



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:06 PM UTC

PDB ID : 4Q47 / pdb_00004q47
Title : Structure of the DrRecQ Catalytic Core in complex with ADP
Authors : Chen, S.C.; Yang, C.S.; Chen, Y.
Deposited on : 2014-04-14
Resolution : 2.90 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

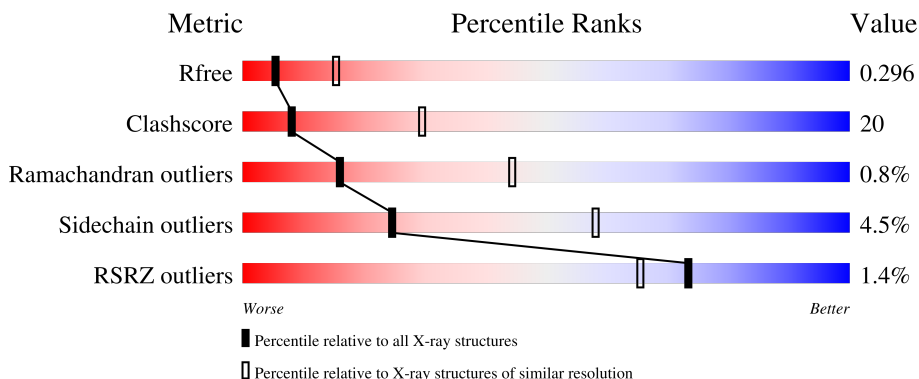
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	525	
1	B	525	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7999 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 DNA helicase RecQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			4012	2522	728	746	16			
1	B	502	Total	C	N	O	S	0	0	0
			3931	2469	713	733	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	518	LEU	-	expression tag	UNP Q9RUU2
A	519	GLU	-	expression tag	UNP Q9RUU2
A	520	HIS	-	expression tag	UNP Q9RUU2
A	521	HIS	-	expression tag	UNP Q9RUU2
A	522	HIS	-	expression tag	UNP Q9RUU2
A	523	HIS	-	expression tag	UNP Q9RUU2
A	524	HIS	-	expression tag	UNP Q9RUU2
A	525	HIS	-	expression tag	UNP Q9RUU2
B	518	LEU	-	expression tag	UNP Q9RUU2
B	519	GLU	-	expression tag	UNP Q9RUU2
B	520	HIS	-	expression tag	UNP Q9RUU2
B	521	HIS	-	expression tag	UNP Q9RUU2
B	522	HIS	-	expression tag	UNP Q9RUU2
B	523	HIS	-	expression tag	UNP Q9RUU2
B	524	HIS	-	expression tag	UNP Q9RUU2
B	525	HIS	-	expression tag	UNP Q9RUU2

- 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	
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

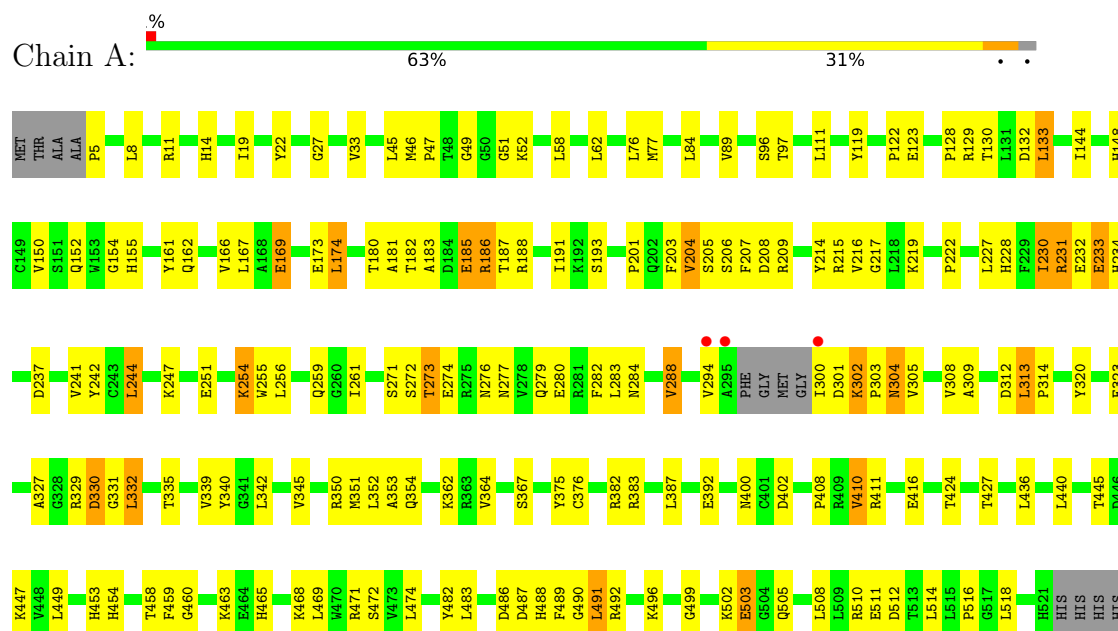
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

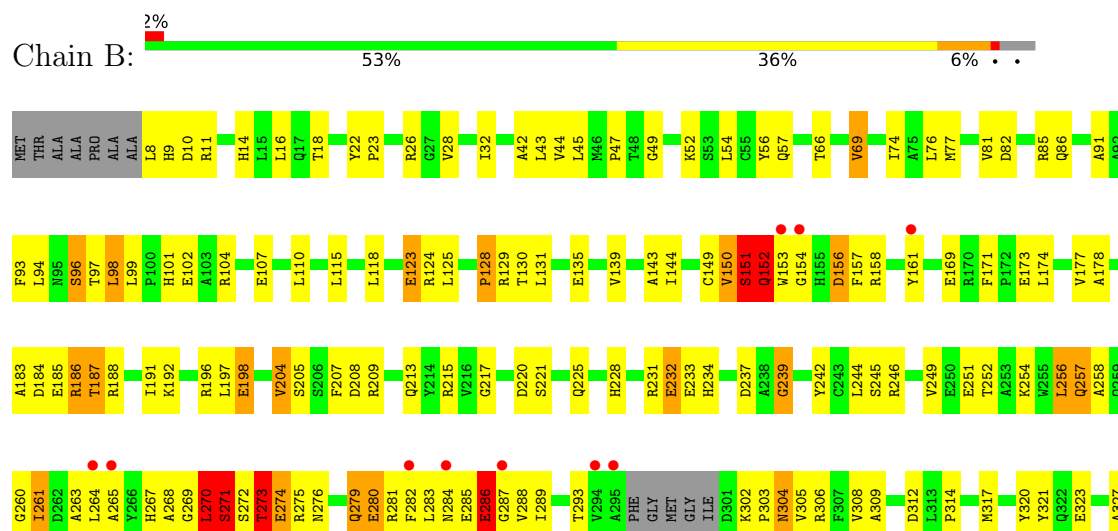
3 Residue-property plots

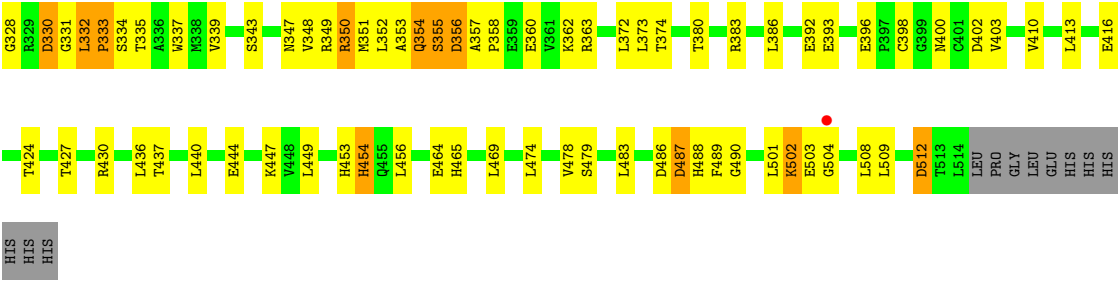
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: DNA helicase RecQ





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.76Å 95.61Å 183.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.56 – 2.90 27.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.56-2.90) 96.5 (27.56-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.222 , 0.295 0.227 , 0.296	Depositor DCC
R_{free} test set	2000 reflections (5.90%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7999	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

5.1 Standard geometry

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

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	0.71	1/4090 (0.0%)	1.13	17/5546 (0.3%)
1	B	0.75	4/4005 (0.1%)	1.33	54/5429 (1.0%)
All	All	0.73	5/8095 (0.1%)	1.23	71/10975 (0.6%)

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	4
1	B	0	11
All	All	0	15

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	GLN	CG-CD	-6.93	1.34	1.52
1	A	458	THR	CA-CB	6.45	1.60	1.52
1	B	186	ARG	CA-C	6.44	1.61	1.52
1	B	152	GLN	CA-C	5.76	1.60	1.52
1	B	151	SER	CA-C	5.55	1.59	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLN	N-CA-CB	-11.49	91.08	110.49
1	B	272	SER	CA-C-N	-10.91	108.15	123.20
1	B	272	SER	C-N-CA	-10.91	108.15	123.20
1	B	152	GLN	N-CA-C	10.86	133.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	THR	N-CA-C	-10.44	99.22	112.90
1	B	258	ALA	N-CA-C	-10.37	100.74	113.50
1	B	354	GLN	N-CA-C	9.45	130.93	110.80
1	B	265	ALA	N-CA-C	9.36	123.18	110.55
1	B	355	SER	N-CA-C	8.84	120.69	111.14
1	A	130	THR	N-CA-C	-8.76	100.92	111.69
1	B	232	GLU	N-CA-C	8.15	119.95	111.14
1	B	332	LEU	CA-C-N	8.03	129.87	119.84
1	B	332	LEU	C-N-CA	8.03	129.87	119.84
1	A	304	ASN	N-CA-C	7.36	121.11	112.72
1	B	98	LEU	N-CA-C	-7.32	96.70	108.55
1	B	272	SER	N-CA-C	7.24	121.71	113.02
1	B	270	LEU	N-CA-CB	-7.04	98.60	110.49
1	B	251	GLU	N-CA-C	-6.97	103.62	111.07
1	B	354	GLN	CA-C-N	6.90	129.82	120.44
1	B	354	GLN	C-N-CA	6.90	129.82	120.44
1	A	313	LEU	CA-C-N	6.78	127.71	120.11
1	A	313	LEU	C-N-CA	6.78	127.71	120.11
1	B	128	PRO	CA-C-O	-6.59	113.92	121.56
1	B	351	MET	N-CA-C	-6.53	104.79	112.89
1	A	490	GLY	N-CA-C	-6.50	101.17	111.18
1	A	162	GLN	N-CA-C	-6.39	104.41	111.82
1	B	274	GLU	N-CA-C	-6.30	104.65	112.90
1	B	280	GLU	CA-CB-CG	-6.25	101.61	114.10
1	A	410	VAL	N-CA-C	6.01	118.03	108.89
1	A	331	GLY	N-CA-C	-6.00	107.74	114.40
1	B	331	GLY	N-CA-C	5.93	120.99	114.40
1	A	233	GLU	N-CA-C	5.93	120.79	113.50
1	B	239	GLY	N-CA-C	5.86	119.65	110.91
1	B	456	LEU	N-CA-C	-5.79	103.48	110.13
1	A	185	GLU	CA-C-N	-5.75	113.39	122.76
1	A	185	GLU	C-N-CA	-5.75	113.39	122.76
1	A	332	LEU	CA-C-N	5.66	125.67	119.90
1	A	332	LEU	C-N-CA	5.66	125.67	119.90
1	B	333	PRO	N-CA-C	5.64	124.09	112.47
1	B	187	THR	CB-CA-C	-5.63	101.28	110.85
1	B	197	LEU	N-CA-C	5.62	120.25	113.17
1	B	273	THR	CA-C-N	5.61	131.84	121.52
1	B	273	THR	C-N-CA	5.61	131.84	121.52
1	B	154	GLY	N-CA-C	5.59	126.42	113.18
1	B	270	LEU	N-CA-C	5.57	122.67	110.80
1	B	281	ARG	N-CA-C	-5.57	105.74	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	ASN	CA-C-N	5.54	131.68	121.70
1	B	284	ASN	C-N-CA	5.54	131.68	121.70
1	B	354	GLN	CB-CA-C	-5.52	99.44	110.42
1	B	271	SER	CA-C-N	-5.46	113.17	122.56
1	B	271	SER	C-N-CA	-5.46	113.17	122.56
1	B	268	ALA	N-CA-C	5.36	119.44	113.01
1	B	330	ASP	N-CA-C	-5.35	101.93	109.96
1	B	490	GLY	N-CA-C	-5.31	102.42	112.51
1	B	151	SER	N-CA-CB	-5.27	101.97	110.71
1	B	270	LEU	CA-C-N	5.24	131.54	121.54
1	B	270	LEU	C-N-CA	5.24	131.54	121.54
1	A	174	LEU	N-CA-C	5.22	116.64	110.07
1	B	151	SER	N-CA-C	5.18	117.81	108.48
1	B	304	ASN	CA-C-N	-5.18	115.79	122.99
1	B	304	ASN	C-N-CA	-5.18	115.79	122.99
1	B	261	ILE	CA-C-N	-5.17	115.54	122.42
1	B	261	ILE	C-N-CA	-5.17	115.54	122.42
1	B	396	GLU	CA-C-N	5.14	125.14	119.89
1	B	396	GLU	C-N-CA	5.14	125.14	119.89
1	B	198	GLU	N-CA-C	5.12	119.15	113.01
1	B	128	PRO	N-CA-C	-5.10	103.10	111.21
1	B	488	HIS	N-CA-C	-5.09	105.98	113.72
1	A	503	GLU	CB-CA-C	-5.06	109.21	115.89
1	B	183	ALA	N-CA-C	5.04	116.99	108.02
1	A	491	LEU	N-CA-C	5.02	117.08	108.90

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Peptide
1	A	230	ILE	Peptide
1	A	272	SER	Peptide
1	A	329	ARG	Peptide
1	B	150	VAL	Peptide
1	B	151	SER	Peptide
1	B	257	GLN	Peptide
1	B	270	LEU	Peptide
1	B	271	SER	Peptide
1	B	273	THR	Peptide
1	B	286	GLU	Peptide
1	B	302	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	454	HIS	Peptide
1	B	486	ASP	Peptide
1	B	487	ASP	Peptide

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	4012	0	4014	127	0
1	B	3931	0	3933	186	0
2	A	27	0	12	6	0
2	B	27	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7999	0	7971	312	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 20.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:OH	2:A:601:ADP:H2'	1.20	1.29
1:A:22:TYR:OH	2:A:601:ADP:C2'	2.03	1.04
1:A:22:TYR:CZ	2:A:601:ADP:H2'	2.01	0.94
1:B:184:ASP:HB3	1:B:187:THR:HG23	1.52	0.91
1:A:499:GLY:HA2	1:A:502:LYS:HE2	1.58	0.85
1:B:308:VAL:HG23	1:B:327:ALA:HB2	1.58	0.84
1:A:314:PRO:HG2	1:A:320:TYR:HB2	1.59	0.84
1:A:271:SER:HG	1:A:273:THR:HG1	1.26	0.83
1:B:305:VAL:HB	1:B:327:ALA:HA	1.61	0.82
1:B:270:LEU:HD11	1:B:275:ARG:HG2	1.61	0.82
1:A:383:ARG:HH21	1:A:400:ASN:HB3	1.44	0.82
1:A:486:ASP:OD1	1:A:487:ASP:N	2.11	0.81
1:B:276:ASN:HA	1:B:279:GLN:HG3	1.62	0.79
1:B:152:GLN:CD	1:B:153:TRP:H	1.92	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLN:NE2	1:B:187:THR:HG22	1.97	0.78
1:B:213:GLN:HB3	1:B:335:THR:HG22	1.67	0.76
1:B:256:LEU:HG	1:B:261:ILE:HD11	1.66	0.76
1:B:169:GLU:HG3	1:B:196:ARG:HH12	1.50	0.76
1:A:410:VAL:HG21	1:A:508:LEU:HD13	1.65	0.76
1:B:271:SER:OG	1:B:274:GLU:OE1	2.05	0.75
1:B:502:LYS:HG2	1:B:504:GLY:H	1.49	0.75
1:B:152:GLN:NE2	1:B:153:TRP:O	2.20	0.74
1:A:353:ALA:O	1:A:362:LYS:NZ	2.20	0.74
1:B:152:GLN:OE1	1:B:153:TRP:CE3	2.42	0.72
1:B:152:GLN:CD	1:B:153:TRP:N	2.48	0.72
1:A:247:LYS:NZ	1:A:251:GLU:OE2	2.18	0.72
1:B:512:ASP:N	1:B:512:ASP:OD1	2.23	0.71
1:A:241:VAL:HG22	1:A:309:ALA:HB3	1.73	0.70
1:B:279:GLN:O	1:B:282:PHE:HB3	1.92	0.69
1:A:510:ARG:NH1	1:A:512:ASP:OD2	2.25	0.69
1:A:129:ARG:O	1:A:133:LEU:HB2	1.92	0.69
1:A:375:TYR:O	1:A:382:ARG:NH1	2.26	0.68
1:B:413:LEU:HD13	1:B:509:LEU:HD22	1.75	0.68
1:B:257:GLN:NE2	1:B:261:ILE:O	2.27	0.67
1:B:123:GLU:HG2	1:B:124:ARG:N	2.09	0.67
1:B:45:LEU:HD11	1:B:188:ARG:HD3	1.77	0.66
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.61	0.65
1:B:184:ASP:HB3	1:B:187:THR:CG2	2.25	0.65
1:B:192:LYS:HD2	1:B:198:GLU:HG2	1.77	0.65
1:B:306:ARG:NH2	1:B:330:ASP:OD1	2.31	0.64
1:B:244:LEU:HD13	1:B:312:ASP:HB3	1.78	0.64
1:A:350:ARG:O	1:A:354:GLN:HG3	1.97	0.64
1:B:220:ASP:OD1	1:B:221:SER:N	2.29	0.63
1:A:209:ARG:NH2	1:A:327:ALA:O	2.32	0.63
1:A:427:THR:OG1	1:A:453:HIS:NE2	2.32	0.63
1:B:271:SER:OG	1:B:271:SER:O	2.11	0.62
1:B:208:ASP:OD1	1:B:209:ARG:N	2.32	0.62
1:B:283:LEU:HA	1:B:285:GLU:OE2	1.99	0.62
1:A:350:ARG:HH21	1:A:351:MET:HE3	1.63	0.62
1:A:152:GLN:CD	1:A:152:GLN:H	2.07	0.62
1:A:185:GLU:HA	1:A:188:ARG:NH2	2.15	0.62
1:A:487:ASP:OD1	1:A:488:HIS:HA	2.00	0.62
1:B:152:GLN:OE1	1:B:153:TRP:CD2	2.53	0.62
1:B:82:ASP:O	1:B:86:GLN:HG3	2.00	0.61
1:A:302:LYS:HE3	1:A:304:ASN:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:OD1	1:A:209:ARG:N	2.33	0.61
1:B:263:ALA:HB1	1:B:289:ILE:O	2.01	0.61
1:B:8:LEU:O	1:B:11:ARG:N	2.31	0.61
1:B:267:HIS:O	1:B:270:LEU:HD22	2.01	0.60
1:B:208:ASP:N	1:B:392:GLU:OE2	2.35	0.60
1:B:85:ARG:NE	1:B:91:ALA:O	2.34	0.60
1:B:332:LEU:HB3	1:B:333:PRO:HD2	1.84	0.60
1:A:387:LEU:HB3	1:A:392:GLU:HB3	1.84	0.59
1:A:228:HIS:HA	1:A:231:ARG:HD3	1.84	0.59
1:B:246:ARG:HG3	1:B:267:HIS:CD2	2.36	0.59
1:A:46:MET:O	1:A:181:ALA:HA	2.03	0.59
1:A:47:PRO:HD2	1:A:206:SER:HB2	1.85	0.59
2:B:601:ADP:H3'	2:B:601:ADP:O1A	2.02	0.59
1:A:308:VAL:HG23	1:A:327:ALA:HB2	1.84	0.59
1:B:125:LEU:HA	1:B:130:THR:HG21	1.85	0.59
1:B:317:MET:HG3	1:B:372:LEU:HD13	1.84	0.58
1:B:124:ARG:HG3	1:B:124:ARG:NH1	2.17	0.58
1:A:201:PRO:HB2	1:A:203:PHE:HE1	1.69	0.58
1:B:273:THR:HG23	1:B:276:ASN:HB2	1.85	0.58
1:A:11:ARG:NH2	1:A:62:LEU:O	2.37	0.57
1:B:54:LEU:HA	1:B:57:GLN:HB2	1.85	0.57
1:A:234:HIS:HB3	1:A:237:ASP:HB2	1.86	0.57
1:A:302:LYS:HG2	1:A:305:VAL:HG23	1.85	0.57
1:B:192:LYS:HB3	1:B:198:GLU:HG3	1.87	0.57
1:A:128:PRO:O	1:A:129:ARG:HB3	2.05	0.57
1:B:104:ARG:HA	1:B:107:GLU:HB2	1.87	0.56
1:B:152:GLN:CD	1:B:187:THR:HG22	2.29	0.56
1:B:26:ARG:NH1	1:B:49:GLY:O	2.38	0.56
1:A:155:HIS:HD2	1:A:155:HIS:O	1.87	0.56
1:A:313:LEU:HD21	1:A:345:VAL:HG22	1.86	0.56
1:B:355:SER:N	1:B:356:ASP:HA	2.19	0.56
1:B:410:VAL:HG21	1:B:508:LEU:HD13	1.87	0.56
1:B:288:VAL:O	1:B:289:ILE:HD13	2.06	0.56
1:B:317:MET:HE3	1:B:386:LEU:HD12	1.89	0.55
1:A:155:HIS:ND1	1:A:182:THR:OG1	2.29	0.55
1:A:242:TYR:CE2	1:A:323:GLU:HB3	2.42	0.55
1:A:486:ASP:HB3	1:A:492:ARG:CZ	2.37	0.55
1:B:96:SER:HB3	1:B:124:ARG:HH12	1.71	0.55
1:A:52:LYS:HZ2	1:A:180:THR:C	2.16	0.54
1:A:183:ALA:HB1	1:A:188:ARG:HG3	1.89	0.54
1:A:364:VAL:O	1:A:367:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PRO:HB2	1:A:203:PHE:CE1	2.43	0.54
1:B:449:LEU:HD23	1:B:454:HIS:CG	2.43	0.54
1:B:304:ASN:HB2	1:B:330:ASP:OD2	2.07	0.54
1:A:111:LEU:HD21	1:A:133:LEU:HD23	1.88	0.53
1:B:221:SER:O	1:B:225:GLN:HG3	2.08	0.53
1:B:157:PHE:CG	1:B:158:ARG:N	2.76	0.53
1:A:330:ASP:C	1:A:332:LEU:H	2.16	0.53
1:B:14:HIS:O	1:B:18:THR:OG1	2.17	0.53
1:A:340:TYR:HE2	1:A:342:LEU:HD23	1.74	0.53
1:B:465:HIS:CG	1:B:469:LEU:HD23	2.43	0.53
1:A:148:HIS:ND1	1:A:180:THR:OG1	2.36	0.53
1:B:184:ASP:OD1	1:B:185:GLU:N	2.42	0.53
1:B:314:PRO:HG3	1:B:320:TYR:HB2	1.90	0.53
1:B:427:THR:HG23	1:B:453:HIS:NE2	2.24	0.52
1:B:263:ALA:CB	1:B:289:ILE:HB	2.39	0.52
1:B:234:HIS:HB3	1:B:237:ASP:HB2	1.91	0.52
1:A:22:TYR:OH	2:A:601:ADP:C3'	2.57	0.52
1:B:149:CYS:C	1:B:151:SER:H	2.16	0.52
1:B:153:TRP:CZ3	1:B:186:ARG:HG3	2.44	0.52
1:B:171:PHE:HD2	1:B:174:LEU:HD12	1.75	0.52
1:B:192:LYS:HB3	1:B:198:GLU:CG	2.40	0.51
1:B:273:THR:HG23	1:B:276:ASN:HD22	1.75	0.51
1:A:122:PRO:HG3	1:A:161:TYR:HE1	1.76	0.51
1:B:156:ASP:OD1	1:B:157:PHE:N	2.43	0.51
1:B:156:ASP:O	1:B:157:PHE:HB3	2.10	0.51
1:A:383:ARG:NH2	1:A:400:ASN:HB3	2.21	0.51
1:A:256:LEU:HD22	1:A:261:ILE:HG12	1.93	0.51
1:B:74:ILE:HG23	1:B:77:MET:HE2	1.92	0.51
1:B:151:SER:CA	1:B:152:GLN:HB3	2.39	0.51
1:B:424:THR:HG21	1:B:483:LEU:HD21	1.92	0.51
1:A:5:PRO:HD2	1:A:8:LEU:HB2	1.92	0.51
1:A:217:GLY:O	1:A:339:VAL:HA	2.11	0.50
1:B:239:GLY:HA2	1:B:305:VAL:HG13	1.94	0.50
1:A:45:LEU:O	1:A:204:VAL:HA	2.12	0.50
1:A:411:ARG:NH2	1:A:511:GLU:OE2	2.39	0.50
1:A:445:THR:HG22	1:A:447:LYS:H	1.77	0.50
1:B:169:GLU:HG3	1:B:196:ARG:NH1	2.24	0.50
1:B:215:ARG:HG2	1:B:402:ASP:HB3	1.93	0.50
1:B:96:SER:CB	1:B:124:ARG:HH12	2.25	0.49
1:B:151:SER:OG	1:B:152:GLN:HB3	2.11	0.49
1:B:353:ALA:C	1:B:354:GLN:HG3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:O	1:A:231:ARG:HB2	2.11	0.49
1:A:204:VAL:HG21	1:A:392:GLU:HA	1.95	0.49
1:B:153:TRP:CH2	1:B:186:ARG:NE	2.79	0.49
1:A:330:ASP:N	1:A:330:ASP:OD1	2.44	0.49
1:B:276:ASN:CA	1:B:279:GLN:HG3	2.39	0.49
1:B:449:LEU:HG	1:B:454:HIS:HB3	1.95	0.49
1:B:306:ARG:C	1:B:334:SER:HG	2.17	0.49
1:B:360:GLU:HA	1:B:363:ARG:CZ	2.43	0.49
1:A:186:ARG:NH2	1:A:486:ASP:O	2.46	0.49
1:B:52:LYS:HE3	2:B:601:ADP:PB	2.52	0.49
1:B:374:THR:HG21	1:B:479:SER:HB2	1.94	0.49
1:B:52:LYS:HB2	2:B:601:ADP:O2B	2.13	0.49
1:B:173:GLU:HG2	1:B:174:LEU:HG	1.93	0.49
1:A:460:GLY:O	1:A:463:LYS:HE3	2.13	0.48
1:A:49:GLY:O	2:A:601:ADP:H5'2	2.13	0.48
1:B:188:ARG:HB3	1:B:192:LYS:NZ	2.29	0.48
1:A:150:VAL:HG21	1:A:191:ILE:HA	1.96	0.48
1:B:99:LEU:HD12	1:B:102:GLU:H	1.78	0.48
1:B:257:GLN:HA	1:B:260:GLY:H	1.79	0.48
1:A:155:HIS:O	1:A:155:HIS:CD2	2.66	0.48
1:A:215:ARG:HG2	1:A:402:ASP:HB3	1.96	0.48
1:A:77:MET:HE2	1:A:119:TYR:HD2	1.77	0.48
1:A:416:GLU:OE2	1:A:465:HIS:NE2	2.46	0.47
1:B:151:SER:CB	1:B:152:GLN:HB3	2.44	0.47
1:A:129:ARG:HA	1:A:132:ASP:HB2	1.95	0.47
1:B:22:TYR:OH	2:B:601:ADP:H2'	2.14	0.47
1:B:99:LEU:HD12	1:B:102:GLU:HG2	1.96	0.47
1:B:280:GLU:HA	1:B:283:LEU:H	1.79	0.47
1:B:416:GLU:OE2	1:B:465:HIS:NE2	2.46	0.47
1:B:508:LEU:O	1:B:509:LEU:HD12	2.14	0.47
1:B:66:THR:OG1	1:B:115:LEU:O	2.13	0.47
1:B:286:GLU:HG2	1:B:287:GLY:C	2.39	0.47
1:A:340:TYR:CE1	1:A:376:CYS:HB3	2.49	0.47
1:A:274:GLU:O	1:A:277:ASN:HB3	2.15	0.46
1:A:436:LEU:O	1:A:440:LEU:HD12	2.15	0.46
1:A:483:LEU:HD22	1:A:491:LEU:HB3	1.96	0.46
1:B:252:THR:O	1:B:256:LEU:HD13	2.15	0.46
1:B:263:ALA:O	1:B:264:LEU:HD12	2.14	0.46
1:A:282:PHE:HA	1:A:288:VAL:HG11	1.97	0.46
1:A:302:LYS:HG2	1:A:305:VAL:CG2	2.45	0.46
1:B:81:VAL:HG21	1:B:93:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:CD1	1:B:102:GLU:HG2	2.45	0.46
1:A:487:ASP:HB3	1:A:488:HIS:ND1	2.30	0.46
1:B:217:GLY:O	1:B:339:VAL:HA	2.15	0.46
1:A:216:VAL:HB	1:A:382:ARG:NH2	2.31	0.46
1:A:186:ARG:CZ	1:A:486:ASP:O	2.63	0.46
1:A:313:LEU:HA	1:A:314:PRO:HD3	1.81	0.46
1:A:465:HIS:HB3	1:A:469:LEU:HD23	1.97	0.46
1:A:33:VAL:HG21	1:A:58:LEU:HD23	1.98	0.46
1:B:347:ASN:HA	1:B:350:ARG:NH2	2.31	0.46
1:A:45:LEU:HD11	1:A:188:ARG:HD3	1.97	0.46
1:A:273:THR:OG1	1:A:274:GLU:N	2.42	0.46
1:A:154:GLY:O	1:A:155:HIS:HB3	2.15	0.45
1:A:271:SER:OG	1:A:273:THR:OG1	2.07	0.45
1:B:9:HIS:CD2	1:B:10:ASP:H	2.34	0.45
1:B:270:LEU:O	1:B:270:LEU:HD23	2.16	0.45
1:B:280:GLU:HG2	1:B:283:LEU:HD13	1.97	0.45
1:B:321:TYR:CD1	1:B:321:TYR:C	2.94	0.45
1:B:487:ASP:N	1:B:487:ASP:OD1	2.47	0.45
1:A:77:MET:HE2	1:A:119:TYR:CD2	2.50	0.45
1:A:256:LEU:O	1:A:261:ILE:HG13	2.17	0.45
1:B:447:LYS:HD3	1:B:447:LYS:HA	1.60	0.45
1:B:449:LEU:HD23	1:B:454:HIS:ND1	2.31	0.45
1:B:128:PRO:O	1:B:129:ARG:HB3	2.16	0.45
1:B:169:GLU:HG3	1:B:196:ARG:HH22	1.81	0.45
1:A:166:VAL:HG13	1:A:167:LEU:HD23	1.98	0.45
1:A:279:GLN:O	1:A:283:LEU:HD13	2.16	0.45
1:A:173:GLU:HG2	1:A:174:LEU:N	2.30	0.45
1:B:487:ASP:C	1:B:489:PHE:H	2.24	0.45
1:B:8:LEU:C	1:B:9:HIS:CG	2.95	0.45
1:B:487:ASP:HA	1:B:489:PHE:H	1.82	0.45
1:A:445:THR:O	1:A:449:LEU:HG	2.17	0.45
1:B:74:ILE:O	1:B:77:MET:HG2	2.16	0.45
1:B:349:ARG:NH2	1:B:373:LEU:HD22	2.31	0.45
1:B:501:LEU:C	1:B:503:GLU:H	2.24	0.45
1:A:27:GLY:HA3	1:A:205:SER:OG	2.16	0.45
1:B:352:LEU:C	1:B:354:GLN:HG3	2.43	0.44
1:B:8:LEU:HD12	1:B:8:LEU:HA	1.80	0.44
1:B:28:VAL:HG12	1:B:32:ILE:HG13	1.98	0.44
1:B:380:THR:C	1:B:403:VAL:HG11	2.42	0.44
1:A:228:HIS:NE2	1:A:232:GLU:OE2	2.49	0.44
1:A:276:ASN:O	1:A:280:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASP:C	1:A:332:LEU:N	2.71	0.44
1:A:454:HIS:HA	1:A:459:PHE:CD1	2.52	0.44
1:B:43:LEU:HD12	1:B:44:VAL:H	1.82	0.44
1:B:150:VAL:CG2	1:B:151:SER:HB2	2.48	0.44
1:B:305:VAL:H	1:B:328:GLY:H	1.64	0.44
1:B:356:ASP:HB2	1:B:362:LYS:CE	2.47	0.44
1:A:14:HIS:O	1:A:14:HIS:ND1	2.51	0.44
1:A:186:ARG:NH1	1:A:487:ASP:OD2	2.51	0.44
1:B:42:ALA:O	1:B:177:VAL:HA	2.18	0.44
1:A:19:ILE:HD11	1:B:246:ARG:NH2	2.33	0.44
1:A:207:PHE:HB2	1:A:392:GLU:OE1	2.18	0.44
1:B:97:THR:O	1:B:97:THR:OG1	2.34	0.44
1:B:231:ARG:HD3	1:B:232:GLU:HG3	2.00	0.44
1:B:263:ALA:HB2	1:B:289:ILE:HB	1.99	0.44
1:A:244:LEU:HD12	1:A:312:ASP:HB3	1.99	0.44
1:B:131:LEU:O	1:B:135:GLU:HG2	2.18	0.44
1:B:357:ALA:HB1	1:B:358:PRO:HD2	1.99	0.44
1:A:465:HIS:CG	1:A:469:LEU:HD23	2.53	0.43
1:B:249:VAL:HG21	1:B:293:THR:HG22	2.00	0.43
1:B:352:LEU:HA	1:B:354:GLN:HG2	1.99	0.43
1:B:129:ARG:HD2	1:B:129:ARG:O	2.19	0.43
1:B:437:THR:HA	1:B:440:LEU:HD12	2.01	0.43
1:A:254:LYS:HE3	1:A:254:LYS:HB3	1.54	0.43
1:B:228:HIS:NE2	1:B:232:GLU:OE1	2.50	0.43
1:A:256:LEU:HB3	1:A:261:ILE:HD11	2.00	0.43
1:B:188:ARG:HB3	1:B:192:LYS:HZ1	1.84	0.43
1:A:503:GLU:C	1:A:505:GLN:H	2.26	0.43
1:B:99:LEU:HD13	1:B:101:HIS:CD2	2.53	0.43
1:B:309:ALA:HA	1:B:337:TRP:O	2.19	0.43
1:B:444:GLU:HB3	1:B:449:LEU:HD11	2.01	0.43
1:B:47:PRO:HG3	1:B:207:PHE:HA	2.00	0.43
1:B:144:ILE:N	1:B:144:ILE:HD12	2.33	0.43
1:B:273:THR:CG2	1:B:276:ASN:HB2	2.48	0.43
1:A:129:ARG:O	1:A:129:ARG:HG2	2.19	0.43
1:B:56:TYR:CE1	1:B:57:GLN:HG3	2.54	0.43
1:A:300:ILE:O	1:A:301:ASP:CG	2.62	0.43
1:B:43:LEU:HD13	1:B:178:ALA:HB3	2.00	0.43
1:B:392:GLU:C	1:B:393:GLU:HG2	2.44	0.43
1:B:436:LEU:O	1:B:440:LEU:HD12	2.19	0.43
1:A:51:GLY:HA2	2:A:601:ADP:H5'1	2.00	0.42
1:B:69:VAL:HA	1:B:143:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:O	1:B:321:TYR:OH	2.13	0.42
1:B:152:GLN:HE22	1:B:153:TRP:HB2	1.83	0.42
1:A:424:THR:HA	1:A:427:THR:HG22	2.01	0.42
1:B:213:GLN:HG3	1:B:400:ASN:O	2.19	0.42
1:B:246:ARG:CZ	1:B:269:GLY:HA3	2.48	0.42
1:A:8:LEU:HD12	1:A:8:LEU:HA	1.87	0.42
1:B:237:ASP:C	1:B:287:GLY:HA2	2.44	0.42
1:A:19:ILE:HD11	1:B:246:ARG:CZ	2.49	0.42
1:A:350:ARG:NH2	1:A:351:MET:HE3	2.33	0.42
1:B:355:SER:HB2	1:B:356:ASP:HA	2.02	0.42
1:A:471:ARG:HD2	1:A:471:ARG:HA	1.73	0.42
1:B:383:ARG:HD2	1:B:398:CYS:CB	2.50	0.42
1:A:144:ILE:HD12	1:A:144:ILE:N	2.35	0.42
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.78	0.42
1:B:282:PHE:HA	1:B:288:VAL:HG21	2.02	0.42
1:A:84:LEU:HD22	1:A:89:VAL:HG11	2.01	0.42
1:B:98:LEU:HG	1:B:102:GLU:HG3	2.01	0.42
1:B:110:LEU:HD22	1:B:118:LEU:HD22	2.01	0.42
1:A:411:ARG:HD2	1:A:514:LEU:HD13	2.02	0.41
1:B:245:SER:O	1:B:249:VAL:HG23	2.20	0.41
1:B:267:HIS:O	1:B:270:LEU:HB3	2.20	0.41
1:B:306:ARG:HA	1:B:334:SER:HB2	2.01	0.41
1:A:424:THR:O	1:A:427:THR:HG22	2.19	0.41
1:B:288:VAL:C	1:B:289:ILE:HD13	2.46	0.41
1:A:219:LYS:HB3	1:A:222:PRO:HG3	2.02	0.41
1:A:280:GLU:HB2	1:A:284:ASN:OD1	2.20	0.41
1:B:171:PHE:CD2	1:B:174:LEU:HD12	2.56	0.41
1:B:173:GLU:HG2	1:B:174:LEU:N	2.34	0.41
1:B:474:LEU:O	1:B:478:VAL:HG23	2.20	0.41
1:A:96:SER:OG	1:A:123:GLU:OE2	2.35	0.41
1:A:487:ASP:HA	1:A:489:PHE:N	2.35	0.41
1:B:502:LYS:HG2	1:B:504:GLY:N	2.26	0.41
1:B:22:TYR:HA	1:B:23:PRO:HD3	1.84	0.41
1:B:205:SER:HA	1:B:392:GLU:OE1	2.20	0.41
1:B:157:PHE:C	1:B:158:ARG:HG3	2.46	0.41
1:B:242:TYR:CE2	1:B:323:GLU:HB3	2.55	0.41
1:B:282:PHE:O	1:B:288:VAL:HG21	2.21	0.41
1:A:204:VAL:HG21	1:A:392:GLU:CA	2.51	0.41
1:B:16:LEU:HG	1:B:22:TYR:HB2	2.02	0.41
1:B:270:LEU:HD21	1:B:275:ARG:HD3	2.01	0.41
1:A:214:TYR:HE1	1:A:383:ARG:NH1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TRP:O	1:A:259:GLN:HG2	2.21	0.40
1:B:45:LEU:HD12	1:B:204:VAL:CG1	2.50	0.40
1:B:98:LEU:HD12	1:B:98:LEU:HA	1.91	0.40
1:B:149:CYS:HB2	1:B:161:TYR:CE2	2.56	0.40
1:A:169:GLU:H	1:A:169:GLU:HG2	1.75	0.40
1:B:43:LEU:HD12	1:B:44:VAL:N	2.36	0.40
1:B:139:VAL:HG11	1:B:174:LEU:HD13	2.04	0.40
1:A:408:PRO:HB3	1:A:510:ARG:NH2	2.36	0.40
1:A:482:TYR:CZ	1:A:496:LYS:HE2	2.57	0.40
1:B:150:VAL:HG21	1:B:191:ILE:HA	2.04	0.40
1:B:348:VAL:O	1:B:352:LEU:HB2	2.22	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	509/525 (97%)	486 (96%)	18 (4%)	5 (1%)	12	39
1	B	498/525 (95%)	468 (94%)	27 (5%)	3 (1%)	21	51
All	All	1007/1050 (96%)	954 (95%)	45 (4%)	8 (1%)	16	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ASP
1	B	271	SER
1	A	230	ILE
1	A	231	ARG
1	A	273	THR
1	A	302	LYS
1	B	303	PRO

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Mol	Chain	Res	Type
1	A	303	PRO

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	428/436 (98%)	410 (96%)	18 (4%)	26	60
1	B	420/436 (96%)	400 (95%)	20 (5%)	23	55
All	All	848/872 (97%)	810 (96%)	38 (4%)	24	58

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	97	THR
1	A	133	LEU
1	A	169	GLU
1	A	193	SER
1	A	204	VAL
1	A	233	GLU
1	A	244	LEU
1	A	254	LYS
1	A	288	VAL
1	A	294	VAL
1	A	330	ASP
1	A	335	THR
1	A	352	LEU
1	A	468	LYS
1	A	472	SER
1	A	516	PRO
1	A	518	LEU
1	B	69	VAL
1	B	76	LEU
1	B	94	LEU
1	B	96	SER

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Mol	Chain	Res	Type
1	B	123	GLU
1	B	152	GLN
1	B	204	VAL
1	B	233	GLU
1	B	254	LYS
1	B	256	LEU
1	B	270	LEU
1	B	279	GLN
1	B	286	GLU
1	B	343	SER
1	B	350	ARG
1	B	356	ASP
1	B	430	ARG
1	B	464	GLU
1	B	502	LYS
1	B	512	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	234	HIS
1	A	257	GLN
1	A	435	HIS
1	A	505	GLN
1	B	267	HIS
1	B	276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	ADP	A	601	-	28,29,29	2.28	10 (35%)	43,45,45	1.74	9 (20%)
2	ADP	B	601	-	28,29,29	2.56	11 (39%)	43,45,45	1.79	9 (20%)

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	A	601	-	-	8/16/32/32	0/3/3/3
2	ADP	B	601	-	-	4/16/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	PA-O5'	7.22	1.87	1.59
2	A	601	ADP	PA-O5'	7.00	1.86	1.59
2	B	601	ADP	PA-O3A	-6.11	1.52	1.59
2	B	601	ADP	O4'-C4'	-4.25	1.35	1.45
2	A	601	ADP	PA-O3A	-3.80	1.55	1.59
2	B	601	ADP	C4-N9	3.72	1.45	1.37
2	A	601	ADP	O4'-C4'	3.54	1.52	1.45
2	A	601	ADP	C2-N1	3.23	1.39	1.33
2	A	601	ADP	C5-C4	2.98	1.44	1.39
2	B	601	ADP	C2-N1	2.69	1.38	1.33
2	A	601	ADP	O5'-C5'	-2.61	1.34	1.44
2	B	601	ADP	C5-C4	2.59	1.43	1.39
2	B	601	ADP	O5'-C5'	-2.57	1.34	1.44
2	B	601	ADP	C6-N6	2.56	1.40	1.34
2	B	601	ADP	C5-C6	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	C4-N3	2.41	1.38	1.34
2	B	601	ADP	C8-N7	2.39	1.36	1.31
2	A	601	ADP	C6-N6	2.38	1.40	1.34
2	B	601	ADP	O3'-C3'	-2.37	1.37	1.43
2	A	601	ADP	O3'-C3'	-2.08	1.37	1.43
2	A	601	ADP	C4-N9	2.01	1.41	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	O4'-C1'-N9	6.54	120.65	108.09
2	A	601	ADP	O4'-C1'-N9	5.29	118.26	108.09
2	B	601	ADP	O2A-PA-O3A	3.77	117.47	107.27
2	A	601	ADP	O2A-PA-O3A	3.62	117.05	107.27
2	A	601	ADP	O3'-C3'-C4'	3.45	121.00	111.08
2	A	601	ADP	C5-C4-N3	-3.44	121.98	126.72
2	A	601	ADP	O5'-PA-O1A	-3.34	95.72	108.94
2	B	601	ADP	O5'-PA-O1A	-3.12	96.56	108.94
2	B	601	ADP	O3'-C3'-C4'	2.94	119.53	111.08
2	B	601	ADP	C5'-C4'-C3'	-2.86	104.91	115.21
2	B	601	ADP	C2'-C1'-N9	2.83	120.34	113.30
2	A	601	ADP	O3A-PA-O1A	2.67	118.73	110.70
2	B	601	ADP	O3A-PA-O1A	2.45	118.07	110.70
2	A	601	ADP	N3-C4-N9	2.31	131.09	127.17
2	B	601	ADP	O2A-PA-O5'	-2.17	97.73	107.57
2	A	601	ADP	O2A-PA-O5'	-2.11	98.00	107.57
2	B	601	ADP	O4'-C4'-C3'	2.07	109.26	105.15
2	A	601	ADP	O3B-PB-O2B	2.00	115.31	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O2A
2	A	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	PB-O3A-PA-O5'
2	B	601	ADP	PA-O3A-PB-O1B
2	A	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	C5'-O5'-PA-O1A

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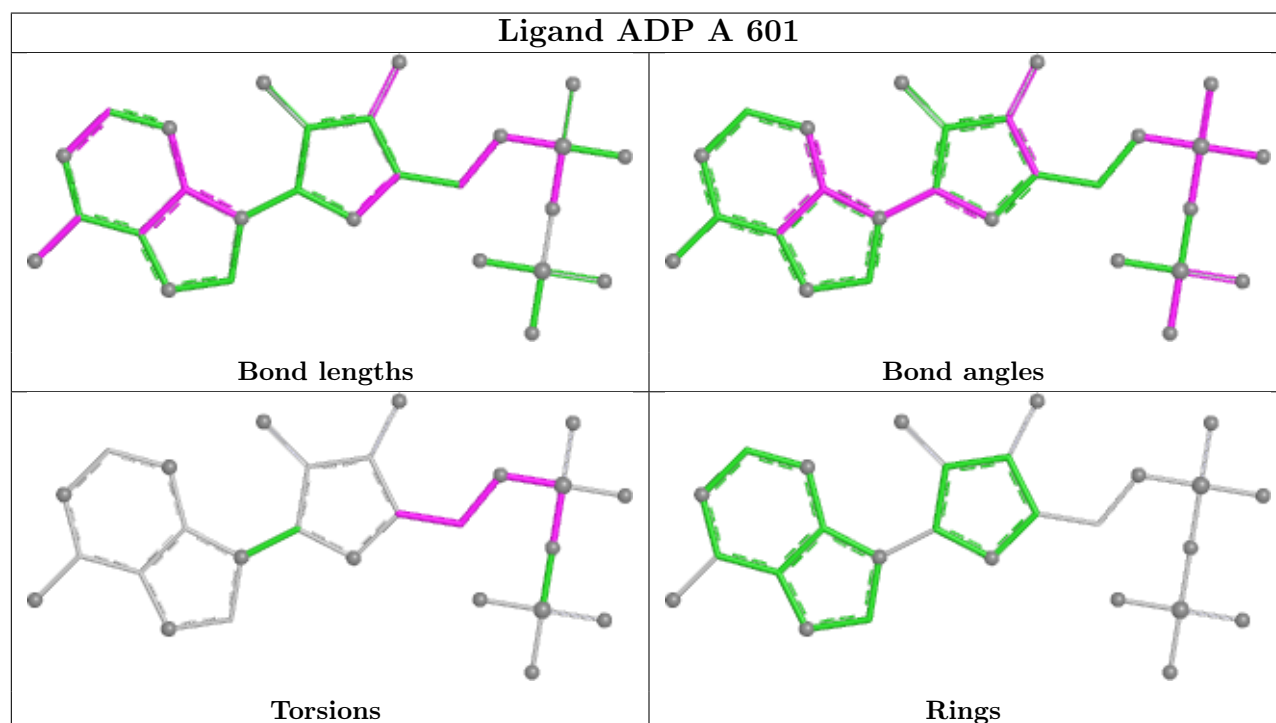
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	PB-O3A-PA-O1A
2	A	601	ADP	C4'-C5'-O5'-PA
2	B	601	ADP	O4'-C4'-C5'-O5'

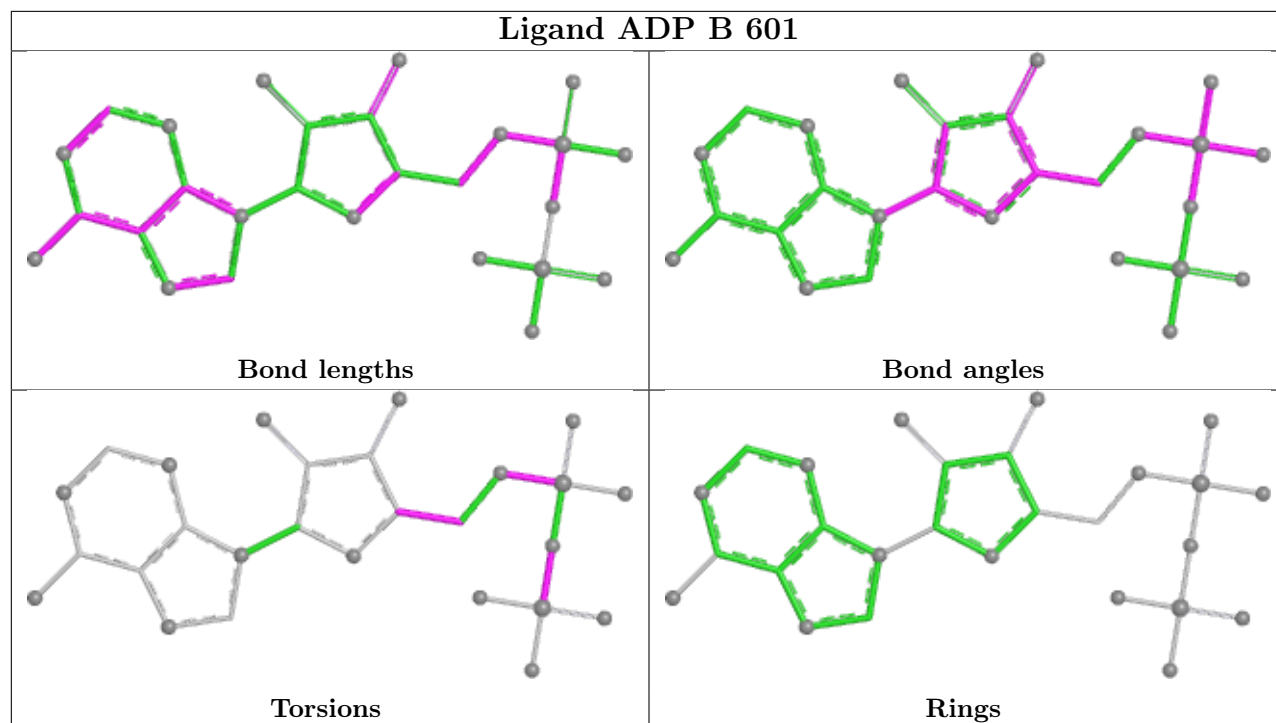
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ADP	6	0
2	B	601	ADP	4	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](#)

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	513/525 (97%)	-0.25	3 (0%) 85 81	40, 63, 87, 99	0
1	B	502/525 (95%)	0.09	11 (2%) 62 53	42, 74, 116, 149	0
All	All	1015/1050 (96%)	-0.08	14 (1%) 73 65	40, 67, 105, 149	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	TYR	3.8
1	A	300	ILE	3.5
1	B	295	ALA	3.3
1	A	295	ALA	3.2
1	B	282	PHE	3.2
1	B	154	GLY	2.9
1	B	294	VAL	2.8
1	B	264	LEU	2.5
1	B	153	TRP	2.3
1	B	504	GLY	2.3
1	B	287	GLY	2.2
1	B	284	ASN	2.1
1	A	294	VAL	2.0
1	B	265	ALA	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](#)

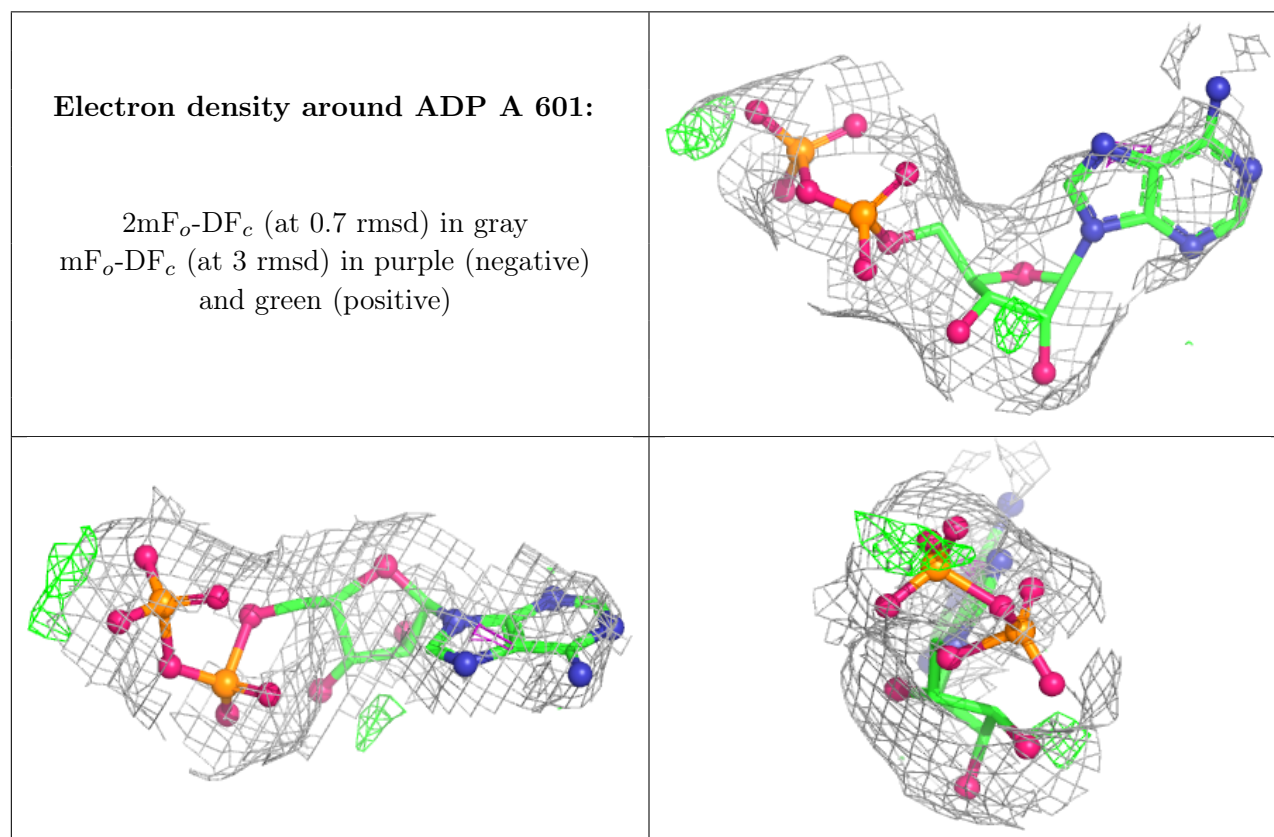
There are no oligosaccharides in this entry.

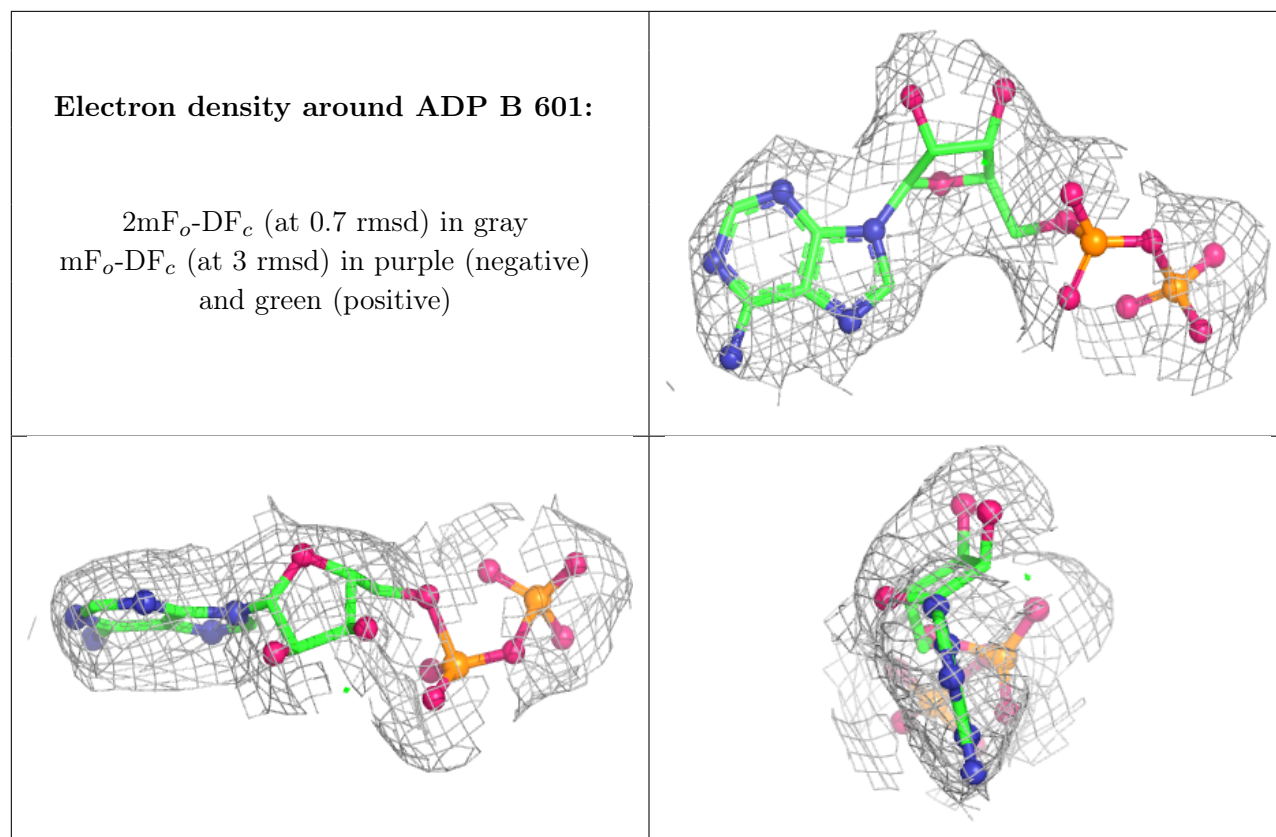
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	ADP	A	601	27/27	0.92	0.09	63,75,90,95	0
2	ADP	B	601	27/27	0.94	0.07	52,67,75,82	0
3	ZN	A	602	1/1	0.99	0.04	63,63,63,63	0
3	ZN	B	602	1/1	1.00	0.02	69,69,69,69	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.