59
1:A:109:GLN:CA	1:A:109:GLN:HE21	2.16	0.58
1:B:235:ILE:HD12	1:B:235:ILE:N	2.18	0.58
1:B:390:LEU:HD13	1:B:453:PHE:CD2	2.38	0.58
1:B:456:VAL:OXT	1:B:456:VAL:HG12	2.04	0.58
1:A:383:GLN:HG2	1:A:387:ARG:NH1	2.19	0.58
1:A:31:LEU:HD11	1:A:39:LEU:HB3	1.84	0.58
1:A:109:GLN:HG3	1:A:139:THR:CB	2.34	0.58
1:A:261:ARG:NH1	1:A:262:ASP:OD1	2.35	0.57
1:A:405:VAL:HG22	1:A:410:TYR:HB2	1.85	0.57
1:B:57:GLN:NE2	1:B:61:GLU:O	2.36	0.57
1:B:424:LEU:O	1:B:427:GLN:HB2	2.05	0.57
1:A:174:ARG:HH11	1:A:317:HIS:HE1	1.51	0.57
1:B:241:VAL:HG12	1:B:245:LEU:HB2	1.87	0.56
1:A:356:ARG:HD3	1:A:356:ARG:N	2.10	0.56
1:A:164:ARG:HB2	1:A:440:ALA:CB	2.36	0.56
1:B:59:GLY:C	1:B:61:GLU:H	2.13	0.56
1:B:387:ARG:HD3	1:B:454:PRO:CG	2.35	0.56
1:A:336:GLN:NE2	1:A:336:GLN:N	2.54	0.56
1:A:385:TYR:O	1:A:389:ARG:HG3	2.05	0.56
1:B:336:GLN:H	1:B:336:GLN:HE21	1.54	0.56
1:A:122:ASP:OD2	1:A:126:LYS:HB2	2.06	0.55
1:A:37:LEU:HD13	1:A:80:MET:HE3	1.88	0.55
1:B:340:ALA:O	1:B:344:ARG:HG3	2.05	0.55
1:B:442:TRP:CE2	1:B:446:LEU:HD11	2.41	0.55
1:A:297:TYR:OH	1:A:339:ILE:HD11	2.07	0.55
1:A:450:ASP:CG	1:A:456:VAL:HG22	2.31	0.55
1:B:185:GLY:HA2	3:B:633:HOH:O	2.07	0.55
1:B:254:THR:HG23	1:B:311:ARG:NH2	2.21	0.55
1:A:363:TYR:HA	1:A:364:PRO:C	2.32	0.55
1:B:385:TYR:HE2	1:B:389:ARG:HH21	1.54	0.55
1:B:110:LEU:O	1:B:139:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:HD3	1:B:454:PRO:HD3	1.89	0.55
1:A:114:PRO:HA	1:A:117:LEU:HD23	1.89	0.55
1:A:164:ARG:NH2	1:A:433:GLN:O	2.40	0.55
1:B:191:LEU:HA	1:B:194:MET:HE3	1.88	0.55
1:A:64:GLU:OE1	1:A:97:ARG:NH2	2.40	0.55
1:A:306:PRO:O	1:A:310:GLU:HB2	2.05	0.55
1:B:25:VAL:HG22	1:B:26:ARG:N	2.22	0.55
1:A:119:ARG:NH2	1:A:132:PRO:O	2.40	0.54
1:B:96:ALA:N	3:B:640:HOH:O	2.40	0.54
1:B:110:LEU:C	1:B:139:THR:HG23	2.32	0.54
1:A:317:HIS:CD2	1:A:318:GLY:H	2.24	0.54
1:A:416:PRO:HA	1:A:419:ASP:OD2	2.07	0.54
1:B:189:SER:HB2	2:B:600:ADP:O2A	2.07	0.54
1:B:453:PHE:HB2	1:B:454:PRO:HD3	1.89	0.54
1:B:197:ARG:HD3	1:B:224:LEU:O	2.08	0.54
1:B:210:GLY:HA3	1:B:276:ARG:CG	2.37	0.54
1:B:194:MET:SD	3:B:625:HOH:O	2.58	0.54
1:A:383:GLN:OE1	1:A:384:HIS:HB2	2.07	0.54
1:A:412:LYS:NZ	1:A:419:ASP:HA	2.23	0.54
1:A:450:ASP:OD1	1:A:456:VAL:HG22	2.09	0.54
1:B:50:ALA:O	1:B:68:GLU:HA	2.08	0.54
1:A:398:PHE:O	1:A:402:ARG:HB2	2.07	0.53
1:B:333:ASP:HB2	3:B:648:HOH:O	2.07	0.53
1:A:401:ASN:ND2	1:A:418:LEU:HD11	2.23	0.53
1:A:142:LEU:HD11	1:A:251:ALA:HB3	1.91	0.53
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.24	0.53
1:B:131:LEU:N	1:B:131:LEU:HD12	2.22	0.53
1:B:301:VAL:O	1:B:305:LEU:HD13	2.08	0.53
1:A:297:TYR:CZ	1:A:339:ILE:HD11	2.44	0.53
1:B:235:ILE:HD11	1:B:256:ILE:HD12	1.90	0.53
1:B:442:TRP:NE1	1:B:446:LEU:HD11	2.23	0.53
1:B:41:ALA:HB1	1:B:94:VAL:HG21	1.91	0.53
1:B:152:ARG:HH12	1:B:177:ARG:HH12	1.55	0.53
1:B:159:LEU:C	1:B:159:LEU:HD23	2.33	0.53
1:B:330:THR:C	1:B:332:GLY:H	2.16	0.53
1:A:453:PHE:HB3	1:A:454:PRO:CD	2.39	0.52
1:A:74:GLY:HA2	3:A:521:HOH:O	2.08	0.52
1:A:117:LEU:HD11	1:A:203:VAL:HG13	1.90	0.52
1:A:336:GLN:H	1:A:336:GLN:HE21	1.57	0.52
1:B:69:VAL:HG21	1:B:77:LEU:HD11	1.91	0.52
1:B:453:PHE:N	1:B:454:PRO:HD2	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:THR:O	1:A:456:VAL:C	2.53	0.52
1:A:109:GLN:HE21	1:A:109:GLN:HA	1.75	0.52
1:A:295:LYS:HB2	1:A:338:PRO:HG3	1.91	0.52
1:B:129:ASP:HB2	3:B:612:HOH:O	2.09	0.52
1:A:164:ARG:HB2	1:A:440:ALA:HB1	1.91	0.52
1:B:195:MET:O	1:B:199:THR:HB	2.10	0.52
1:A:148:ASN:C	1:A:150:LEU:N	2.66	0.52
1:B:387:ARG:HD3	1:B:454:PRO:HG3	1.91	0.52
1:A:54:ILE:HG21	1:A:88:ILE:HD13	1.92	0.51
1:A:65:VAL:HG13	1:A:83:GLU:HB2	1.92	0.51
1:A:205:VAL:CG2	1:A:269:LEU:CD1	2.88	0.51
1:B:109:GLN:N	1:B:109:GLN:HE21	2.08	0.51
1:A:205:VAL:HG23	1:A:269:LEU:HD12	1.92	0.51
1:A:387:ARG:HG2	1:A:454:PRO:HD3	1.92	0.51
1:B:241:VAL:HG12	1:B:242:SER:N	2.25	0.51
1:B:443:GLU:HG2	1:B:447:GLN:HE21	1.76	0.51
1:B:335:GLN:NE2	1:B:335:GLN:N	2.58	0.51
1:B:377:THR:HG23	3:B:631:HOH:O	2.11	0.51
1:B:401:ASN:O	1:B:405:VAL:HG23	2.10	0.51
1:B:112:LEU:HA	1:B:116:LEU:CD2	2.41	0.51
1:B:407:VAL:HG13	1:B:407:VAL:O	2.10	0.51
1:B:85:VAL:HG22	1:B:88:ILE:CD1	2.40	0.51
1:A:391:PHE:CZ	1:A:428:LEU:HB2	2.45	0.51
1:B:190:VAL:HG12	1:B:194:MET:HE2	1.92	0.50
1:B:204:ILE:O	1:B:232:SER:HA	2.11	0.50
1:B:335:GLN:O	1:B:337:ASP:N	2.44	0.50
1:A:109:GLN:O	1:A:110:LEU:HD23	2.11	0.50
1:B:152:ARG:HH12	1:B:177:ARG:NH1	2.08	0.50
1:A:225:GLY:O	1:A:229:ARG:HG3	2.11	0.50
1:A:331:GLU:HG3	1:A:331:GLU:O	2.11	0.50
1:B:191:LEU:HG	1:B:195:MET:HE2	1.94	0.50
1:B:336:GLN:NE2	1:B:336:GLN:N	2.58	0.50
1:A:294:THR:C	1:A:296:GLY:H	2.20	0.50
1:B:56:ARG:HD3	1:B:57:GLN:C	2.36	0.50
1:A:142:LEU:HD23	1:A:142:LEU:O	2.11	0.50
1:B:108:LYS:O	1:B:141:ALA:HA	2.11	0.50
1:A:46:LEU:HB2	1:A:69:VAL:HG21	1.92	0.50
1:A:357:LEU:HD13	1:A:362:HIS:CD2	2.47	0.50
1:A:160:ASP:O	1:A:199:THR:HA	2.12	0.49
1:A:397:SER:O	1:A:401:ASN:HB3	2.12	0.49
1:B:144:THR:HB	1:B:145:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.77	0.49
1:B:54:ILE:HA	1:B:94:VAL:HG12	1.94	0.49
1:B:131:LEU:HB3	1:B:132:PRO:HD2	1.94	0.49
1:A:218:ASP:OD1	1:A:222:ASN:ND2	2.36	0.49
1:B:112:LEU:HA	1:B:116:LEU:HD22	1.94	0.49
1:A:354:SER:OG	1:A:356:ARG:NE	2.45	0.49
1:B:62:THR:HG21	3:B:613:HOH:O	2.12	0.49
1:A:28:TYR:HD2	1:A:93:ARG:HB3	1.78	0.49
1:A:193:GLY:HA3	1:A:223:ILE:HG22	1.95	0.49
1:A:455:THR:O	1:A:455:THR:HG23	2.12	0.49
1:B:295:LYS:HD3	1:B:338:PRO:HD2	1.91	0.49
1:A:352:VAL:H	1:A:371:SER:HB3	1.78	0.48
1:B:118:GLY:HA2	1:B:229:ARG:O	2.12	0.48
1:B:241:VAL:CG1	1:B:245:LEU:HB2	2.42	0.48
1:A:288:ILE:HD12	1:A:288:ILE:C	2.38	0.48
1:B:67:SER:HB2	1:B:80:MET:O	2.14	0.48
1:B:325:PHE:HE2	1:B:351:ILE:HD12	1.79	0.48
1:A:148:ASN:ND2	1:A:151:GLN:HG3	2.28	0.48
1:A:451:LEU:N	1:A:451:LEU:HD23	2.27	0.48
1:B:34:ALA:O	1:B:35:THR:C	2.55	0.48
1:B:203:VAL:HG12	1:B:204:ILE:N	2.28	0.48
1:B:261:ARG:HG3	1:B:320:GLY:C	2.39	0.48
1:B:158:VAL:HG21	1:B:442:TRP:CZ3	2.48	0.48
1:A:204:ILE:HB	1:A:232:SER:HB3	1.96	0.48
1:A:368:ILE:HD12	1:A:368:ILE:N	2.29	0.48
1:B:109:GLN:HG3	1:B:139:THR:CG2	2.37	0.48
1:B:394:LEU:HD11	1:B:453:PHE:HE2	1.79	0.48
1:B:419:ASP:O	1:B:423:THR:CG2	2.57	0.47
1:A:136:THR:OG1	1:A:137:LEU:N	2.47	0.47
1:A:153:THR:HG22	1:A:314:ASN:HB3	1.97	0.47
1:A:204:ILE:HD11	1:A:231:ARG:NH1	2.29	0.47
1:A:119:ARG:NH2	1:A:131:LEU:HB2	2.30	0.47
1:A:148:ASN:ND2	1:A:151:GLN:NE2	2.50	0.47
1:B:357:LEU:HG	1:B:362:HIS:CD2	2.50	0.47
1:A:205:VAL:CG2	1:A:269:LEU:HD12	2.44	0.47
1:B:109:GLN:HE21	1:B:109:GLN:CA	2.26	0.47
1:A:425:TRP:N	1:A:426:PRO:HD2	2.30	0.47
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.79	0.47
1:B:330:THR:C	1:B:332:GLY:N	2.72	0.47
1:B:188:LYS:HE2	1:B:272:ASP:OD2	2.15	0.47
1:A:336:GLN:N	1:A:336:GLN:HE21	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ILE:HG23	1:B:268:LEU:CD1	2.44	0.46
1:B:424:LEU:O	1:B:427:GLN:N	2.48	0.46
1:A:75:GLN:O	1:A:76:ARG:HB2	2.14	0.46
1:A:204:ILE:O	1:A:232:SER:HB2	2.15	0.46
1:A:241:VAL:HG13	1:A:242:SER:N	2.30	0.46
1:A:269:LEU:HB3	1:A:324:ALA:HB2	1.95	0.46
1:A:274:LEU:HD22	1:A:305:LEU:CD2	2.45	0.46
1:B:387:ARG:HD3	1:B:454:PRO:CD	2.45	0.46
1:A:33:ARG:HG2	1:A:34:ALA:N	2.30	0.46
1:A:122:ASP:OD1	1:A:124:GLY:N	2.45	0.46
1:B:219:PHE:O	1:B:223:ILE:HB	2.15	0.46
1:A:142:LEU:HD23	1:A:142:LEU:C	2.39	0.46
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.26	0.46
1:B:434:GLN:NE2	3:B:625:HOH:O	2.49	0.46
1:A:68:GLU:OE1	1:A:244:LEU:HD22	2.15	0.46
1:A:305:LEU:CB	1:A:306:PRO:HD3	2.45	0.46
1:A:391:PHE:O	1:A:395:LEU:HB2	2.16	0.46
1:A:282:ARG:HH11	1:A:282:ARG:CG	2.24	0.46
1:B:109:GLN:CG	1:B:139:THR:HG22	2.38	0.46
1:B:332:GLY:O	1:B:333:ASP:HB2	2.15	0.46
1:A:241:VAL:CG1	1:A:242:SER:N	2.78	0.46
1:A:422:ILE:HG13	1:A:423:THR:N	2.26	0.46
1:B:149:PRO:HG2	3:B:662:HOH:O	2.14	0.46
1:B:204:ILE:HD13	1:B:268:LEU:HB3	1.97	0.46
1:B:245:LEU:HD13	3:B:659:HOH:O	2.16	0.46
1:A:200:ARG:NE	1:A:439:ARG:NH2	2.60	0.45
1:A:212:ARG:HB2	1:A:215:GLU:HG3	1.98	0.45
1:B:261:ARG:HD2	1:B:315:GLY:CA	2.45	0.45
1:B:305:LEU:N	1:B:305:LEU:HD12	2.32	0.45
1:B:272:ASP:HA	1:B:273:SER:HA	1.69	0.45
1:B:89:LEU:HB3	1:B:90:PRO:HD2	1.99	0.45
1:B:80:MET:SD	1:B:244:LEU:HG	2.56	0.45
1:B:159:LEU:HD13	1:B:323:THR:HG21	1.98	0.45
1:B:288:ILE:HG23	1:B:288:ILE:O	2.16	0.45
1:A:117:LEU:N	1:A:117:LEU:HD22	2.31	0.45
1:A:336:GLN:NE2	1:A:336:GLN:H	2.13	0.45
1:B:95:TYR:O	1:B:96:ALA:O	2.35	0.45
1:B:131:LEU:N	1:B:131:LEU:CD1	2.79	0.45
1:B:32:THR:HG21	1:B:40:GLU:OE2	2.17	0.45
1:B:54:ILE:CG2	1:B:65:VAL:HB	2.35	0.44
1:B:86:GLU:CD	1:B:86:GLU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HD2	1:B:315:GLY:HA3	1.99	0.44
1:A:149:PRO:O	1:A:150:LEU:HD23	2.15	0.44
1:A:414:SER:O	1:A:415:ASP:C	2.60	0.44
1:B:317:HIS:C	3:B:605:HOH:O	2.60	0.44
1:A:96:ALA:O	1:A:97:ARG:CB	2.65	0.44
1:A:293:ALA:HB2	1:A:299:PRO:HG3	1.98	0.44
1:A:219:PHE:HA	1:A:223:ILE:CG1	2.47	0.44
1:B:85:VAL:CG2	1:B:88:ILE:HD12	2.46	0.44
1:B:418:LEU:O	1:B:422:ILE:HG12	2.17	0.44
1:A:453:PHE:CB	1:A:454:PRO:CD	2.92	0.44
1:B:210:GLY:HA3	1:B:276:ARG:HG2	1.99	0.44
1:B:246:ARG:HD2	3:B:634:HOH:O	2.17	0.44
1:B:145:PRO:HA	1:B:146:PRO:HD2	1.92	0.44
1:B:209:ILE:HD12	1:B:209:ILE:N	2.32	0.44
1:A:425:TRP:O	1:A:428:LEU:HG	2.18	0.44
1:B:188:LYS:HD2	2:B:600:ADP:O2B	2.17	0.44
1:B:214:ARG:NH1	1:B:214:ARG:HG3	2.33	0.43
1:A:182:ALA:HB1	1:A:186:VAL:CG2	2.48	0.43
1:B:305:LEU:N	1:B:306:PRO:HD2	2.33	0.43
1:B:330:THR:O	1:B:332:GLY:N	2.50	0.43
1:A:56:ARG:O	1:A:56:ARG:HG3	2.18	0.43
1:A:184:SER:O	1:A:355:ARG:NH2	2.51	0.43
1:A:267:VAL:HG12	1:A:268:LEU:N	2.33	0.43
1:A:258:GLU:HA	1:A:322:ILE:HD11	1.98	0.43
1:A:398:PHE:CD1	1:A:422:ILE:HG22	2.54	0.43
1:B:58:ASP:O	1:B:61:GLU:HB3	2.18	0.43
1:A:119:ARG:CZ	1:A:131:LEU:HB2	2.49	0.43
1:A:294:THR:O	1:A:296:GLY:N	2.46	0.43
1:A:384:HIS:C	1:A:384:HIS:CD2	2.97	0.43
1:B:37:LEU:HD11	1:B:283:GLU:HG2	2.01	0.43
1:B:314:ASN:HD22	1:B:314:ASN:HA	1.68	0.43
1:A:148:ASN:HD22	1:A:151:GLN:HG3	1.84	0.43
1:A:261:ARG:HD3	1:A:322:ILE:HG13	2.01	0.43
1:A:418:LEU:O	1:A:421:ALA:HB3	2.19	0.43
1:A:142:LEU:CD2	1:A:251:ALA:HB1	2.40	0.42
1:A:273:SER:HA	1:A:327:THR:OG1	2.19	0.42
1:B:241:VAL:CG1	1:B:242:SER:N	2.81	0.42
1:B:181:PHE:CD2	1:B:181:PHE:N	2.87	0.42
1:B:32:THR:HG23	1:B:33:ARG:N	2.34	0.42
1:A:254:THR:O	1:A:258:GLU:HG3	2.19	0.42
1:B:187:GLY:CA	2:B:600:ADP:H8	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:NH1	1:B:129:ASP:OD1	2.53	0.42
1:A:205:VAL:HG23	1:A:269:LEU:CD1	2.50	0.42
1:A:325:PHE:HE2	1:A:351:ILE:HD12	1.85	0.42
1:A:181:PHE:N	1:A:181:PHE:CD2	2.87	0.42
1:A:205:VAL:CG2	1:A:269:LEU:HD13	2.50	0.42
1:B:319:GLY:N	3:B:605:HOH:O	2.53	0.42
1:B:86:GLU:CD	1:B:86:GLU:H	2.27	0.42
1:B:91:GLY:O	1:B:92:ALA:C	2.62	0.42
1:B:85:VAL:CG1	1:B:88:ILE:HD12	2.47	0.42
1:A:369:GLU:HG3	1:A:392:LYS:NZ	2.34	0.41
1:A:401:ASN:OD1	1:A:418:LEU:HD11	2.20	0.41
1:B:117:LEU:O	1:B:119:ARG:HG2	2.20	0.41
1:A:202:ASP:OD1	1:A:266:HIS:HB2	2.20	0.41
1:B:425:TRP:N	1:B:426:PRO:HD2	2.35	0.41
1:A:144:THR:HG21	1:A:255:ARG:HE	1.85	0.41
1:A:153:THR:CB	1:A:317:HIS:HB2	2.50	0.41
1:A:72:PHE:O	1:A:73:ASN:C	2.63	0.41
1:A:132:PRO:O	1:A:133:ALA:C	2.62	0.41
1:A:272:ASP:HA	1:A:273:SER:HA	1.66	0.41
1:B:109:GLN:CA	1:B:109:GLN:NE2	2.84	0.41
1:A:350:HIS:O	1:A:371:SER:HB2	2.21	0.41
1:A:75:GLN:O	1:A:76:ARG:HD3	2.21	0.41
1:A:198:TYR:HB3	1:A:439:ARG:NH1	2.35	0.41
1:B:57:GLN:O	1:B:59:GLY:N	2.54	0.41
1:A:406:SER:HB2	3:A:510:HOH:O	2.19	0.41
1:A:182:ALA:HB1	1:A:186:VAL:HG21	2.03	0.41
1:A:200:ARG:HH21	1:A:439:ARG:HH21	1.69	0.41
1:A:412:LYS:HZ2	1:A:419:ASP:HA	1.86	0.41
1:A:425:TRP:CZ3	1:A:428:LEU:HD11	2.54	0.41
1:A:428:LEU:HD12	1:A:428:LEU:C	2.46	0.41
1:B:332:GLY:C	1:B:334:ASP:H	2.28	0.41
1:B:335:GLN:NE2	1:B:335:GLN:H	2.18	0.41
1:A:200:ARG:NH2	1:A:439:ARG:HH21	2.18	0.41
1:B:219:PHE:CD1	1:B:219:PHE:C	2.98	0.41
1:A:424:LEU:HD23	1:A:427:GLN:HE22	1.85	0.40
1:B:390:LEU:O	1:B:394:LEU:HG	2.20	0.40
1:A:80:MET:HA	1:A:81:PRO:HD3	1.83	0.40
1:B:188:LYS:HB3	2:B:600:ADP:O1B	2.21	0.40
1:A:137:LEU:CD2	1:B:26:ARG:HB3	2.52	0.40
1:A:274:LEU:HG	1:A:326:TYR:HB3	2.03	0.40
1:B:86:GLU:OE1	1:B:87:GLY:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:CG2	1:B:210:GLY:N	2.85	0.40

There are no symmetry-related clashes.

## 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	418/438 (95%)	379 (91%)	28 (7%)	11 (3%)	4	4
1	B	422/438 (96%)	368 (87%)	42 (10%)	12 (3%)	4	3
All	All	840/876 (96%)	747 (89%)	70 (8%)	23 (3%)	4	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	GLY
1	A	136	THR
1	A	144	THR
1	A	454	PRO
1	B	34	ALA
1	B	35	THR
1	B	96	ALA
1	B	316	ILE
1	B	336	GLN
1	B	412	LYS
1	B	453	PHE
1	A	453	PHE
1	B	454	PRO
1	B	331	GLU
1	B	332	GLY
1	A	76	ARG
1	A	295	LYS

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Mol	Chain	Res	Type
1	A	60	PRO
1	A	75	GLN
1	B	83	GLU
1	B	107	GLY
1	A	49	GLY
1	A	143	ILE

### 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	332/342 (97%)	307 (92%)	25 (8%)	12	21
1	B	334/342 (98%)	309 (92%)	25 (8%)	12	21
All	All	666/684 (97%)	616 (92%)	50 (8%)	12	21

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	48	LEU
1	A	109	GLN
1	A	112	LEU
1	A	148	ASN
1	A	205	VAL
1	A	224	LEU
1	A	241	VAL
1	A	282	ARG
1	A	309	VAL
1	A	317	HIS
1	A	334	ASP
1	A	336	GLN
1	A	353	LEU
1	A	356	ARG
1	A	369	GLU
1	A	383	GLN

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Mol	Chain	Res	Type
1	A	390	LEU
1	A	392	LYS
1	A	418	LEU
1	A	422	ILE
1	A	443	GLU
1	A	447	GLN
1	A	451	LEU
1	A	454	PRO
1	B	33	ARG
1	B	57	GLN
1	B	86	GLU
1	B	109	GLN
1	B	150	LEU
1	B	180	LEU
1	B	188	LYS
1	B	199	THR
1	B	235	ILE
1	B	254	THR
1	B	255	ARG
1	B	268	LEU
1	B	288	ILE
1	B	335	GLN
1	B	346	ILE
1	B	347	LEU
1	B	354	SER
1	B	357	LEU
1	B	390	LEU
1	B	399	GLN
1	B	403	ASP
1	B	407	VAL
1	B	412	LYS
1	B	418	LEU
1	B	423	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	73	ASN
1	A	109	GLN
1	A	148	ASN
1	A	281	GLN

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Mol	Chain	Res	Type
1	A	314	ASN
1	A	317	HIS
1	A	335	GLN
1	A	336	GLN
1	A	427	GLN
1	A	433	GLN
1	B	57	GLN
1	B	109	GLN
1	B	248	GLN
1	B	266	HIS
1	B	314	ASN
1	B	317	HIS
1	B	335	GLN
1	B	336	GLN
1	B	350	HIS
1	B	393	GLN
1	B	399	GLN
1	B	427	GLN
1	B	433	GLN
1	B	447	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](#)

1 ligand is 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	ADP	B	600	-	28,29,29	2.20	10 (35%)	43,45,45	2.04	12 (27%)

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	ADP	B	600	-	-	4/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ADP	C1'-N9	5.07	1.60	1.46
2	B	600	ADP	C5-N7	-4.55	1.30	1.39
2	B	600	ADP	PA-O2A	-4.16	1.36	1.55
2	B	600	ADP	PB-O2B	3.29	1.67	1.54
2	B	600	ADP	PA-O3A	3.27	1.63	1.59
2	B	600	ADP	C8-N9	-2.80	1.32	1.37
2	B	600	ADP	C2-N1	2.65	1.38	1.33
2	B	600	ADP	O4'-C1'	2.51	1.47	1.42
2	B	600	ADP	C2-N3	2.39	1.38	1.33
2	B	600	ADP	C4-N3	2.12	1.38	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ADP	C5-C4-N3	-5.59	119.02	126.72
2	B	600	ADP	N3-C2-N1	-5.47	120.31	128.58
2	B	600	ADP	C2-N3-C4	3.89	121.33	111.83
2	B	600	ADP	N3-C4-N9	3.82	133.67	127.17
2	B	600	ADP	O2A-PA-O3A	3.54	116.85	107.27
2	B	600	ADP	C5-N7-C8	3.48	108.93	103.45
2	B	600	ADP	N9-C8-N7	-3.23	109.36	113.94
2	B	600	ADP	C4-C5-N7	-3.19	106.93	110.58
2	B	600	ADP	O4'-C1'-N9	2.88	113.61	108.09
2	B	600	ADP	O3B-PB-O3A	2.32	112.40	104.64
2	B	600	ADP	O2A-PA-O5'	2.22	117.61	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ADP	O3A-PA-O1A	-2.13	104.29	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

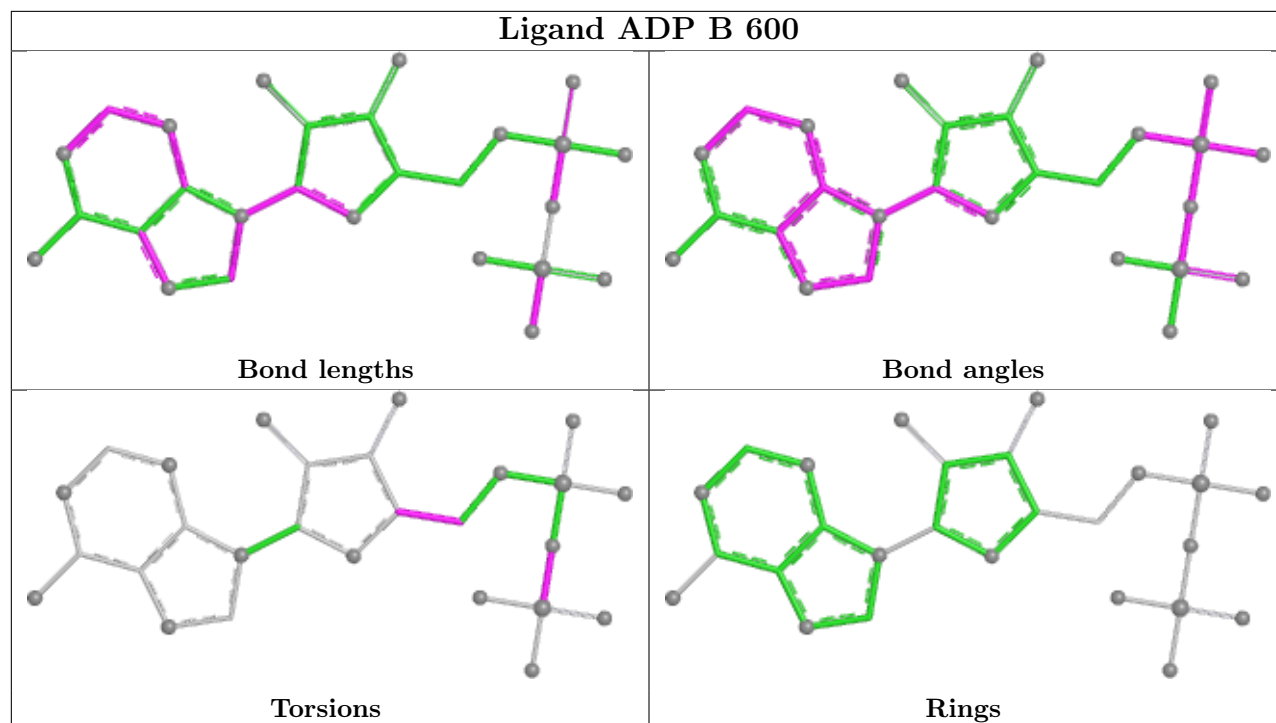
Mol	Chain	Res	Type	Atoms
2	B	600	ADP	PA-O3A-PB-O2B
2	B	600	ADP	O4'-C4'-C5'-O5'
2	B	600	ADP	PA-O3A-PB-O3B
2	B	600	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	ADP	6	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	422/438 (96%)	0.55	39 (9%) 14 12	22, 47, 96, 111	0
1	B	426/438 (97%)	0.59	35 (8%) 17 14	23, 48, 93, 113	0
All	All	848/876 (96%)	0.57	74 (8%) 16 13	22, 48, 94, 113	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	6.0
1	B	85	VAL	4.6
1	B	60	PRO	4.4
1	A	409	ALA	4.3
1	B	333	ASP	4.2
1	B	334	ASP	4.2
1	B	25	VAL	4.2
1	A	404	LEU	4.1
1	B	149	PRO	4.1
1	B	54	ILE	4.1
1	B	24	ALA	4.1
1	A	147	PHE	3.9
1	B	65	VAL	3.9
1	A	74	GLY	3.8
1	A	455	THR	3.7
1	A	73	ASN	3.7
1	B	456	VAL	3.6
1	A	145	PRO	3.5
1	B	320	GLY	3.5
1	B	59	GLY	3.4
1	A	25	VAL	3.3
1	A	456	VAL	3.3
1	A	146	PRO	3.1
1	A	454	PRO	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	106	SER	3.1
1	B	135	ASP	3.0
1	B	34	ALA	3.0
1	B	332	GLY	3.0
1	A	397	SER	3.0
1	A	416	PRO	2.9
1	A	316	ILE	2.9
1	A	332	GLY	2.9
1	B	23	PRO	2.9
1	A	333	ASP	2.8
1	A	414	SER	2.8
1	A	398	PHE	2.8
1	B	147	PHE	2.8
1	A	452	ILE	2.8
1	A	411	ALA	2.8
1	B	31	LEU	2.8
1	B	68	GLU	2.8
1	B	150	LEU	2.7
1	A	317	HIS	2.7
1	A	451	LEU	2.7
1	A	76	ARG	2.7
1	B	88	ILE	2.7
1	A	149	PRO	2.7
1	B	455	THR	2.6
1	A	408	GLY	2.5
1	B	331	GLU	2.5
1	A	453	PHE	2.5
1	A	141	ALA	2.5
1	A	75	GLN	2.4
1	A	422	ILE	2.4
1	B	317	HIS	2.4
1	A	410	TYR	2.4
1	A	150	LEU	2.3
1	B	82	LEU	2.3
1	A	334	ASP	2.2
1	B	37	LEU	2.2
1	B	337	ASP	2.2
1	A	144	THR	2.2
1	A	142	LEU	2.2
1	A	59	GLY	2.2
1	B	27	ARG	2.2
1	B	94	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	79	LEU	2.1
1	B	97	ARG	2.1
1	A	60	PRO	2.1
1	B	81	PRO	2.1
1	B	57	GLN	2.0
1	B	335	GLN	2.0
1	A	420	LYS	2.0
1	A	294	THR	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](#)

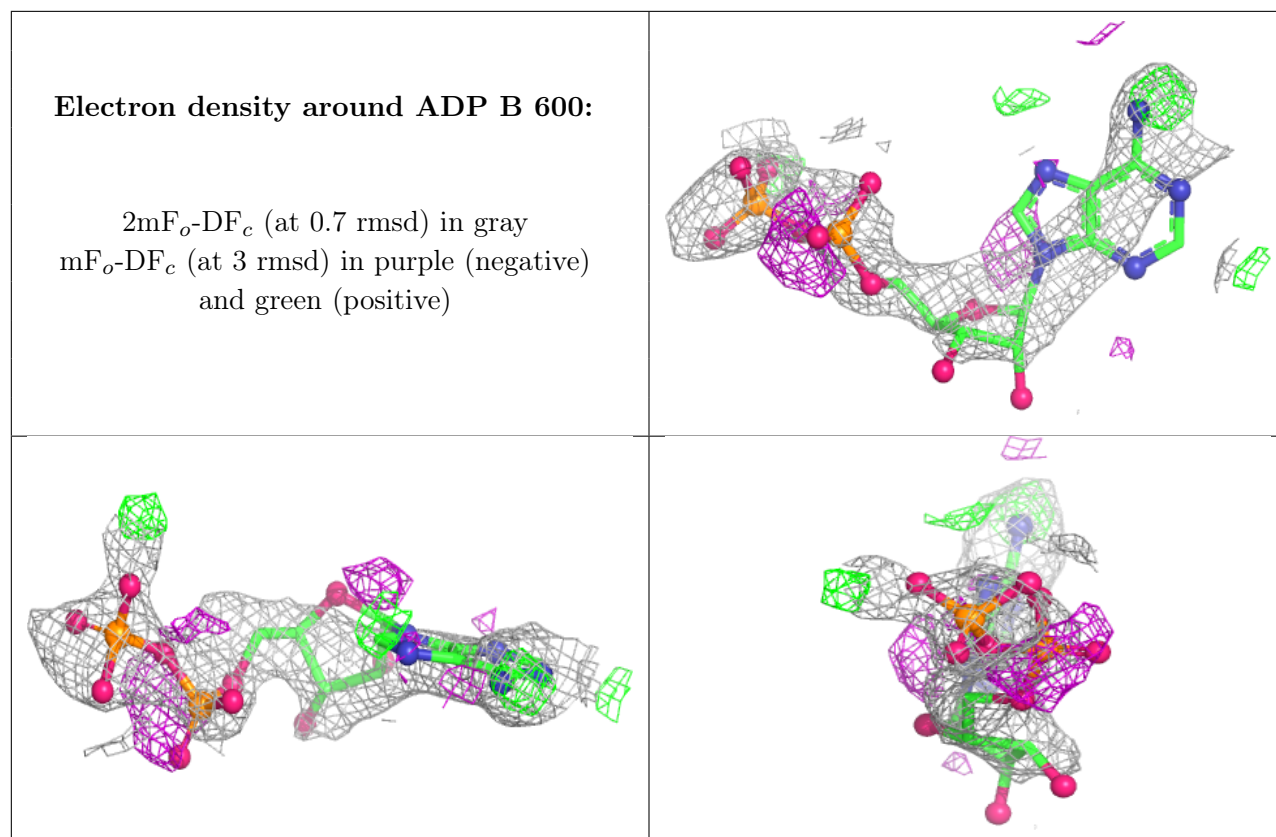
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	B	600	27/27	0.55	0.22	127,130,133,133	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.