



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:55 pm BST

PDB ID : 2AWN
Title : Crystal structure of the ADP-Mg-bound E. Coli MALK (Crystallized with ATP-Mg)
Authors : Lu, G.; Westbrook, J.M.; Davidson, A.L.; Chen, J.
Deposited on : 2005-09-01
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

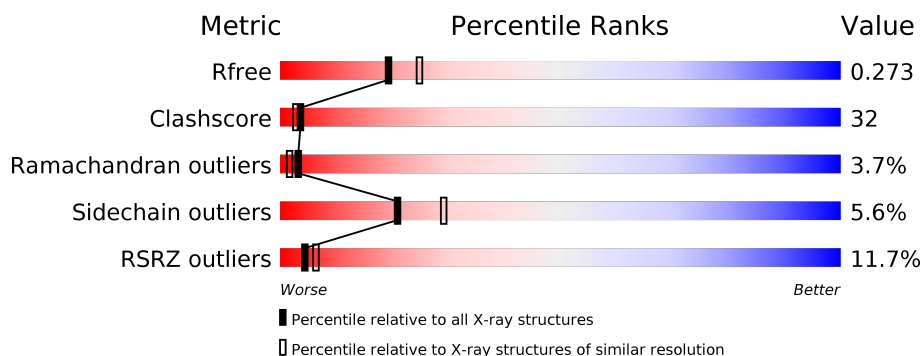
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	381	
1	B	381	
1	C	381	
1	D	381	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10669 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 Maltose/maltodextrin import ATP-binding protein malK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2534	1605	445	472	12			
1	B	374	Total	C	N	O	S	0	0	0
			2887	1825	515	534	13			
1	C	344	Total	C	N	O	S	0	0	0
			2596	1642	466	476	12			
1	D	301	Total	C	N	O	S	0	0	0
			2334	1475	412	435	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	CLONING ARTIFACT	UNP P68187
A	373	SER	-	CLONING ARTIFACT	UNP P68187
A	374	ALA	-	CLONING ARTIFACT	UNP P68187
A	375	SER	-	CLONING ARTIFACT	UNP P68187
A	376	HIS	-	CLONING ARTIFACT	UNP P68187
A	377	HIS	-	CLONING ARTIFACT	UNP P68187
A	378	HIS	-	CLONING ARTIFACT	UNP P68187
A	379	HIS	-	CLONING ARTIFACT	UNP P68187
A	380	HIS	-	CLONING ARTIFACT	UNP P68187
A	381	HIS	-	CLONING ARTIFACT	UNP P68187
B	372	ALA	-	CLONING ARTIFACT	UNP P68187
B	373	SER	-	CLONING ARTIFACT	UNP P68187
B	374	ALA	-	CLONING ARTIFACT	UNP P68187
B	375	SER	-	CLONING ARTIFACT	UNP P68187
B	376	HIS	-	CLONING ARTIFACT	UNP P68187
B	377	HIS	-	CLONING ARTIFACT	UNP P68187
B	378	HIS	-	CLONING ARTIFACT	UNP P68187
B	379	HIS	-	CLONING ARTIFACT	UNP P68187
B	380	HIS	-	CLONING ARTIFACT	UNP P68187
B	381	HIS	-	CLONING ARTIFACT	UNP P68187
C	372	ALA	-	CLONING ARTIFACT	UNP P68187

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	SER	-	CLONING ARTIFACT	UNP P68187
C	374	ALA	-	CLONING ARTIFACT	UNP P68187
C	375	SER	-	CLONING ARTIFACT	UNP P68187
C	376	HIS	-	CLONING ARTIFACT	UNP P68187
C	377	HIS	-	CLONING ARTIFACT	UNP P68187
C	378	HIS	-	CLONING ARTIFACT	UNP P68187
C	379	HIS	-	CLONING ARTIFACT	UNP P68187
C	380	HIS	-	CLONING ARTIFACT	UNP P68187
C	381	HIS	-	CLONING ARTIFACT	UNP P68187
D	372	ALA	-	CLONING ARTIFACT	UNP P68187
D	373	SER	-	CLONING ARTIFACT	UNP P68187
D	374	ALA	-	CLONING ARTIFACT	UNP P68187
D	375	SER	-	CLONING ARTIFACT	UNP P68187
D	376	HIS	-	CLONING ARTIFACT	UNP P68187
D	377	HIS	-	CLONING ARTIFACT	UNP P68187
D	378	HIS	-	CLONING ARTIFACT	UNP P68187
D	379	HIS	-	CLONING ARTIFACT	UNP P68187
D	380	HIS	-	CLONING ARTIFACT	UNP P68187
D	381	HIS	-	CLONING ARTIFACT	UNP P68187

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

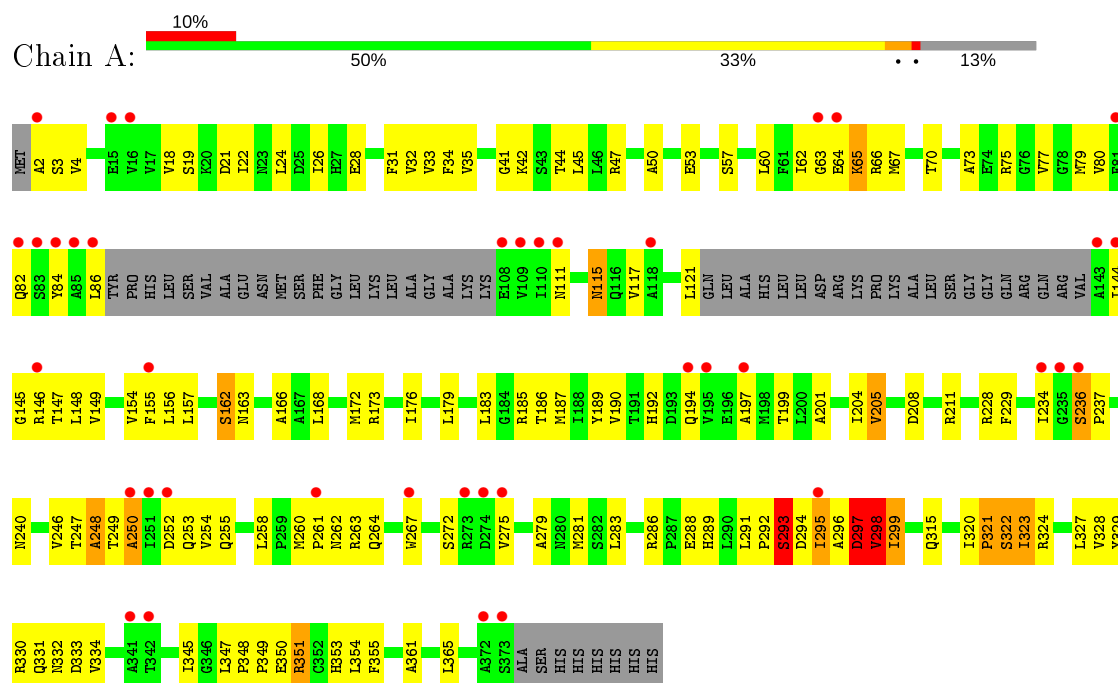
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	81	Total O 81 81	0	0
4	C	36	Total O 36 36	0	0
4	D	45	Total O 45 45	0	0

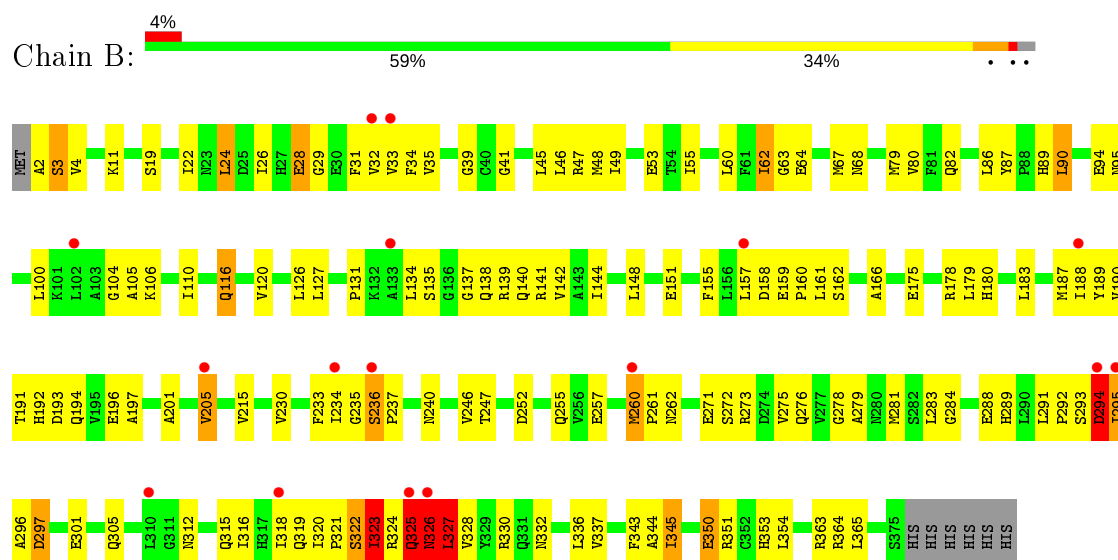
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

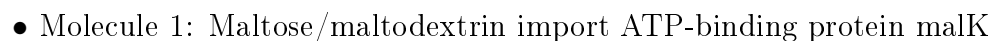
- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK



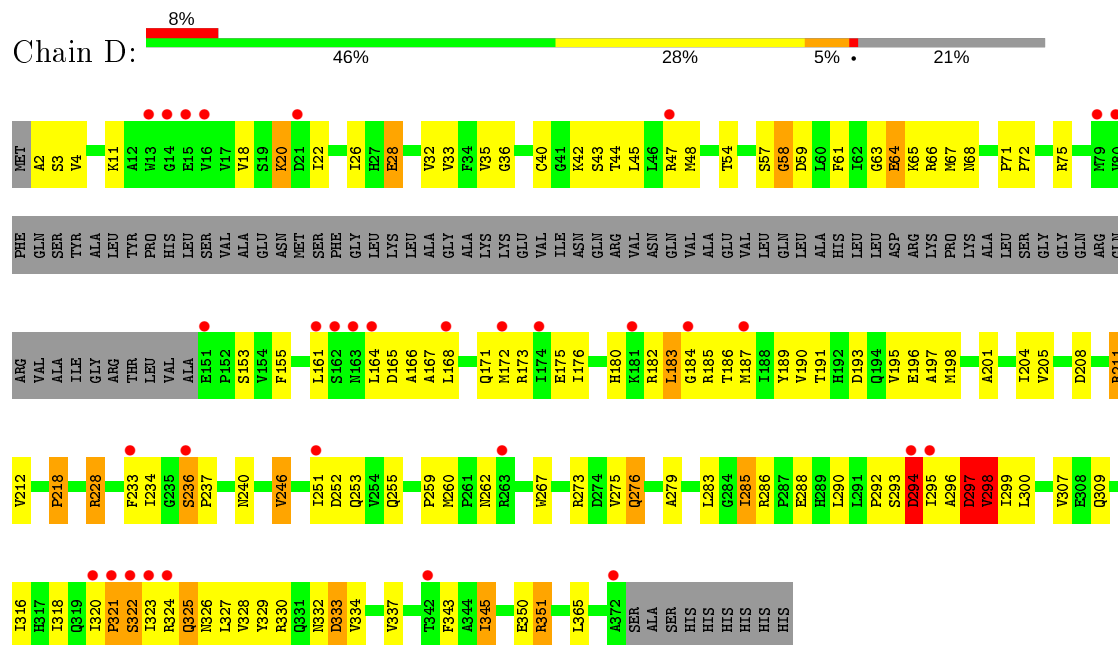
- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK



Chain C:



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.31Å 102.67Å 130.78Å 90.00° 90.81° 90.00°	Depositor
Resolution (Å)	37.28 – 2.30 37.28 – 2.28	Depositor EDS
% Data completeness (in resolution range)	85.0 (37.28-2.30) 93.9 (37.28-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.271 0.230 , 0.273	Depositor DCC
R_{free} test set	3843 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10669	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: MG, 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	0.90	3/2576 (0.1%)	0.91	9/3500 (0.3%)
1	B	0.54	2/2937 (0.1%)	0.82	11/3984 (0.3%)
1	C	0.49	2/2637 (0.1%)	0.79	7/3581 (0.2%)
1	D	0.76	3/2375 (0.1%)	0.82	7/3224 (0.2%)
All	All	0.69	10/10525 (0.1%)	0.84	34/14289 (0.2%)

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	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	ILE	N-CA	32.04	2.10	1.46
1	D	298	VAL	N-CA	30.24	2.06	1.46
1	A	298	VAL	N-CA	24.84	1.96	1.46
1	C	297	ASP	N-CA	17.16	1.80	1.46
1	B	327	LEU	N-CA	15.96	1.78	1.46
1	A	294	ASP	N-CA	10.09	1.66	1.46
1	D	58	GLY	N-CA	7.93	1.57	1.46
1	D	294	ASP	N-CA	7.23	1.60	1.46
1	B	326	ASN	N-CA	6.03	1.58	1.46
1	C	298	VAL	N-CA	-5.14	1.36	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	VAL	N-CA-CB	19.45	154.29	111.50
1	A	298	VAL	N-CA-CB	18.42	152.02	111.50
1	A	298	VAL	C-N-CA	-16.37	80.79	121.70
1	C	297	ASP	N-CA-CB	15.98	139.37	110.60
1	C	297	ASP	C-N-CA	14.99	159.17	121.70
1	A	294	ASP	N-CA-C	-13.68	74.07	111.00
1	B	327	LEU	N-CA-CB	13.67	137.75	110.40
1	D	297	ASP	C-N-CA	-13.34	88.36	121.70
1	A	297	ASP	C-N-CA	-12.88	89.50	121.70
1	A	298	VAL	N-CA-C	-12.86	76.27	111.00
1	C	297	ASP	N-CA-C	-11.28	80.56	111.00
1	A	294	ASP	N-CA-CB	10.65	129.77	110.60
1	D	298	VAL	N-CA-C	-9.23	86.09	111.00
1	C	296	ALA	C-N-CA	-9.14	98.86	121.70
1	C	18	VAL	CA-C-N	-8.82	97.80	117.20
1	C	18	VAL	O-C-N	8.46	136.24	122.70
1	B	296	ALA	N-CA-C	-8.39	88.35	111.00
1	A	299	ILE	N-CA-CB	-7.90	92.63	110.80
1	D	58	GLY	N-CA-C	7.82	132.65	113.10
1	B	322	SER	C-N-CA	7.08	139.40	121.70
1	D	326	ASN	N-CA-C	6.59	128.81	111.00
1	A	297	ASP	N-CA-C	-6.41	93.71	111.00
1	A	293	SER	C-N-CA	5.90	136.44	121.70
1	B	323	ILE	N-CA-C	5.76	126.56	111.00
1	B	324	ARG	C-N-CA	5.60	135.70	121.70
1	B	323	ILE	C-N-CA	-5.53	107.87	121.70
1	B	323	ILE	CB-CA-C	-5.50	100.60	111.60
1	B	294	ASP	N-CA-C	-5.47	96.22	111.00
1	C	298	VAL	N-CA-CB	5.39	123.36	111.50
1	B	325	GLN	N-CA-C	5.31	125.33	111.00
1	B	294	ASP	N-CA-CB	5.15	119.87	110.60
1	B	326	ASN	N-CA-CB	5.14	119.85	110.60
1	D	57	SER	C-N-CA	-5.12	111.55	122.30
1	D	294	ASP	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	SER	Peptide
1	B	326	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	C	18	VAL	Mainchain
1	C	296	ALA	Peptide
1	D	297	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	2534	0	2562	150	0
1	B	2887	0	2946	161	0
1	C	2596	0	2624	226	1
1	D	2334	0	2367	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	3	0
3	C	27	0	12	3	0
3	D	27	0	12	0	0
4	A	44	0	0	1	0
4	B	81	0	0	6	1
4	C	36	0	0	2	0
4	D	45	0	0	1	0
All	All	10669	0	10547	663	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 32.

All (663) 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:C:18:VAL:CG2	1:C:44:THR:HG21	1.31	1.58
1:C:296:ALA:CB	1:C:299:ILE:CG1	1.83	1.54
1:B:327:LEU:N	1:B:327:LEU:CA	1.78	1.45
1:C:297:ASP:N	1:C:297:ASP:CA	1.80	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLN:CA	1:B:326:ASN:HD21	1.29	1.41
1:B:319:GLN:HA	1:B:326:ASN:ND2	1.39	1.33
1:A:298:VAL:N	1:A:298:VAL:CA	1.96	1.29
1:C:294:ASP:O	1:C:295:ILE:HG13	1.14	1.23
1:C:18:VAL:HG21	1:C:44:THR:CG2	1.68	1.22
1:C:18:VAL:CG2	1:C:44:THR:CG2	2.19	1.21
1:D:320:ILE:HD11	1:D:327:LEU:HD22	1.22	1.20
1:D:298:VAL:CA	1:D:298:VAL:N	2.06	1.18
1:A:22:ILE:HD13	1:A:45:LEU:HD21	1.24	1.16
1:D:236:SER:HB3	1:D:237:PRO:HD3	1.24	1.16
1:C:296:ALA:HB3	1:C:299:ILE:CD1	1.76	1.16
1:C:259:PRO:HG2	1:C:323:ILE:CD1	1.76	1.16
1:A:299:ILE:CA	1:A:299:ILE:N	2.10	1.15
1:C:259:PRO:CG	1:C:323:ILE:HG12	1.75	1.14
1:A:298:VAL:O	1:A:299:ILE:CA	1.97	1.12
1:C:294:ASP:O	1:C:295:ILE:CG1	1.96	1.11
1:C:259:PRO:CB	1:C:323:ILE:HG12	1.79	1.11
1:B:318:ILE:O	1:B:326:ASN:ND2	1.83	1.10
1:C:286:ARG:HB2	1:C:289:HIS:HD2	1.11	1.10
1:C:296:ALA:CB	1:C:299:ILE:HG13	1.61	1.10
1:C:296:ALA:CB	1:C:299:ILE:HG12	1.61	1.08
1:C:296:ALA:HB3	1:C:299:ILE:HD11	1.23	1.07
1:B:236:SER:HB3	1:B:237:PRO:HD3	1.32	1.06
1:B:319:GLN:CA	1:B:326:ASN:ND2	2.05	1.05
1:B:319:GLN:N	1:B:326:ASN:HD21	1.54	1.04
1:C:259:PRO:HB2	1:C:323:ILE:CG1	1.89	1.03
1:C:296:ALA:HB3	1:C:299:ILE:CG1	1.87	1.03
1:D:26:ILE:HD12	1:D:32:VAL:HG21	1.39	1.03
1:C:296:ALA:HB2	1:C:299:ILE:HG12	1.02	1.01
1:A:298:VAL:C	1:A:299:ILE:CA	2.30	1.00
1:B:135:SER:H	1:B:138:GLN:HE21	1.02	1.00
1:C:191:THR:HG22	1:C:193:ASP:H	1.27	0.98
1:C:296:ALA:HB1	1:C:299:ILE:HG13	0.99	0.98
1:C:286:ARG:HB2	1:C:289:HIS:CD2	1.98	0.97
1:A:298:VAL:C	1:A:298:VAL:N	2.18	0.97
1:C:297:ASP:N	1:C:297:ASP:C	2.16	0.97
1:B:4:VAL:HG22	1:B:62:ILE:HD13	1.46	0.96
1:C:296:ALA:HB1	1:C:299:ILE:CG1	1.69	0.96
1:D:285:ILE:HD12	1:D:290:LEU:HG	1.48	0.96
1:B:318:ILE:C	1:B:326:ASN:ND2	2.20	0.95
1:C:259:PRO:HB2	1:C:323:ILE:HG12	1.39	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LEU:HB3	1:C:234:ILE:HD13	1.47	0.95
1:A:297:ASP:C	1:A:298:VAL:CA	2.36	0.94
1:C:204:ILE:HD11	1:C:218:PRO:HG3	1.50	0.94
1:A:240:ASN:HD21	1:A:328:VAL:H	1.08	0.94
1:C:296:ALA:C	1:C:297:ASP:CA	2.37	0.93
1:C:288:GLU:HG3	1:C:330:ARG:HD3	1.51	0.93
1:C:18:VAL:HG22	1:C:44:THR:HG21	1.48	0.92
1:D:22:ILE:HD12	1:D:212:VAL:HG23	1.49	0.92
1:C:259:PRO:CG	1:C:323:ILE:CG1	2.48	0.92
1:A:197:ALA:HB1	1:A:204:ILE:HD12	1.49	0.92
1:C:26:ILE:HD12	1:C:32:VAL:HG21	1.52	0.92
1:A:298:VAL:O	1:A:299:ILE:HA	1.70	0.92
1:D:183:LEU:HD12	1:D:184:GLY:H	1.35	0.91
1:A:22:ILE:CD1	1:A:45:LEU:HD21	2.01	0.91
1:A:79:MET:HG2	1:A:156:LEU:HB2	1.52	0.91
1:B:288:GLU:HG3	1:B:330:ARG:HD3	1.53	0.90
1:D:236:SER:HB3	1:D:237:PRO:CD	2.02	0.89
1:B:135:SER:H	1:B:138:GLN:NE2	1.72	0.88
1:D:297:ASP:C	1:D:298:VAL:CA	2.42	0.88
1:C:18:VAL:HG11	3:C:403:ADP:O4'	1.74	0.88
1:D:240:ASN:HD21	1:D:328:VAL:H	1.21	0.88
1:D:320:ILE:HD11	1:D:327:LEU:CD2	2.04	0.88
1:B:48:MET:SD	1:B:55:ILE:HD13	2.14	0.88
1:A:62:ILE:HD13	1:A:67:MET:HG3	1.54	0.87
1:B:260:MET:HG3	1:B:323:ILE:HB	1.56	0.86
1:C:18:VAL:HG21	1:C:44:THR:HG21	0.87	0.86
1:B:236:SER:CB	1:B:237:PRO:HD3	2.05	0.86
1:B:297:ASP:N	1:B:297:ASP:OD1	2.09	0.85
1:D:2:ALA:N	1:D:186:THR:HG1	1.74	0.85
1:C:260:MET:SD	1:C:262:ASN:HB3	2.15	0.85
1:C:296:ALA:CB	1:C:299:ILE:CD1	2.44	0.85
1:C:259:PRO:HG2	1:C:323:ILE:HD13	1.59	0.85
1:D:320:ILE:CD1	1:D:327:LEU:HD22	2.05	0.84
1:C:322:SER:C	1:C:323:ILE:HD12	1.98	0.84
1:A:297:ASP:O	1:A:298:VAL:CA	2.26	0.83
1:B:236:SER:HB3	1:B:237:PRO:CD	2.08	0.83
1:C:260:MET:HA	1:C:322:SER:HB3	1.60	0.83
1:C:300:LEU:HB3	1:C:320:ILE:HD13	1.61	0.82
1:D:35:VAL:HG11	1:D:197:ALA:HB2	1.59	0.82
1:D:285:ILE:HD13	1:D:286:ARG:O	1.79	0.81
1:B:319:GLN:HA	1:B:326:ASN:HD22	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:CD1	1:D:290:LEU:HG	2.10	0.81
1:A:299:ILE:HG13	1:A:299:ILE:N	1.97	0.80
1:C:236:SER:CB	1:C:237:PRO:HD3	2.10	0.80
1:B:260:MET:HB3	1:B:261:PRO:CD	2.12	0.80
1:B:46:LEU:HB3	1:B:79:MET:HE1	1.65	0.79
1:A:86:LEU:HA	1:A:146:ARG:HH22	1.47	0.79
1:C:259:PRO:HG2	1:C:323:ILE:CG1	2.10	0.79
1:C:272:SER:O	1:C:275:VAL:HG12	1.83	0.79
1:C:259:PRO:CB	1:C:323:ILE:CG1	2.52	0.78
1:B:2:ALA:HB1	1:B:28:GLU:CD	2.03	0.78
1:D:297:ASP:O	1:D:298:VAL:HA	1.84	0.78
1:B:272:SER:O	1:B:275:VAL:HG12	1.84	0.78
1:C:221:LEU:HB3	1:C:234:ILE:CD1	2.14	0.78
1:C:107:LYS:H	1:C:107:LYS:HD3	1.50	0.77
1:B:323:ILE:O	1:B:323:ILE:CG2	2.31	0.77
1:B:87:TYR:H	1:B:95:ASN:HD21	1.31	0.77
1:B:323:ILE:O	1:B:323:ILE:HG22	1.81	0.77
1:A:33:VAL:HB	1:A:204:ILE:HD13	1.68	0.76
1:C:259:PRO:CG	1:C:323:ILE:CD1	2.62	0.76
1:C:260:MET:N	1:C:323:ILE:HD11	1.99	0.76
1:B:294:ASP:O	1:B:295:ILE:HG22	1.86	0.76
1:C:31:PHE:HE1	1:C:189:TYR:HB2	1.48	0.75
1:A:236:SER:CB	1:A:237:PRO:HD3	2.16	0.75
1:B:260:MET:HB3	1:B:261:PRO:HD3	1.66	0.74
1:D:292:PRO:O	1:D:294:ASP:N	2.21	0.74
1:A:288:GLU:HG3	1:A:330:ARG:HD3	1.68	0.74
1:B:301:GLU:HG3	1:B:344:ALA:HB2	1.68	0.74
1:C:183:LEU:HD11	1:C:185:ARG:HE	1.51	0.74
1:B:158:ASP:HA	1:B:190:VAL:HG22	1.70	0.74
1:B:144:ILE:HD11	1:B:160:PRO:HB2	1.69	0.73
1:C:259:PRO:HG2	1:C:323:ILE:HD11	1.70	0.73
1:A:240:ASN:ND2	1:A:328:VAL:H	1.85	0.73
1:D:297:ASP:O	1:D:298:VAL:CA	2.37	0.73
1:C:22:ILE:HD12	1:C:212:VAL:HG23	1.70	0.73
1:B:320:ILE:HG22	1:B:322:SER:H	1.54	0.72
1:A:236:SER:OG	1:A:237:PRO:HD3	1.89	0.72
1:B:100:LEU:HD23	1:B:110:ILE:HD13	1.72	0.72
1:D:18:VAL:HG21	1:D:44:THR:HG21	1.72	0.72
1:D:183:LEU:HD13	1:D:185:ARG:H	1.53	0.72
1:B:26:ILE:HG21	1:B:188:ILE:HD11	1.71	0.71
1:C:80:VAL:HG11	1:C:144:ILE:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ALA:N	1:A:28:GLU:HG3	2.06	0.71
1:C:40:CYS:SG	1:C:42:LYS:HG3	2.30	0.70
1:C:159:GLU:O	1:C:162:SER:HB2	1.91	0.70
1:C:182:ARG:O	1:C:183:LEU:HB2	1.91	0.70
1:D:228:ARG:HH11	1:D:228:ARG:HG3	1.56	0.70
1:C:18:VAL:HG21	1:C:44:THR:CB	2.21	0.69
1:B:35:VAL:HG11	1:B:197:ALA:HB2	1.72	0.69
1:B:89:HIS:ND1	4:B:673:HOH:O	2.26	0.69
1:C:290:LEU:HD22	1:C:345:ILE:HD13	1.73	0.69
1:B:318:ILE:O	1:B:326:ASN:HA	1.93	0.68
1:B:41:GLY:HA2	3:B:402:ADP:O2A	1.92	0.68
1:B:345:ILE:HD13	1:B:345:ILE:H	1.58	0.68
1:A:236:SER:HB3	1:A:237:PRO:CD	2.24	0.68
1:C:31:PHE:CE1	1:C:189:TYR:HB2	2.29	0.67
1:C:204:ILE:CD1	1:C:218:PRO:HG3	2.24	0.67
1:D:183:LEU:HD12	1:D:184:GLY:N	2.08	0.67
1:D:240:ASN:ND2	1:D:328:VAL:H	1.90	0.67
1:A:292:PRO:O	1:A:293:SER:HB2	1.94	0.67
1:C:236:SER:HB2	1:C:237:PRO:HD3	1.75	0.67
1:A:19:SER:HB3	1:A:22:ILE:CD1	2.24	0.67
1:B:86:LEU:HD12	1:B:131:PRO:HB3	1.77	0.67
1:B:26:ILE:HD12	1:B:32:VAL:HG21	1.77	0.67
1:C:155:PHE:C	1:C:156:LEU:HD12	2.15	0.67
1:B:80:VAL:HG21	1:B:144:ILE:HD13	1.77	0.67
1:A:253:GLN:HG2	1:A:267:TRP:CE3	2.30	0.66
1:D:298:VAL:C	1:D:298:VAL:N	2.48	0.66
1:C:101:LYS:C	1:C:103:ALA:H	1.98	0.66
1:D:2:ALA:CB	1:D:153:SER:HB3	2.25	0.66
1:C:236:SER:HB3	1:C:237:PRO:HD3	1.77	0.66
1:A:62:ILE:HD13	1:A:67:MET:CG	2.24	0.66
1:C:240:ASN:HD21	1:C:328:VAL:H	1.43	0.66
1:D:2:ALA:HB2	1:D:153:SER:HB3	1.77	0.66
1:C:123:LEU:HD12	1:C:141:ARG:NH2	2.10	0.66
1:A:183:LEU:HD11	1:A:185:ARG:NE	2.11	0.66
1:B:281:MET:HE3	1:B:354:LEU:HD21	1.78	0.66
1:C:18:VAL:HG23	1:C:44:THR:CG2	2.25	0.65
1:A:252:ASP:HB3	1:A:365:LEU:HD13	1.76	0.65
1:A:67:MET:HA	1:A:67:MET:HE2	1.77	0.65
1:B:252:ASP:HB3	1:B:365:LEU:CD1	2.27	0.65
1:B:260:MET:CB	1:B:261:PRO:CD	2.74	0.65
1:B:33:VAL:HG23	1:B:201:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LYS:N	1:C:107:LYS:HD3	2.10	0.65
1:B:246:VAL:HG11	1:B:276:GLN:O	1.96	0.65
1:B:144:ILE:HD11	1:B:160:PRO:CB	2.27	0.65
1:D:324:ARG:HG2	1:D:325:GLN:H	1.60	0.65
1:C:293:SER:HB3	1:C:345:ILE:HA	1.79	0.65
1:D:276:GLN:NE2	1:D:276:GLN:H	1.95	0.65
1:B:318:ILE:O	1:B:326:ASN:CG	2.35	0.64
1:C:33:VAL:HG22	1:C:189:TYR:HB3	1.80	0.64
1:C:204:ILE:N	1:C:204:ILE:HD12	2.13	0.64
1:A:22:ILE:HD13	1:A:45:LEU:CD2	2.15	0.64
1:B:33:VAL:CG2	1:B:201:ALA:HB2	2.27	0.64
1:A:41:GLY:HA2	3:A:401:ADP:O2A	1.98	0.63
1:C:259:PRO:HG3	1:C:323:ILE:HG12	1.75	0.63
1:A:65:LYS:HG2	1:A:66:ARG:H	1.63	0.63
1:A:236:SER:HB3	1:A:237:PRO:HD3	1.80	0.63
1:A:236:SER:CB	1:A:237:PRO:CD	2.75	0.63
1:B:294:ASP:O	1:B:295:ILE:CG2	2.46	0.63
1:C:291:LEU:HB3	1:C:292:PRO:HD2	1.80	0.63
1:C:148:LEU:HD23	1:C:155:PHE:HE2	1.63	0.63
1:C:157:LEU:HD12	1:C:157:LEU:N	2.14	0.63
1:C:322:SER:CB	1:C:323:ILE:HD12	2.28	0.63
1:A:173:ARG:NH1	1:A:199:THR:HG21	2.13	0.63
1:C:244:VAL:HG23	1:C:281:MET:HB2	1.80	0.63
1:B:48:MET:HB3	1:B:55:ILE:HD11	1.80	0.63
1:C:259:PRO:HB2	1:C:323:ILE:HG13	1.75	0.63
1:D:296:ALA:O	1:D:297:ASP:HB2	1.98	0.63
1:C:161:LEU:HB3	1:C:169:ARG:HG2	1.80	0.62
1:A:197:ALA:HB1	1:A:204:ILE:CD1	2.27	0.62
1:C:294:ASP:O	1:C:295:ILE:CB	2.47	0.62
1:A:19:SER:HB3	1:A:22:ILE:HD12	1.81	0.62
1:B:191:THR:HG23	4:B:758:HOH:O	1.97	0.62
1:B:316:ILE:CG2	1:B:318:ILE:HD11	2.29	0.62
1:C:260:MET:HB2	1:C:261:PRO:HD2	1.80	0.62
1:B:3:SER:HB3	4:B:744:HOH:O	1.99	0.62
1:A:291:LEU:HD13	1:A:295:ILE:CD1	2.29	0.62
1:A:34:PHE:HB2	1:A:190:VAL:HG22	1.81	0.62
1:B:316:ILE:HG21	1:B:318:ILE:HD11	1.82	0.62
1:D:63:GLY:O	1:D:64:GLU:HB2	2.00	0.62
1:D:66:ARG:NH1	1:D:68:ASN:HB2	2.15	0.62
1:A:260:MET:C	1:A:262:ASN:H	2.03	0.62
1:A:253:GLN:HG2	1:A:267:TRP:HE3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HD13	1:A:295:ILE:HG12	1.82	0.62
1:A:65:LYS:HD3	1:A:67:MET:HE3	1.81	0.61
1:A:295:ILE:O	1:A:295:ILE:HD12	2.01	0.61
1:C:237:PRO:HD2	4:C:706:HOH:O	1.99	0.61
1:D:161:LEU:HD22	1:D:172:MET:HG2	1.80	0.61
1:B:292:PRO:O	1:B:293:SER:HB3	2.01	0.61
1:B:151:GLU:HG2	1:B:183:LEU:HD21	1.83	0.61
1:D:172:MET:O	1:D:176:ILE:HG12	2.01	0.61
1:C:236:SER:CB	1:C:237:PRO:CD	2.79	0.61
1:D:307:VAL:HG13	1:D:316:ILE:CD1	2.30	0.61
1:D:42:LYS:HD2	1:D:190:VAL:HG13	1.83	0.60
1:C:123:LEU:HD12	1:C:141:ARG:HH21	1.65	0.60
1:D:11:LYS:HB2	1:D:48:MET:SD	2.41	0.60
1:D:36:GLY:O	1:D:42:LYS:HE3	2.00	0.60
1:A:286:ARG:HD2	1:A:289:HIS:CE1	2.36	0.60
1:A:327:LEU:HD23	1:A:345:ILE:HD11	1.83	0.60
1:C:103:ALA:C	1:C:105:ALA:H	2.04	0.60
1:A:272:SER:O	1:A:275:VAL:HG12	2.02	0.60
1:C:183:LEU:HG	1:C:185:ARG:HD2	1.82	0.60
1:D:285:ILE:CD1	1:D:286:ARG:O	2.48	0.60
1:A:247:THR:O	1:A:248:ALA:HB2	2.01	0.60
1:B:350:GLU:CD	1:B:350:GLU:H	2.05	0.60
1:D:161:LEU:HD22	1:D:172:MET:CG	2.31	0.60
1:B:87:TYR:H	1:B:95:ASN:ND2	1.96	0.60
1:C:77:VAL:HG12	1:C:154:VAL:HB	1.83	0.60
1:C:35:VAL:HG11	1:C:197:ALA:HB2	1.84	0.59
1:C:294:ASP:C	1:C:295:ILE:HG13	2.10	0.59
1:B:191:THR:HG22	1:B:193:ASP:H	1.67	0.59
1:B:230:VAL:HG13	1:B:234:ILE:HD13	1.84	0.59
1:B:281:MET:CE	1:B:354:LEU:HD21	2.32	0.59
1:C:260:MET:CA	1:C:322:SER:HB3	2.32	0.59
1:D:33:VAL:HG23	1:D:201:ALA:HB2	1.84	0.58
1:D:288:GLU:HG3	1:D:330:ARG:HD3	1.85	0.58
1:A:34:PHE:HD2	1:A:205:VAL:HG13	1.68	0.58
1:B:325:GLN:O	1:B:326:ASN:HB2	2.02	0.58
1:D:22:ILE:CD1	1:D:212:VAL:HG23	2.30	0.58
1:A:293:SER:C	1:A:296:ALA:H	2.06	0.58
1:B:319:GLN:N	1:B:326:ASN:ND2	2.28	0.58
1:D:285:ILE:HD13	1:D:285:ILE:C	2.23	0.58
1:C:18:VAL:HG11	3:C:403:ADP:C1'	2.32	0.58
1:A:297:ASP:O	1:A:298:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:HB3	1:A:187:MET:HG2	1.85	0.58
1:A:299:ILE:CB	1:A:299:ILE:N	2.66	0.58
1:B:63:GLY:O	1:B:64:GLU:HB2	2.04	0.58
1:A:192:HIS:CD2	1:B:166:ALA:H	2.22	0.58
1:C:101:LYS:O	1:C:103:ALA:N	2.37	0.58
1:C:9:VAL:HG11	1:C:48:MET:SD	2.43	0.58
1:B:327:LEU:N	1:B:327:LEU:HA	2.04	0.57
1:D:43:SER:O	1:D:47:ARG:HG3	2.03	0.57
1:D:236:SER:CB	1:D:237:PRO:HD3	2.17	0.57
1:C:146:ARG:HG2	1:C:146:ARG:HH11	1.70	0.57
1:C:22:ILE:CD1	1:C:212:VAL:HG23	2.35	0.57
1:B:26:ILE:HG23	1:B:32:VAL:HG21	1.87	0.57
1:B:345:ILE:HD13	1:B:345:ILE:N	2.19	0.56
1:A:258:LEU:O	1:A:263:ARG:HA	2.05	0.56
1:D:173:ARG:NE	1:D:196:GLU:HG2	2.20	0.56
1:A:42:LYS:HB3	1:A:190:VAL:CG1	2.35	0.56
1:C:252:ASP:HB3	1:C:365:LEU:CD1	2.36	0.56
1:B:318:ILE:HD12	1:B:343:PHE:HB3	1.87	0.56
1:C:259:PRO:C	1:C:323:ILE:HD11	2.24	0.56
1:A:293:SER:O	1:A:296:ALA:N	2.38	0.56
1:C:162:SER:C	1:C:163:ASN:HD22	2.09	0.56
1:C:295:ILE:HG22	1:C:295:ILE:O	2.05	0.56
1:D:67:MET:SD	1:D:75:ARG:HG2	2.46	0.56
1:A:173:ARG:HH11	1:A:199:THR:HG21	1.70	0.56
1:C:296:ALA:O	1:C:297:ASP:CA	2.53	0.56
1:D:33:VAL:CG2	1:D:201:ALA:HB2	2.35	0.56
1:C:26:ILE:HG21	1:C:188:ILE:HD11	1.88	0.56
1:C:191:THR:HG22	1:C:192:HIS:N	2.20	0.56
1:C:318:ILE:HD11	1:C:343:PHE:HD2	1.71	0.56
1:B:140:GLN:OE1	1:B:140:GLN:HA	2.04	0.56
1:C:296:ALA:HB2	1:C:299:ILE:CG1	1.73	0.56
1:D:155:PHE:HB2	1:D:187:MET:HG2	1.87	0.56
1:D:233:PHE:HB3	1:D:234:ILE:HD12	1.86	0.55
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.71	0.55
1:A:299:ILE:CG1	1:A:299:ILE:N	2.67	0.55
1:B:46:LEU:HB3	1:B:79:MET:CE	2.35	0.55
1:B:87:TYR:N	1:B:95:ASN:HD21	2.00	0.55
1:C:89:HIS:CD2	1:C:90:LEU:HD13	2.42	0.55
1:A:201:ALA:HB3	1:A:204:ILE:HD11	1.89	0.55
1:B:234:ILE:HD12	1:B:234:ILE:N	2.21	0.55
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:VAL:O	1:C:151:GLU:HG2	2.07	0.55
1:D:259:PRO:HG2	1:D:260:MET:CE	2.37	0.55
1:A:320:ILE:O	1:A:322:SER:N	2.40	0.55
1:B:271:GLU:HG2	1:B:363:ARG:HB3	1.88	0.55
1:A:144:ILE:HG23	1:A:155:PHE:CZ	2.42	0.55
1:A:147:THR:HG21	1:A:155:PHE:HE2	1.71	0.55
1:B:294:ASP:O	1:B:295:ILE:O	2.25	0.55
1:B:240:ASN:HD21	1:B:328:VAL:H	1.55	0.54
1:D:285:ILE:HD12	1:D:290:LEU:CG	2.29	0.54
1:C:137:GLY:HA2	1:C:172:MET:CE	2.38	0.54
1:C:163:ASN:O	1:C:164:LEU:HG	2.06	0.54
1:A:64:GLU:O	1:A:65:LYS:HB2	2.07	0.54
1:B:246:VAL:HG13	1:B:278:GLY:H	1.73	0.54
1:C:148:LEU:HD23	1:C:155:PHE:CE2	2.42	0.54
1:B:106:LYS:O	1:B:110:ILE:HG12	2.07	0.54
1:C:300:LEU:HB3	1:C:320:ILE:CD1	2.34	0.54
1:C:26:ILE:HD12	1:C:32:VAL:HG11	1.90	0.54
1:A:33:VAL:CG2	1:A:201:ALA:HB2	2.38	0.54
1:B:35:VAL:HG11	1:B:197:ALA:CB	2.36	0.54
1:B:60:LEU:H	1:B:68:ASN:HD21	1.56	0.54
1:B:246:VAL:HG13	1:B:278:GLY:N	2.22	0.54
1:A:145:GLY:O	1:A:149:VAL:HG23	2.07	0.54
1:C:112:GLN:HA	1:C:112:GLN:HE21	1.71	0.54
1:C:228:ARG:HG3	1:C:228:ARG:NH1	2.21	0.54
1:C:228:ARG:HH11	1:C:228:ARG:HG3	1.72	0.54
1:D:300:LEU:O	1:D:345:ILE:HD13	2.08	0.54
1:C:107:LYS:H	1:C:107:LYS:CD	2.19	0.54
1:C:240:ASN:ND2	1:C:328:VAL:H	2.06	0.54
1:C:289:HIS:HD1	1:C:351:ARG:NH1	2.06	0.53
1:B:353:HIS:HD2	4:B:624:HOH:O	1.92	0.53
1:C:111:ASN:O	1:C:115:ASN:ND2	2.41	0.53
1:D:276:GLN:NE2	1:D:276:GLN:N	2.56	0.53
1:B:120:VAL:HG13	1:B:175:GLU:OE1	2.08	0.53
1:B:2:ALA:HB1	1:B:28:GLU:CG	2.37	0.53
1:B:47:ARG:HB3	1:B:53:GLU:HG2	1.91	0.53
1:C:97:SER:O	1:C:99:GLY:N	2.39	0.53
1:A:293:SER:O	1:A:296:ALA:CA	2.56	0.53
1:A:18:VAL:HG21	1:A:44:THR:HG21	1.90	0.53
1:B:137:GLY:O	1:B:141:ARG:HD3	2.08	0.53
1:B:326:ASN:C	1:B:327:LEU:CA	2.69	0.53
1:C:173:ARG:HE	1:C:196:GLU:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:CG1	1:C:197:ALA:HB2	2.39	0.53
1:C:38:SER:HB2	1:D:165:ASP:OD1	2.08	0.53
1:A:347:LEU:O	1:A:349:PRO:HD3	2.09	0.53
1:B:194:GLN:NE2	1:B:236:SER:HA	2.24	0.53
1:B:236:SER:CB	1:B:237:PRO:CD	2.78	0.53
1:D:67:MET:HE2	1:D:67:MET:HA	1.90	0.53
1:D:198:MET:HE2	1:D:204:ILE:CD1	2.39	0.53
1:D:33:VAL:HA	1:D:189:TYR:O	2.09	0.53
1:B:80:VAL:HG11	1:B:144:ILE:HD13	1.91	0.52
1:B:321:PRO:C	1:B:323:ILE:H	2.10	0.52
1:B:318:ILE:C	1:B:326:ASN:CG	2.67	0.52
1:C:294:ASP:CG	1:C:294:ASP:O	2.48	0.52
1:C:45:LEU:HD23	1:C:45:LEU:O	2.09	0.52
1:D:11:LYS:HD3	1:D:54:THR:O	2.09	0.52
1:C:106:LYS:HB3	1:C:109:VAL:HB	1.90	0.52
1:D:228:ARG:HG3	1:D:228:ARG:NH1	2.20	0.52
1:B:252:ASP:HB3	1:B:365:LEU:HD13	1.91	0.52
1:A:333:ASP:CG	1:A:334:VAL:H	2.13	0.52
1:D:316:ILE:CG2	1:D:318:ILE:HD11	2.39	0.52
1:A:144:ILE:HG23	1:A:155:PHE:HZ	1.75	0.52
1:C:283:LEU:C	1:C:283:LEU:HD23	2.30	0.52
1:A:260:MET:C	1:A:262:ASN:N	2.63	0.52
1:C:26:ILE:CD1	1:C:32:VAL:HG11	2.40	0.52
1:D:252:ASP:HB3	1:D:365:LEU:HD13	1.90	0.52
1:A:298:VAL:N	1:A:299:ILE:N	2.57	0.51
1:D:259:PRO:HG2	1:D:260:MET:HE2	1.92	0.51
1:D:345:ILE:N	1:D:345:ILE:HD13	2.25	0.51
1:A:67:MET:HE1	1:A:70:THR:HG21	1.92	0.51
1:D:61:PHE:HA	1:D:65:LYS:O	2.10	0.51
1:A:291:LEU:HD13	1:A:295:ILE:CG1	2.40	0.51
1:B:305:GLN:HG3	1:B:326:ASN:OD1	2.10	0.51
1:B:41:GLY:HA2	3:B:402:ADP:PA	2.51	0.51
1:D:316:ILE:HG22	1:D:318:ILE:CD1	2.41	0.51
1:A:33:VAL:HG23	1:A:201:ALA:HB2	1.91	0.51
1:D:260:MET:HA	1:D:322:SER:OG	2.10	0.51
1:B:157:LEU:N	1:B:157:LEU:HD12	2.26	0.51
1:C:129:ARG:HD3	4:C:791:HOH:O	2.10	0.51
1:A:201:ALA:HB3	1:A:204:ILE:CD1	2.41	0.51
1:C:173:ARG:NE	1:C:196:GLU:HG2	2.25	0.51
1:A:283:LEU:HD23	1:A:283:LEU:C	2.31	0.51
1:B:148:LEU:HD13	1:B:179:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:VAL:HG22	1:C:277:VAL:HA	1.93	0.51
1:A:260:MET:HG2	1:A:322:SER:OG	2.11	0.51
1:B:2:ALA:HB1	1:B:28:GLU:HG2	1.93	0.51
1:C:322:SER:O	1:C:323:ILE:HG13	2.11	0.51
1:A:117:VAL:O	1:A:121:LEU:HG	2.11	0.50
1:C:236:SER:HB2	1:C:237:PRO:CD	2.40	0.50
1:D:316:ILE:HG22	1:D:318:ILE:HD11	1.93	0.50
1:A:19:SER:HB3	1:A:22:ILE:HD11	1.93	0.50
1:D:4:VAL:HB	1:D:26:ILE:HB	1.93	0.50
1:C:164:LEU:HB2	1:C:169:ARG:HG3	1.92	0.50
1:C:208:ASP:HB2	1:C:229:PHE:CD2	2.46	0.50
1:C:47:ARG:HB3	1:C:52:LEU:HB2	1.93	0.50
1:A:65:LYS:HG2	1:A:66:ARG:N	2.26	0.50
1:C:26:ILE:HG23	1:C:32:VAL:HG21	1.93	0.50
1:D:183:LEU:CD1	1:D:185:ARG:H	2.22	0.50
1:A:33:VAL:HB	1:A:204:ILE:CD1	2.39	0.50
1:B:126:LEU:HD13	1:B:134:LEU:HD22	1.92	0.50
1:B:325:GLN:O	1:B:326:ASN:CB	2.59	0.50
1:D:208:ASP:O	1:D:211:ARG:HG2	2.12	0.50
1:B:230:VAL:CG1	1:B:234:ILE:HD13	2.41	0.50
1:B:34:PHE:HB2	1:B:190:VAL:HG12	1.94	0.49
1:C:351:ARG:HG2	1:C:351:ARG:HH11	1.77	0.49
1:C:118:ALA:O	1:C:123:LEU:N	2.45	0.49
1:C:42:LYS:HB2	3:C:403:ADP:O2B	2.11	0.49
1:A:194:GLN:HB2	1:A:234:ILE:HD13	1.94	0.49
1:C:322:SER:C	1:C:323:ILE:CD1	2.77	0.49
1:C:113:ARG:O	1:C:117:VAL:HG22	2.12	0.49
1:D:237:PRO:HD2	1:D:330:ARG:NH1	2.26	0.49
1:B:237:PRO:HD2	1:B:330:ARG:NH1	2.27	0.49
1:C:161:LEU:HG	1:C:189:TYR:OH	2.13	0.49
1:A:42:LYS:HB3	1:A:190:VAL:HG13	1.95	0.49
1:B:293:SER:O	1:B:293:SER:OG	2.24	0.49
1:C:208:ASP:O	1:C:210:GLY:N	2.45	0.49
1:C:345:ILE:HD12	1:C:345:ILE:O	2.11	0.49
1:C:92:VAL:HG12	1:C:96:MET:HE1	1.94	0.49
1:A:315:GLN:HG2	1:A:330:ARG:HG2	1.95	0.49
1:B:22:ILE:HD13	1:B:45:LEU:HD11	1.93	0.49
1:C:156:LEU:HD12	1:C:156:LEU:N	2.28	0.49
1:A:60:LEU:HG	1:A:62:ILE:CD1	2.42	0.49
1:C:112:GLN:HA	1:C:112:GLN:NE2	2.28	0.49
1:C:79:MET:HG3	1:C:156:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:CD1	1:D:218:PRO:HG3	2.43	0.49
1:D:237:PRO:HD2	1:D:330:ARG:HH11	1.78	0.49
1:C:121:LEU:HD11	1:C:145:GLY:CA	2.43	0.48
1:A:320:ILE:HB	1:A:323:ILE:HD12	1.94	0.48
1:D:33:VAL:HG12	1:D:35:VAL:HG13	1.94	0.48
1:D:18:VAL:CG2	1:D:44:THR:HG21	2.42	0.48
1:D:324:ARG:HE	1:D:325:GLN:HE21	1.61	0.48
1:A:260:MET:HA	1:A:322:SER:OG	2.14	0.48
1:C:46:LEU:HG	1:C:190:VAL:HG21	1.96	0.48
1:D:3:SER:N	1:D:28:GLU:HG2	2.29	0.48
1:B:320:ILE:HD12	1:B:320:ILE:N	2.28	0.48
1:C:101:LYS:C	1:C:103:ALA:N	2.64	0.48
1:B:283:LEU:HD23	1:B:283:LEU:C	2.34	0.48
1:C:97:SER:C	1:C:99:GLY:H	2.16	0.48
1:D:234:ILE:N	1:D:234:ILE:HD12	2.27	0.48
1:B:283:LEU:HD23	1:B:284:GLY:N	2.29	0.48
1:C:191:THR:HG22	1:C:192:HIS:H	1.78	0.48
1:C:208:ASP:C	1:C:210:GLY:H	2.18	0.48
1:D:193:ASP:OD2	1:D:195:VAL:HB	2.14	0.48
1:A:166:ALA:H	1:B:192:HIS:CD2	2.32	0.47
1:A:197:ALA:O	1:A:204:ILE:HD11	2.13	0.47
1:C:121:LEU:HB2	1:C:123:LEU:HD13	1.96	0.47
1:C:312:ASN:HB2	1:D:288:GLU:HG2	1.96	0.47
1:B:159:GLU:HB3	4:B:758:HOH:O	2.13	0.47
1:C:252:ASP:HB3	1:C:365:LEU:HD13	1.95	0.47
1:B:161:LEU:HD12	1:B:196:GLU:OE1	2.14	0.47
1:A:33:VAL:HG22	1:A:189:TYR:HB3	1.96	0.47
1:C:163:ASN:N	1:C:163:ASN:HD22	2.12	0.47
1:A:353:HIS:HD2	4:A:644:HOH:O	1.96	0.47
1:B:138:GLN:O	1:B:142:VAL:HG23	2.13	0.47
1:C:2:ALA:O	1:C:3:SER:CB	2.63	0.47
1:A:321:PRO:O	1:A:322:SER:OG	2.29	0.47
1:B:29:GLY:O	1:B:180:HIS:HE1	1.98	0.47
1:D:180:HIS:HA	1:D:183:LEU:HD11	1.96	0.47
1:D:253:GLN:HG2	1:D:267:TRP:CE3	2.49	0.47
1:A:26:ILE:HG23	1:A:32:VAL:HG21	1.95	0.47
1:C:183:LEU:CG	1:C:185:ARG:HD2	2.45	0.47
1:C:283:LEU:HD23	1:C:284:GLY:N	2.30	0.47
1:A:183:LEU:HD21	1:A:185:ARG:HE	1.80	0.47
1:B:90:LEU:HG	1:B:94:GLU:HB3	1.97	0.47
1:C:159:GLU:HG2	1:C:190:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:HA	1:C:205:VAL:HG22	1.97	0.47
1:D:251:ILE:O	1:D:252:ASP:HB2	2.14	0.47
1:D:255:GLN:HB2	1:D:267:TRP:CD2	2.49	0.47
1:A:262:ASN:OD1	1:A:264:GLN:HB2	2.14	0.47
1:B:89:HIS:CE1	1:B:90:LEU:HD13	2.50	0.47
1:D:318:ILE:HD12	1:D:343:PHE:HB3	1.96	0.47
1:B:289:HIS:ND1	4:B:640:HOH:O	1.96	0.47
1:C:9:VAL:HG11	1:C:48:MET:CE	2.44	0.47
1:A:252:ASP:HB3	1:A:365:LEU:CD1	2.43	0.46
1:C:36:GLY:HA3	1:C:40:CYS:SG	2.55	0.46
1:A:172:MET:O	1:A:176:ILE:HG12	2.16	0.46
1:D:253:GLN:HG2	1:D:267:TRP:HE3	1.81	0.46
1:A:50:ALA:HA	1:A:77:VAL:HG21	1.96	0.46
1:A:80:VAL:HB	1:A:84:TYR:OH	2.15	0.46
1:C:44:THR:O	1:C:44:THR:HG22	2.16	0.46
1:A:157:LEU:N	1:A:157:LEU:HD12	2.31	0.46
1:C:35:VAL:HG11	1:C:197:ALA:CB	2.46	0.46
1:C:171:GLN:HE21	1:C:171:GLN:HB3	1.59	0.46
1:D:260:MET:HA	1:D:322:SER:CB	2.45	0.46
1:A:62:ILE:HD13	1:A:67:MET:HB2	1.98	0.46
1:C:80:VAL:HG21	1:C:144:ILE:HD13	1.98	0.46
1:C:260:MET:HG3	1:C:263:ARG:N	2.31	0.46
1:C:26:ILE:HD12	1:C:32:VAL:CG2	2.34	0.46
1:C:92:VAL:HG12	1:C:96:MET:CE	2.45	0.46
1:D:40:CYS:SG	1:D:42:LYS:HG3	2.54	0.46
1:C:260:MET:HG3	1:C:263:ARG:H	1.80	0.46
1:C:323:ILE:HD12	1:C:323:ILE:N	2.29	0.46
1:A:260:MET:HA	1:A:322:SER:CB	2.46	0.46
1:B:315:GLN:HG2	1:B:330:ARG:HG2	1.98	0.46
1:C:205:VAL:CG2	1:C:205:VAL:O	2.63	0.46
1:A:348:PRO:HG2	1:A:351:ARG:CB	2.46	0.46
1:A:288:GLU:HG2	1:B:312:ASN:HB2	1.98	0.46
1:B:246:VAL:HG12	1:B:279:ALA:N	2.31	0.45
1:B:336:LEU:O	1:B:337:VAL:HG13	2.16	0.45
1:D:246:VAL:HG12	1:D:279:ALA:O	2.15	0.45
1:B:2:ALA:O	1:B:3:SER:HB3	2.16	0.45
1:C:368:GLU:OE1	1:C:369:PRO:HD2	2.16	0.45
1:A:291:LEU:HB3	1:A:295:ILE:HG12	1.97	0.45
1:A:323:ILE:HG12	1:A:324:ARG:O	2.17	0.45
1:B:34:PHE:HD2	1:B:205:VAL:HG13	1.82	0.45
1:B:316:ILE:HG22	1:B:318:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLU:HA	1:C:264:GLN:O	2.16	0.45
1:A:246:VAL:HG12	1:A:279:ALA:O	2.15	0.45
1:A:295:ILE:HG13	1:A:296:ALA:N	2.30	0.45
1:B:327:LEU:N	1:B:327:LEU:C	2.62	0.45
1:C:211:ARG:HG2	1:C:211:ARG:HH11	1.80	0.45
1:D:298:VAL:H	1:D:299:ILE:HG13	1.82	0.45
1:A:111:ASN:O	1:A:115:ASN:HB2	2.16	0.45
1:A:292:PRO:HG2	1:A:295:ILE:HG23	1.98	0.45
1:C:99:GLY:O	1:C:101:LYS:N	2.48	0.45
1:B:175:GLU:OE1	1:B:178:ARG:HD2	2.17	0.45
1:A:323:ILE:HD13	1:A:323:ILE:O	2.17	0.45
1:C:121:LEU:HD21	1:C:148:LEU:HD11	1.99	0.45
1:D:276:GLN:H	1:D:276:GLN:HE21	1.61	0.45
1:D:324:ARG:NE	1:D:325:GLN:HE21	2.13	0.45
1:A:34:PHE:CD2	1:A:205:VAL:HG13	2.50	0.45
1:B:148:LEU:HD22	1:B:179:LEU:CD1	2.47	0.45
1:B:179:LEU:C	1:B:179:LEU:HD23	2.37	0.45
1:A:147:THR:HG21	1:A:155:PHE:CE2	2.52	0.44
1:A:62:ILE:HD13	1:A:67:MET:CB	2.47	0.44
1:B:233:PHE:HB3	1:B:234:ILE:HD12	2.00	0.44
1:A:254:VAL:HG22	1:A:275:VAL:HG11	1.99	0.44
1:D:167:ALA:O	1:D:171:GLN:HG3	2.16	0.44
1:D:283:LEU:HD23	1:D:283:LEU:C	2.38	0.44
1:D:285:ILE:O	1:D:285:ILE:HG23	2.17	0.44
1:A:293:SER:O	1:A:296:ALA:HA	2.17	0.44
1:C:121:LEU:CB	1:C:123:LEU:HD13	2.48	0.44
1:A:291:LEU:HD13	1:A:295:ILE:HD11	2.00	0.44
1:C:103:ALA:C	1:C:105:ALA:N	2.71	0.44
1:C:18:VAL:CG2	1:C:44:THR:CB	2.88	0.44
1:D:164:LEU:HD13	1:D:172:MET:HE2	1.98	0.44
1:D:65:LYS:HD3	1:D:67:MET:HE1	1.99	0.44
1:D:204:ILE:HD11	1:D:218:PRO:HG3	2.00	0.44
1:D:295:ILE:HD12	1:D:296:ALA:N	2.32	0.44
1:C:111:ASN:O	1:C:114:VAL:HG12	2.18	0.44
1:B:260:MET:SD	1:D:182:ARG:HG3	2.58	0.44
1:D:260:MET:C	1:D:262:ASN:N	2.71	0.44
1:A:260:MET:O	1:A:263:ARG:N	2.45	0.44
1:A:295:ILE:C	1:A:295:ILE:HD12	2.38	0.44
1:C:29:GLY:HA2	1:C:184:GLY:O	2.17	0.44
1:A:329:TYR:OH	1:A:331:GLN:NE2	2.51	0.44
1:B:33:VAL:HA	1:B:189:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASP:HB3	1:D:365:LEU:CD1	2.48	0.44
1:B:272:SER:C	1:B:275:VAL:HG12	2.36	0.43
1:C:104:GLY:O	1:C:105:ALA:HB2	2.17	0.43
1:C:199:THR:HG22	1:C:200:LEU:HG	1.99	0.43
1:A:86:LEU:HD23	1:A:146:ARG:NH2	2.33	0.43
1:D:290:LEU:HB2	1:D:329:TYR:HD1	1.83	0.43
1:A:297:ASP:O	1:A:298:VAL:CG2	2.67	0.43
1:C:281:MET:SD	1:C:356:ARG:HA	2.59	0.43
1:C:290:LEU:HB2	1:C:329:TYR:HD1	1.82	0.43
1:D:185:ARG:HH11	1:D:185:ARG:HG2	1.83	0.43
1:A:208:ASP:HB2	1:A:229:PHE:CE2	2.53	0.43
1:C:161:LEU:O	1:C:162:SER:C	2.57	0.43
1:D:2:ALA:O	1:D:3:SER:HB3	2.19	0.43
1:C:2:ALA:HB3	1:C:186:THR:OG1	2.18	0.43
1:B:295:ILE:HG23	1:B:295:ILE:O	2.18	0.43
1:C:10:THR:HG23	1:C:19:SER:O	2.18	0.43
1:C:320:ILE:O	1:C:322:SER:N	2.52	0.43
1:A:248:ALA:HB3	1:A:255:GLN:HB3	2.01	0.43
1:B:22:ILE:HD13	1:B:45:LEU:CD1	2.49	0.43
1:C:82:GLN:CB	1:C:85:ALA:HB2	2.48	0.43
1:C:6:LEU:HD22	1:C:9:VAL:HG21	2.01	0.43
1:A:260:MET:HA	1:A:322:SER:HB3	2.00	0.43
1:B:316:ILE:HG22	1:B:318:ILE:HD11	2.00	0.43
1:B:39:GLY:N	3:B:402:ADP:O3B	2.35	0.43
1:C:192:HIS:CD2	1:C:192:HIS:H	2.36	0.43
1:C:356:ARG:HB2	1:C:358:ASP:OD1	2.19	0.43
1:D:323:ILE:HG13	1:D:324:ARG:N	2.33	0.43
1:C:126:LEU:HD22	1:C:126:LEU:N	2.34	0.43
1:C:201:ALA:CB	1:C:204:ILE:HG13	2.49	0.43
1:C:230:VAL:HG12	1:C:234:ILE:HD12	2.00	0.43
1:A:62:ILE:N	1:A:62:ILE:HD12	2.34	0.42
1:C:345:ILE:C	1:C:345:ILE:HD12	2.39	0.42
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.86	0.42
1:B:134:LEU:O	1:B:139:ARG:NH1	2.52	0.42
1:D:252:ASP:HA	1:D:365:LEU:HD11	2.00	0.42
1:B:247:THR:OG1	1:B:255:GLN:NE2	2.48	0.42
1:C:123:LEU:O	1:C:124:ALA:HB3	2.19	0.42
1:D:44:THR:HG22	1:D:48:MET:HE1	2.00	0.42
1:C:146:ARG:HG2	1:C:146:ARG:NH1	2.32	0.42
1:B:235:GLY:O	1:B:236:SER:C	2.57	0.42
1:C:286:ARG:HD2	1:C:289:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HA	1:D:45:LEU:HD23	1.84	0.42
1:C:205:VAL:O	1:C:205:VAL:HG23	2.19	0.42
1:B:48:MET:HB3	1:B:55:ILE:CD1	2.46	0.42
1:C:138:GLN:O	1:C:142:VAL:HG23	2.19	0.42
1:D:168:LEU:O	1:D:172:MET:HB2	2.20	0.42
1:D:246:VAL:HG13	1:D:279:ALA:H	1.85	0.42
1:C:208:ASP:C	1:C:210:GLY:N	2.73	0.42
1:C:293:SER:HB3	1:C:345:ILE:CA	2.49	0.42
1:A:148:LEU:HD11	1:A:179:LEU:HD11	2.01	0.42
1:B:22:ILE:HG23	1:B:24:LEU:HD23	2.00	0.42
1:C:297:ASP:N	1:C:298:VAL:N	2.67	0.42
1:D:20:LYS:N	1:D:20:LYS:HD3	2.34	0.42
1:D:320:ILE:O	1:D:322:SER:N	2.52	0.42
1:C:125:HIS:CE1	1:C:126:LEU:HD21	2.55	0.42
1:A:60:LEU:HG	1:A:62:ILE:HD12	2.02	0.41
1:B:262:ASN:HB2	1:B:322:SER:OG	2.20	0.41
1:B:301:GLU:O	1:B:321:PRO:HD2	2.20	0.41
1:C:126:LEU:HD12	1:C:129:ARG:NH1	2.35	0.41
1:C:161:LEU:HD22	1:C:172:MET:HG2	2.03	0.41
1:A:47:ARG:HB3	1:A:53:GLU:HG2	2.02	0.41
1:A:67:MET:SD	1:A:75:ARG:HG2	2.60	0.41
1:A:260:MET:HE2	1:A:261:PRO:HD2	2.01	0.41
1:B:116:GLN:HE21	1:B:116:GLN:HB3	1.66	0.41
1:A:183:LEU:HD11	1:A:185:ARG:CZ	2.49	0.41
1:A:355:PHE:CE2	1:A:361:ALA:HB2	2.55	0.41
1:B:104:GLY:O	1:B:105:ALA:HB2	2.19	0.41
1:B:320:ILE:HD11	1:B:327:LEU:HB2	2.03	0.41
1:D:332:ASN:ND2	4:D:717:HOH:O	2.52	0.41
1:A:42:LYS:HB3	1:A:190:VAL:HG11	2.01	0.41
1:B:155:PHE:HB2	1:B:187:MET:HG2	2.01	0.41
1:B:257:GLU:HG3	1:B:257:GLU:O	2.19	0.41
1:C:292:PRO:O	1:C:293:SER:CB	2.68	0.41
1:C:319:GLN:O	1:C:321:PRO:HD3	2.20	0.41
1:B:205:VAL:HB	1:B:215:VAL:HG22	2.01	0.41
1:D:2:ALA:HA	1:D:28:GLU:CD	2.41	0.41
1:D:316:ILE:HD12	1:D:337:VAL:HG21	2.03	0.41
1:D:345:ILE:H	1:D:345:ILE:HD13	1.86	0.41
1:A:154:VAL:HG13	1:A:186:THR:HG22	2.02	0.41
1:C:183:LEU:HD11	1:C:185:ARG:NE	2.27	0.41
1:C:322:SER:HB2	1:C:323:ILE:HD12	2.01	0.41
1:C:87:TYR:HA	1:C:88:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ASP:C	1:B:295:ILE:HG22	2.40	0.41
1:B:82:GLN:HG3	1:B:162:SER:OG	2.20	0.41
1:C:228:ARG:HH11	1:C:228:ARG:CG	2.33	0.41
1:D:173:ARG:HE	1:D:196:GLU:HG2	1.85	0.41
1:D:260:MET:HA	1:D:322:SER:HB3	2.01	0.41
1:D:36:GLY:O	1:D:42:LYS:CE	2.68	0.41
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.85	0.41
1:A:281:MET:CE	1:A:354:LEU:HD21	2.51	0.41
1:B:319:GLN:CB	1:B:326:ASN:HD21	2.17	0.41
1:B:305:GLN:CG	1:B:326:ASN:OD1	2.68	0.41
1:C:159:GLU:HG2	1:C:191:THR:HA	2.01	0.41
1:D:260:MET:C	1:D:262:ASN:H	2.24	0.41
1:B:240:ASN:O	1:B:284:GLY:HA2	2.20	0.41
1:B:68:ASN:H	1:B:68:ASN:HD22	1.68	0.41
1:C:204:ILE:HD11	1:C:218:PRO:CG	2.36	0.41
1:C:221:LEU:HD23	1:C:234:ILE:HD11	2.03	0.41
1:D:161:LEU:HD22	1:D:172:MET:HG3	1.99	0.41
1:D:351:ARG:HA	1:D:351:ARG:HD2	1.82	0.41
1:A:291:LEU:HA	1:A:292:PRO:HD2	1.84	0.41
1:A:3:SER:O	1:A:63:GLY:N	2.52	0.41
1:A:65:LYS:CD	1:A:67:MET:HE3	2.48	0.41
1:B:45:LEU:O	1:B:49:ILE:HG13	2.20	0.41
1:C:122:GLN:O	1:C:125:HIS:HE1	2.03	0.41
1:D:42:LYS:HD2	1:D:190:VAL:CG1	2.48	0.41
1:A:82:GLN:CG	1:A:162:SER:HB3	2.51	0.40
1:A:291:LEU:CD1	1:A:295:ILE:HD11	2.51	0.40
1:B:11:LYS:HB3	1:B:19:SER:HB2	2.03	0.40
1:B:353:HIS:CD2	1:B:364:ARG:HD2	2.56	0.40
1:C:114:VAL:O	1:C:118:ALA:HB2	2.21	0.40
1:C:203:LYS:C	1:C:204:ILE:HD12	2.41	0.40
1:D:190:VAL:HG12	1:D:191:THR:N	2.36	0.40
1:D:309:GLN:OE1	1:D:334:VAL:HG13	2.22	0.40
1:A:348:PRO:HG2	1:A:351:ARG:HB2	2.04	0.40
1:C:155:PHE:CZ	1:C:185:ARG:HD3	2.55	0.40
1:D:320:ILE:HA	1:D:321:PRO:HD3	1.84	0.40
1:A:249:THR:O	1:A:250:ALA:HB2	2.21	0.40
1:A:60:LEU:HD21	1:A:62:ILE:HD11	2.03	0.40
1:B:63:GLY:O	1:B:64:GLU:CB	2.66	0.40
1:C:157:LEU:H	1:C:157:LEU:HD12	1.86	0.40
1:A:4:VAL:CG2	1:A:154:VAL:HG21	2.51	0.40
1:B:67:MET:O	1:B:68:ASN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD12	1:C:345:ILE:HD11	2.04	0.40
1:D:295:ILE:O	1:D:296:ALA:HB3	2.21	0.40
1:D:324:ARG:HG2	1:D:325:GLN:N	2.32	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:C:102:LEU:CD2	4:B:765:HOH:O[2_556]	1.97	0.23

5.3 Torsion angles

5.3.1 Protein backbone

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	324/381 (85%)	294 (91%)	20 (6%)	10 (3%)	4	2
1	B	372/381 (98%)	339 (91%)	24 (6%)	9 (2%)	6	4
1	C	338/381 (89%)	290 (86%)	29 (9%)	19 (6%)	2	1
1	D	297/381 (78%)	263 (89%)	23 (8%)	11 (4%)	3	2
All	All	1331/1524 (87%)	1186 (89%)	96 (7%)	49 (4%)	3	2

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	SER
1	A	293	SER
1	A	298	VAL
1	B	236	SER
1	B	323	ILE
1	B	325	GLN
1	B	326	ASN

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Mol	Chain	Res	Type
1	B	327	LEU
1	C	85	ALA
1	C	105	ALA
1	C	183	LEU
1	C	236	SER
1	C	273	ARG
1	C	295	ILE
1	C	296	ALA
1	C	297	ASP
1	D	64	GLU
1	D	293	SER
1	D	298	VAL
1	A	65	LYS
1	A	322	SER
1	B	260	MET
1	B	273	ARG
1	B	295	ILE
1	C	3	SER
1	C	98	PHE
1	C	99	GLY
1	C	209	ALA
1	C	294	ASP
1	D	58	GLY
1	D	236	SER
1	A	321	PRO
1	C	162	SER
1	C	322	SER
1	D	322	SER
1	D	325	GLN
1	A	73	ALA
1	A	162	SER
1	A	248	ALA
1	B	3	SER
1	C	102	LEU
1	D	273	ARG
1	D	333	ASP
1	A	250	ALA
1	C	238	LYS
1	C	325	GLN
1	D	166	ALA
1	D	321	PRO
1	C	321	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	277/323 (86%)	261 (94%)	16 (6%)	20	27
1	B	315/323 (98%)	299 (95%)	16 (5%)	24	33
1	C	277/323 (86%)	265 (96%)	12 (4%)	29	40
1	D	258/323 (80%)	239 (93%)	19 (7%)	13	17
All	All	1127/1292 (87%)	1064 (94%)	63 (6%)	21	29

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	24	LEU
1	A	31	PHE
1	A	35	VAL
1	A	57	SER
1	A	115	ASN
1	A	163	ASN
1	A	168	LEU
1	A	205	VAL
1	A	228	ARG
1	A	295	ILE
1	A	297	ASP
1	A	323	ILE
1	A	332	ASN
1	A	350	GLU
1	A	351	ARG
1	B	24	LEU
1	B	28	GLU
1	B	31	PHE
1	B	62	ILE
1	B	90	LEU
1	B	116	GLN
1	B	127	LEU
1	B	205	VAL

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Mol	Chain	Res	Type
1	B	294	ASP
1	B	297	ASP
1	B	326	ASN
1	B	327	LEU
1	B	332	ASN
1	B	345	ILE
1	B	350	GLU
1	B	351	ARG
1	C	31	PHE
1	C	90	LEU
1	C	107	LYS
1	C	126	LEU
1	C	168	LEU
1	C	192	HIS
1	C	199	THR
1	C	228	ARG
1	C	246	VAL
1	C	297	ASP
1	C	350	GLU
1	C	351	ARG
1	D	20	LYS
1	D	28	GLU
1	D	59	ASP
1	D	175	GLU
1	D	183	LEU
1	D	205	VAL
1	D	211	ARG
1	D	218	PRO
1	D	228	ARG
1	D	246	VAL
1	D	275	VAL
1	D	276	GLN
1	D	285	ILE
1	D	294	ASP
1	D	297	ASP
1	D	333	ASP
1	D	345	ILE
1	D	350	GLU
1	D	351	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	GLN
1	A	163	ASN
1	A	171	GLN
1	A	192	HIS
1	A	240	ASN
1	A	264	GLN
1	A	331	GLN
1	A	332	ASN
1	A	353	HIS
1	B	68	ASN
1	B	95	ASN
1	B	111	ASN
1	B	122	GLN
1	B	138	GLN
1	B	171	GLN
1	B	180	HIS
1	B	192	HIS
1	B	240	ASN
1	B	253	GLN
1	B	255	GLN
1	B	264	GLN
1	B	326	ASN
1	B	331	GLN
1	B	332	ASN
1	B	353	HIS
1	C	112	GLN
1	C	115	ASN
1	C	163	ASN
1	C	171	GLN
1	C	240	ASN
1	C	253	GLN
1	C	255	GLN
1	C	264	GLN
1	C	331	GLN
1	C	332	ASN
1	D	7	GLN
1	D	163	ASN
1	D	240	ASN
1	D	255	GLN
1	D	264	GLN
1	D	276	GLN
1	D	325	GLN

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Mol	Chain	Res	Type
1	D	331	GLN
1	D	353	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	401	2	24,29,29	1.22	2 (8%)	29,45,45	2.45	7 (24%)
3	ADP	D	404	2	24,29,29	1.12	1 (4%)	29,45,45	2.30	8 (27%)
3	ADP	C	403	2	24,29,29	1.03	1 (4%)	29,45,45	2.34	8 (27%)
3	ADP	B	402	2	24,29,29	1.28	3 (12%)	29,45,45	2.43	9 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	401	2	-	6/12/32/32	0/3/3/3
3	ADP	D	404	2	-	2/12/32/32	0/3/3/3
3	ADP	C	403	2	-	4/12/32/32	0/3/3/3
3	ADP	B	402	2	-	6/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	ADP	C2-N1	3.31	1.40	1.33
3	D	404	ADP	C2-N1	3.31	1.40	1.33
3	A	401	ADP	C2-N1	3.29	1.40	1.33
3	C	403	ADP	C2-N1	3.18	1.39	1.33
3	B	402	ADP	O4'-C1'	2.18	1.44	1.41
3	B	402	ADP	C5'-C4'	2.04	1.58	1.51
3	A	401	ADP	O4'-C1'	2.01	1.43	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	O5'-PA-O1A	-8.74	74.93	109.07
3	C	403	ADP	O5'-PA-O1A	-8.43	76.14	109.07
3	D	404	ADP	O5'-PA-O1A	-8.18	77.12	109.07
3	B	402	ADP	O5'-PA-O1A	-8.08	77.51	109.07
3	B	402	ADP	O2A-PA-O5'	-4.28	87.88	107.75
3	A	401	ADP	O2A-PA-O5'	-4.08	88.79	107.75
3	D	404	ADP	O2A-PA-O5'	-3.86	89.84	107.75
3	C	403	ADP	C5-C6-N6	3.79	126.11	120.35
3	D	404	ADP	C5-C6-N6	3.76	126.06	120.35
3	A	401	ADP	O2A-PA-O1A	3.74	130.75	112.24
3	C	403	ADP	O2A-PA-O5'	-3.70	90.54	107.75
3	B	402	ADP	C5-C6-N6	3.63	125.87	120.35
3	A	401	ADP	C5-C6-N6	3.60	125.82	120.35
3	C	403	ADP	N3-C2-N1	-3.52	123.18	128.68
3	B	402	ADP	O2A-PA-O1A	3.51	129.60	112.24
3	A	401	ADP	N3-C2-N1	-3.49	123.22	128.68
3	B	402	ADP	N3-C2-N1	-3.49	123.23	128.68
3	D	404	ADP	N3-C2-N1	-3.40	123.36	128.68
3	C	403	ADP	O2A-PA-O1A	3.12	127.67	112.24
3	D	404	ADP	O2A-PA-O1A	3.07	127.44	112.24
3	D	404	ADP	C5-C6-N1	-2.86	113.88	120.35
3	A	401	ADP	C2-N1-C6	2.84	123.61	118.75
3	C	403	ADP	C5-C6-N1	-2.83	113.93	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5-C6-N1	-2.82	113.95	120.35
3	C	403	ADP	C2-N1-C6	2.79	123.53	118.75
3	B	402	ADP	C2-N1-C6	2.76	123.47	118.75
3	D	404	ADP	C2-N1-C6	2.73	123.43	118.75
3	B	402	ADP	C5-C6-N1	-2.73	114.16	120.35
3	D	404	ADP	C3'-C2'-C1'	2.67	104.99	100.98
3	C	403	ADP	C3'-C2'-C1'	2.46	104.69	100.98
3	B	402	ADP	O5'-C5'-C4'	2.36	117.10	108.99
3	B	402	ADP	O2B-PB-O3A	-2.06	97.74	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

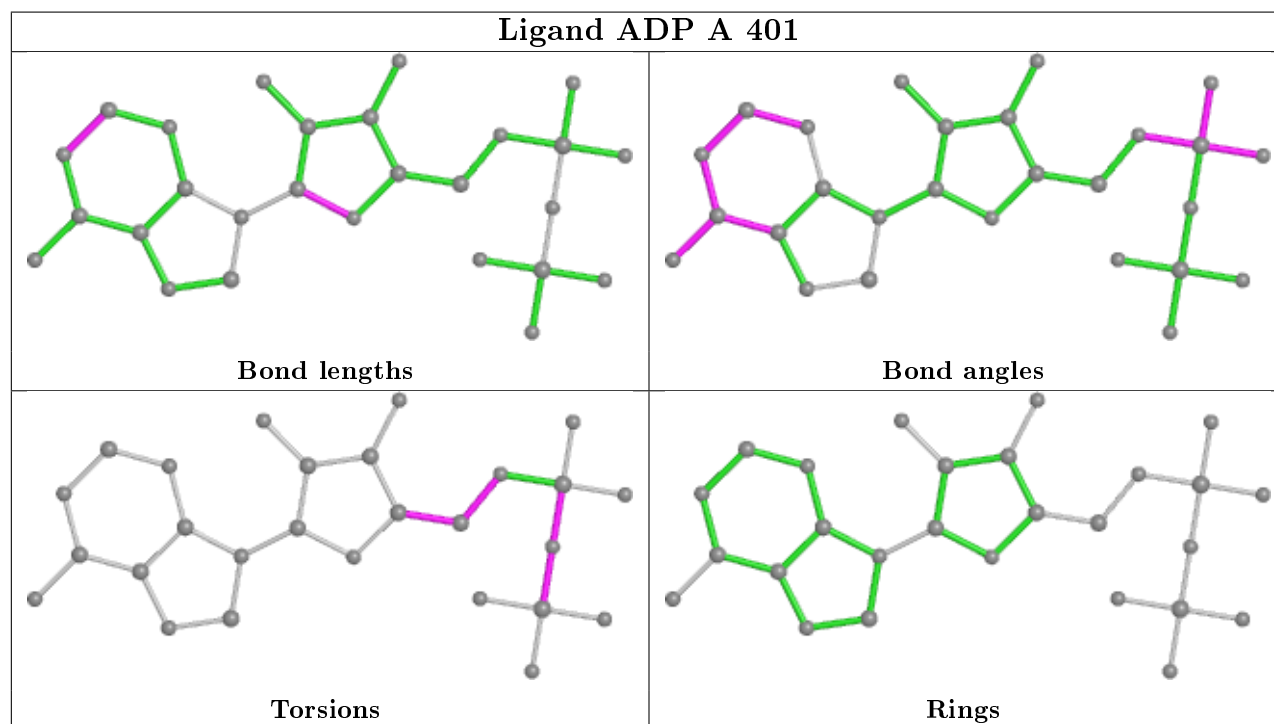
Mol	Chain	Res	Type	Atoms
3	D	404	ADP	PA-O3A-PB-O2B
3	C	403	ADP	PA-O3A-PB-O3B
3	B	402	ADP	PA-O3A-PB-O3B
3	C	403	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	O4'-C4'-C5'-O5'
3	C	403	ADP	O4'-C4'-C5'-O5'
3	A	401	ADP	C3'-C4'-C5'-O5'
3	B	402	ADP	C4'-C5'-O5'-PA
3	A	401	ADP	C4'-C5'-O5'-PA
3	A	401	ADP	PA-O3A-PB-O3B
3	B	402	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	PA-O3A-PB-O1B
3	A	401	ADP	PB-O3A-PA-O1A
3	B	402	ADP	PA-O3A-PB-O1B
3	B	402	ADP	O4'-C4'-C5'-O5'
3	D	404	ADP	PA-O3A-PB-O3B
3	C	403	ADP	PA-O3A-PB-O2B
3	B	402	ADP	PB-O3A-PA-O1A

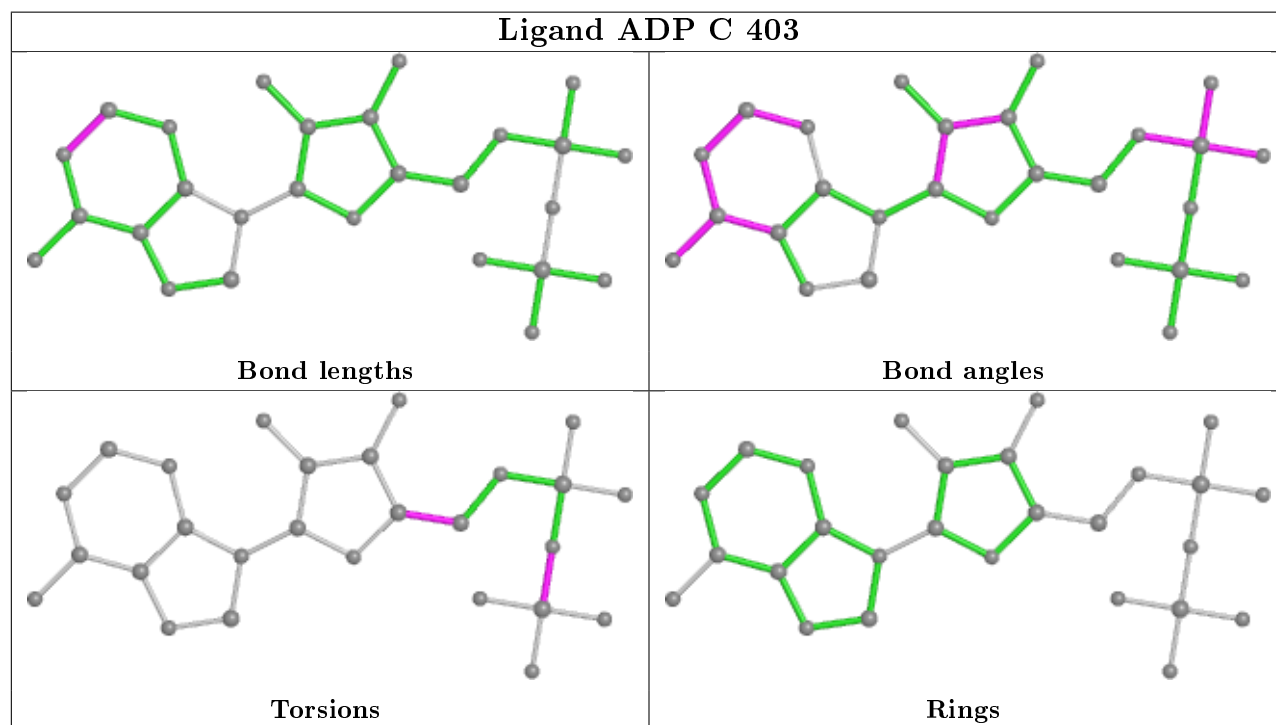
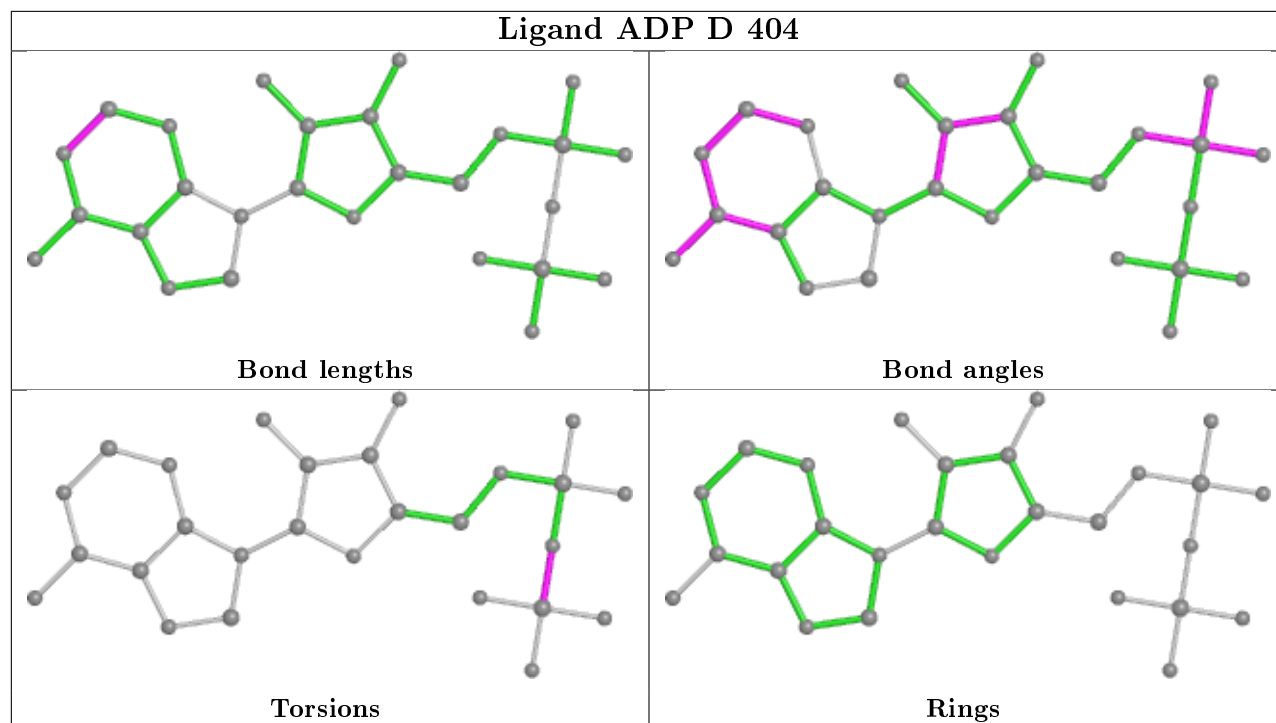
There are no ring outliers.

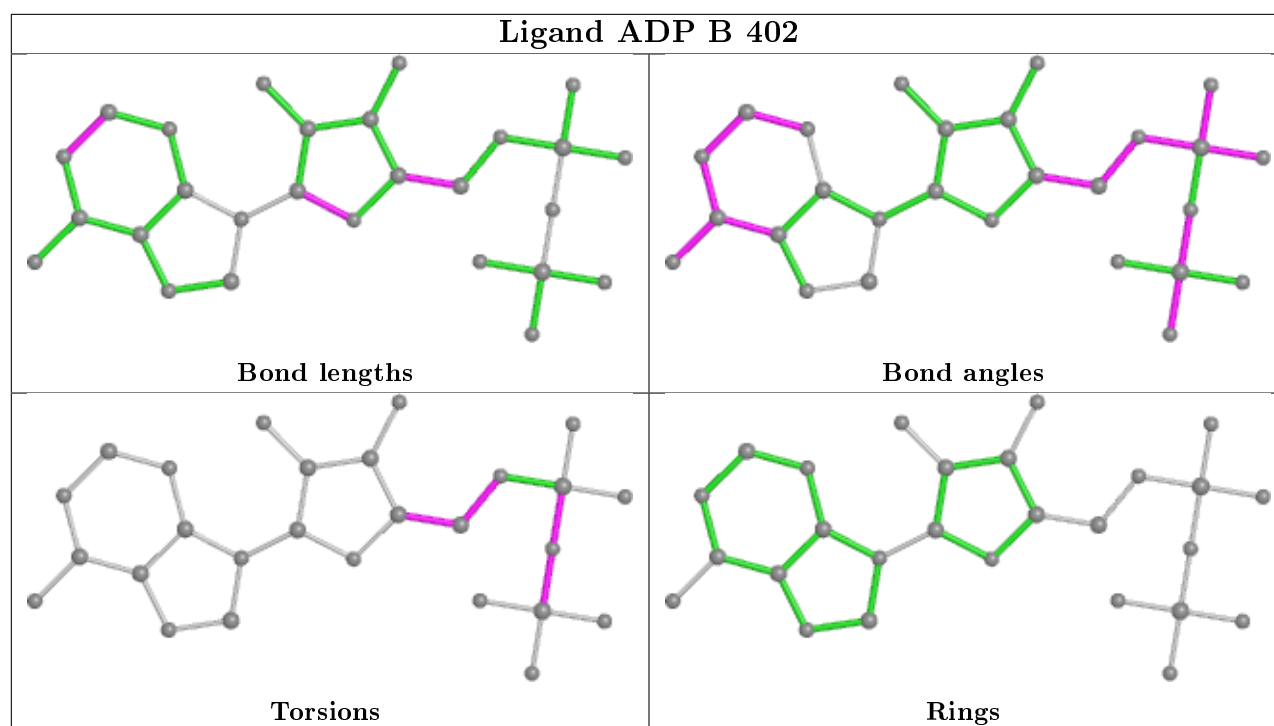
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	1	0
3	C	403	ADP	3	0
3	B	402	ADP	3	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	330/381 (86%)	0.72	39 (11%) 4 6	39, 63, 107, 146	0
1	B	374/381 (98%)	0.40	16 (4%) 35 42	32, 52, 87, 119	0
1	C	344/381 (90%)	1.06	71 (20%) 1 1	38, 76, 130, 148	0
1	D	301/381 (79%)	0.67	32 (10%) 6 8	34, 64, 102, 115	0
All	All	1349/1524 (88%)	0.71	158 (11%) 4 6	32, 62, 113, 148	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	9.2
1	C	103	ALA	8.8
1	C	102	LEU	8.8
1	A	84	TYR	8.3
1	C	48	MET	7.7
1	D	80	VAL	7.7
1	A	85	ALA	7.4
1	C	6	LEU	6.8
1	C	109	VAL	6.7
1	B	325	GLN	6.3
1	D	15	GLU	5.6
1	C	110	ILE	5.4
1	C	4	VAL	5.4
1	C	18	VAL	5.3
1	D	13	TRP	5.1
1	C	22	ILE	5.1
1	D	323	ILE	5.0
1	C	47	ARG	5.0
1	A	82	GLN	5.0
1	A	251	ILE	5.0
1	C	295	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	321	PRO	4.9
1	C	126	LEU	4.6
1	A	111	ASN	4.4
1	C	50	ALA	4.4
1	C	323	ILE	4.3
1	C	105	ALA	4.2
1	B	295	ILE	4.1
1	A	83	SER	4.1
1	A	146	ARG	4.1
1	A	373	SER	4.1
1	C	127	LEU	4.0
1	D	162	SER	4.0
1	D	320	ILE	4.0
1	D	163	ASN	3.9
1	D	14	GLY	3.9
1	D	295	ILE	3.8
1	B	294	ASP	3.8
1	C	80	VAL	3.8
1	A	15	GLU	3.8
1	A	267	TRP	3.7
1	A	295	ILE	3.7
1	A	252	ASP	3.7
1	C	261	PRO	3.7
1	C	294	ASP	3.6
1	C	81	PHE	3.6
1	C	46	LEU	3.6
1	C	77	VAL	3.6
1	C	113	ARG	3.5
1	D	184	GLY	3.5
1	D	79	MET	3.5
1	C	120	VAL	3.5
1	D	181	LYS	3.5
1	D	324	ARG	3.5
1	A	110	ILE	3.4
1	C	52	LEU	3.4
1	B	236	SER	3.3
1	A	372	ALA	3.3
1	C	106	LYS	3.3
1	C	51	GLY	3.2
1	C	9	VAL	3.2
1	D	321	PRO	3.2
1	D	16	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	3.1
1	C	296	ALA	3.1
1	A	16	VAL	3.1
1	A	342	THR	3.1
1	B	260	MET	3.0
1	A	64	GLU	3.0
1	D	164	LEU	3.0
1	C	117	VAL	3.0
1	C	129	ARG	3.0
1	C	21	ASP	2.9
1	C	10	THR	2.9
1	A	250	ALA	2.9
1	A	341	ALA	2.9
1	C	151	GLU	2.9
1	C	100	LEU	2.9
1	C	183	LEU	2.9
1	C	260	MET	2.9
1	D	263	ARG	2.9
1	C	123	LEU	2.9
1	A	235	GLY	2.8
1	C	114	VAL	2.8
1	D	47	ARG	2.8
1	D	161	LEU	2.8
1	A	236	SER	2.8
1	A	81	PHE	2.8
1	C	82	GLN	2.8
1	D	372	ALA	2.7
1	C	234	ILE	2.7
1	A	144	ILE	2.7
1	C	19	SER	2.7
1	C	2	ALA	2.7
1	A	274	ASP	2.6
1	A	273	ARG	2.6
1	C	322	SER	2.6
1	A	143	ALA	2.6
1	C	182	ARG	2.6
1	C	262	ASN	2.6
1	B	32	VAL	2.5
1	C	26	ILE	2.5
1	D	21	ASP	2.5
1	C	116	GLN	2.5
1	C	101	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	83	SER	2.5
1	A	155	PHE	2.4
1	A	2	ALA	2.4
1	C	150	ALA	2.4
1	A	195	VAL	2.4
1	C	92	VAL	2.4
1	C	108	GLU	2.4
1	C	124	ALA	2.4
1	A	109	VAL	2.4
1	D	294	ASP	2.3
1	C	5	GLN	2.3
1	C	125	HIS	2.3
1	A	118	ALA	2.3
1	D	236	SER	2.3
1	C	148	LEU	2.2
1	C	99	GLY	2.2
1	C	128	ASP	2.2
1	B	102	LEU	2.2
1	D	342	THR	2.2
1	D	168	LEU	2.2
1	D	187	MET	2.2
1	B	133	ALA	2.2
1	A	63	GLY	2.2
1	A	275	VAL	2.2
1	B	33	VAL	2.2
1	C	112	GLN	2.2
1	A	197	ALA	2.2
1	B	234	ILE	2.2
1	C	144	ILE	2.2
1	A	108	GLU	2.2
1	C	8	ASN	2.1
1	C	170	VAL	2.1
1	B	157	LEU	2.1
1	B	326	ASN	2.1
1	B	205	VAL	2.1
1	C	85	ALA	2.1
1	C	204	ILE	2.1
1	D	251	ILE	2.1
1	C	136	GLY	2.1
1	D	151	GLU	2.1
1	B	310	LEU	2.1
1	C	291	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	199	THR	2.1
1	D	233	PHE	2.1
1	B	188	ILE	2.1
1	C	20	LYS	2.1
1	B	318	ILE	2.0
1	D	322	SER	2.0
1	C	149	VAL	2.0
1	A	261	PRO	2.0
1	D	174	ILE	2.0
1	A	194	GLN	2.0
1	D	172	MET	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 carbohydrates in this entry.

6.4 Ligands [i](#)

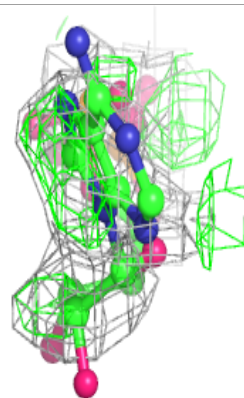
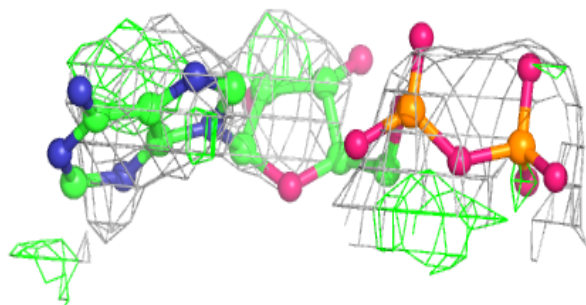
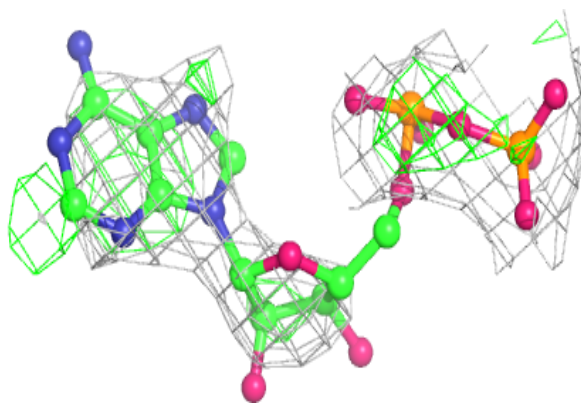
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	C	503	1/1	0.39	0.14	109,109,109,109	0
3	ADP	C	403	27/27	0.80	0.32	85,110,116,117	27
2	MG	B	502	1/1	0.81	0.18	48,48,48,48	0
2	MG	D	504	1/1	0.87	0.06	76,76,76,76	0
3	ADP	B	402	27/27	0.93	0.18	40,56,73,81	0
3	ADP	A	401	27/27	0.94	0.16	38,74,84,94	0
3	ADP	D	404	27/27	0.95	0.16	54,92,100,106	0
2	MG	A	501	1/1	0.96	0.05	55,55,55,55	0

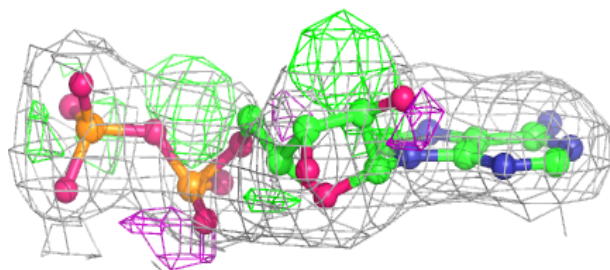
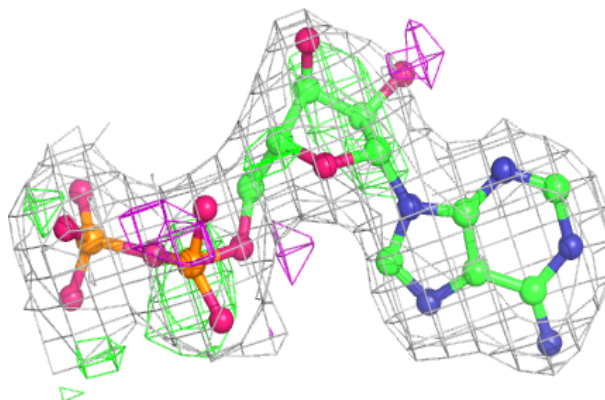
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

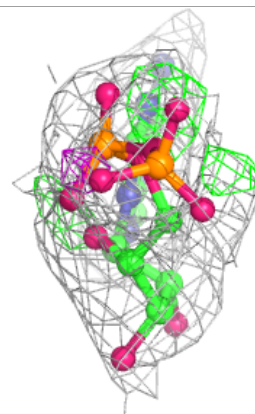
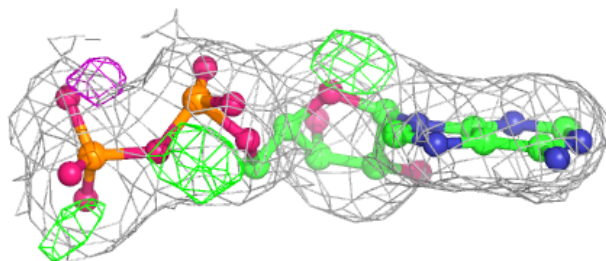
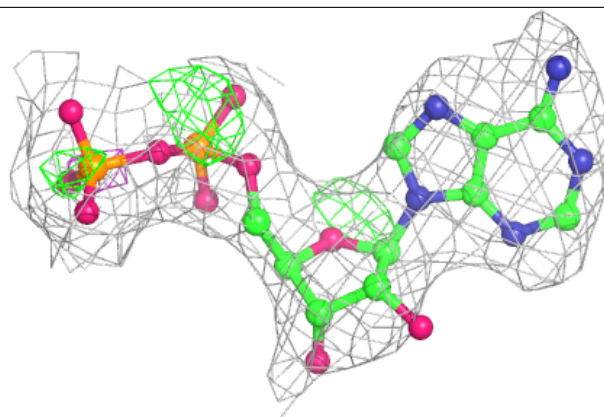
**Electron density around ADP B 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

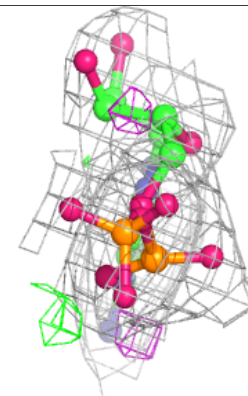
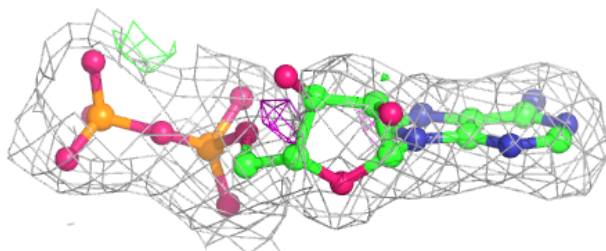
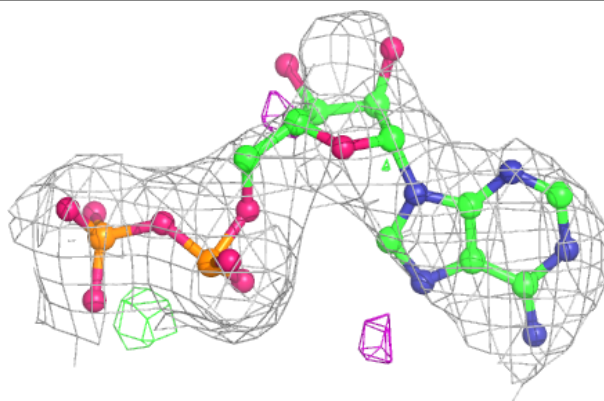


Electron density around ADP A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP D 404:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.