



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:34 am BST

PDB ID : 2AWO  
Title : Crystal structure of the ADP-Mg-bound E. Coli MALK (Crystallized with ADP-Mg)  
Authors : Lu, G.; Westbrook, J.M.; Davidson, A.L.; Chen, J.  
Deposited on : 2005-09-01  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

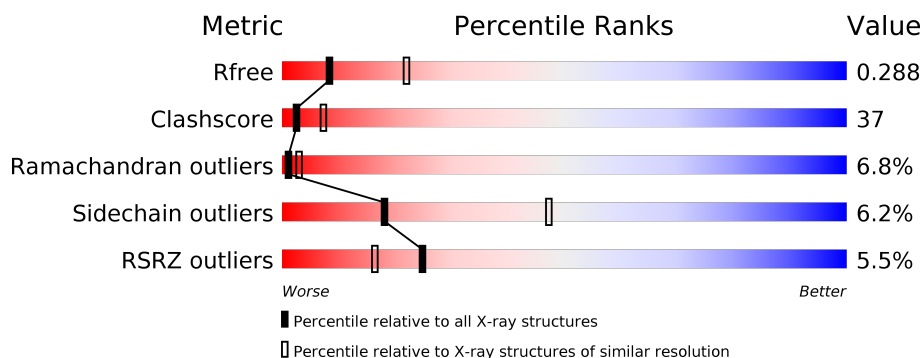
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	381	<div> <div>7%</div> <div>45%</div> <div>44%</div> <div>8%</div> <div>••</div> </div>
1	B	381	<div> <div>3%</div> <div>50%</div> <div>39%</div> <div>8%</div> <div>••</div> </div>
1	C	381	<div> <div>6%</div> <div>44%</div> <div>43%</div> <div>8%</div> <div>• 5%</div> </div>
1	D	381	<div> <div>4%</div> <div>43%</div> <div>29%</div> <div>6%</div> <div>• 22%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11005 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	372	Total	C	N	O	S	0	0	0
			2882	1822	516	531	13			
1	B	374	Total	C	N	O	S	0	0	0
			2893	1828	518	534	13			
1	C	363	Total	C	N	O	S	0	0	0
			2800	1765	504	518	13			
1	D	299	Total	C	N	O	S	0	0	0
			2318	1465	409	432	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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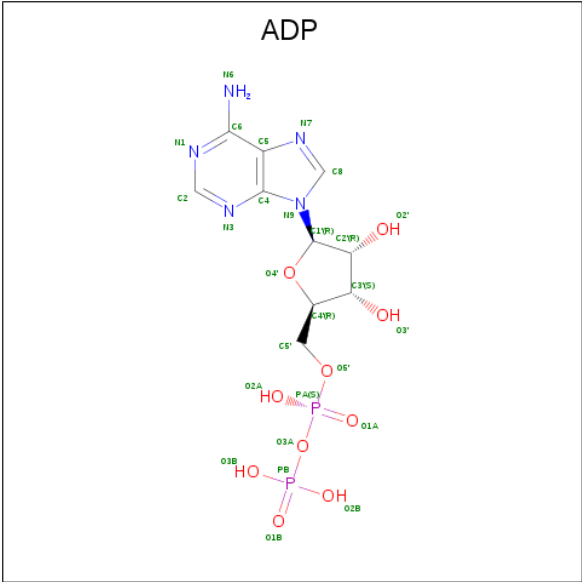
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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	SER	-	CLONING ARTIFACT	UNP P68187
C	374	ALA	-	CLONING ARTIFACT	UNP P68187
C	375	SER	-	CLONING ARTIFACT	UNP P68187
C	376	HIS	-	CLONING ARTIFACT	UNP P68187
C	377	HIS	-	CLONING ARTIFACT	UNP P68187
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: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

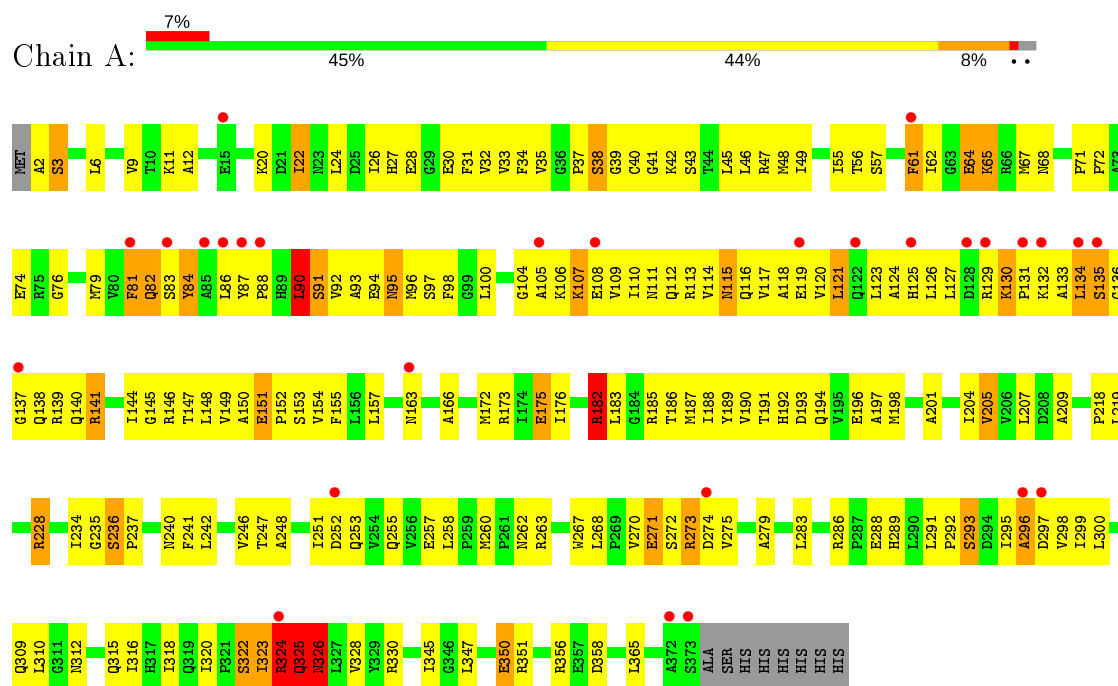


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

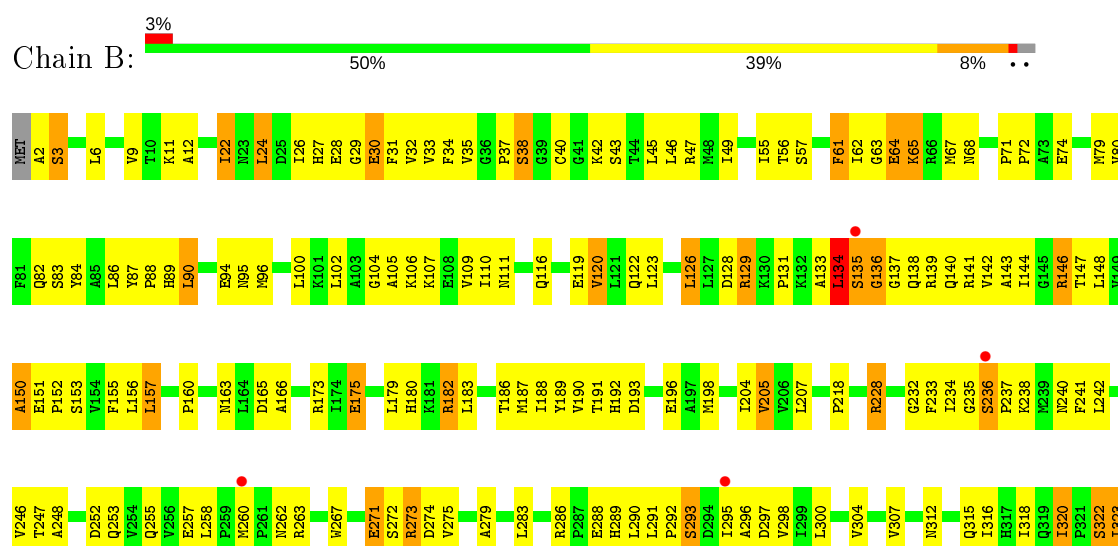
### 3 Residue-property plots

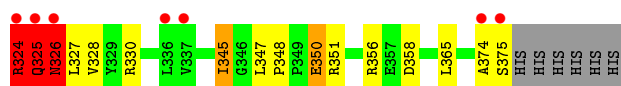
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

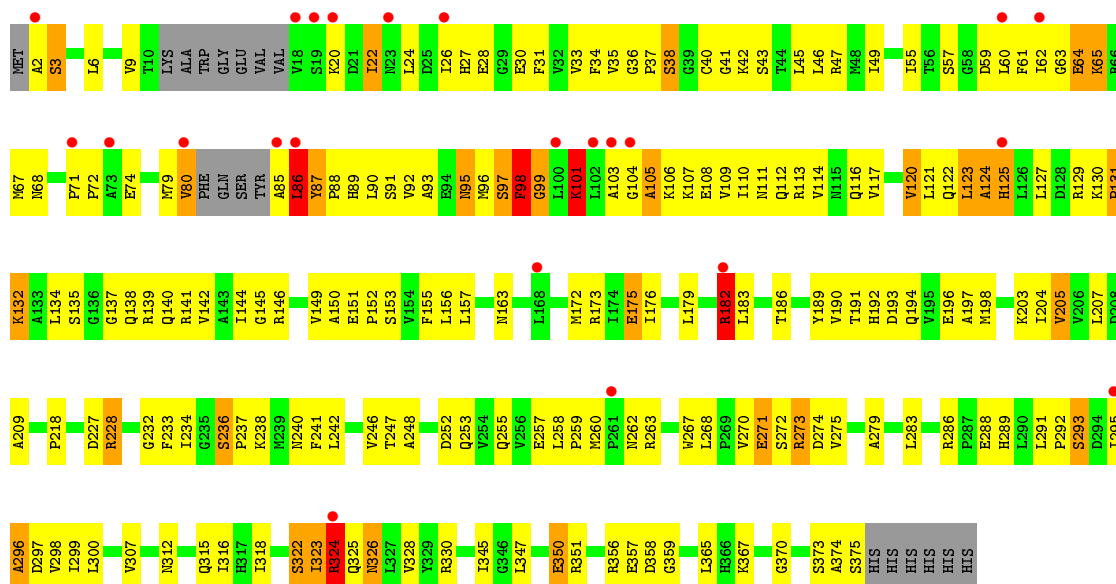
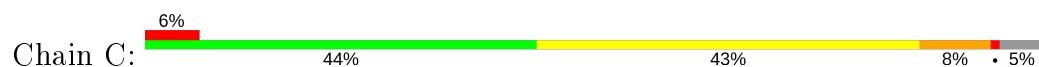


- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK

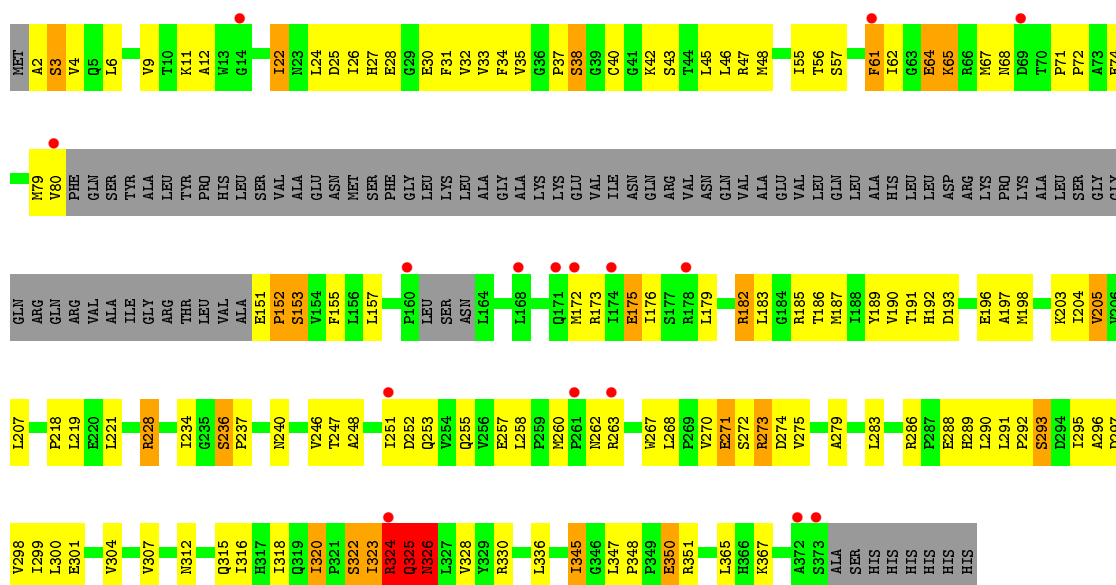
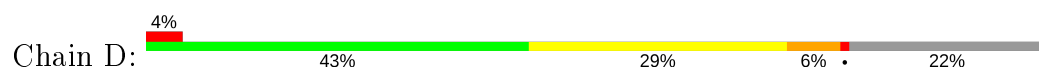




- Molecule 1: Maltose/maltodextrin import ATP-binding protein malK



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.21Å 101.97Å 131.50Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	29.93 – 2.80 29.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.5 (29.93-2.80) 88.8 (29.93-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.277 0.246 , 0.288	Depositor DCC
$R_{free}$ test set	2024 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 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	0.58	3/2932 (0.1%)	1.02	11/3976 (0.3%)
1	B	0.74	2/2943 (0.1%)	0.91	13/3991 (0.3%)
1	C	0.91	4/2844 (0.1%)	0.88	11/3853 (0.3%)
1	D	0.66	1/2358 (0.0%)	1.08	10/3199 (0.3%)
All	All	0.74	10/11077 (0.1%)	0.97	45/15019 (0.3%)

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	2
1	C	0	1
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	C	86	LEU	N-CA	33.60	2.13	1.46
1	B	326	ASN	N-CA	30.26	2.06	1.46
1	C	87	TYR	N-CA	26.08	1.98	1.46
1	D	326	ASN	N-CA	25.10	1.96	1.46
1	A	326	ASN	N-CA	21.33	1.89	1.46
1	B	135	SER	N-CA	8.65	1.63	1.46
1	C	125	HIS	N-CA	6.41	1.59	1.46
1	A	107	LYS	N-CA	6.35	1.59	1.46
1	A	83	SER	N-CA	6.11	1.58	1.46
1	C	59	ASP	C-N	-5.83	1.20	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ARG	NE-CZ-NH1	-26.03	107.29	120.30
1	D	324	ARG	NE-CZ-NH1	-25.87	107.36	120.30
1	D	324	ARG	NE-CZ-NH2	25.27	132.93	120.30
1	A	182	ARG	NE-CZ-NH2	24.97	132.79	120.30
1	B	326	ASN	N-CA-CB	-21.18	72.48	110.60
1	D	326	ASN	N-CA-CB	-19.37	75.73	110.60
1	A	326	ASN	N-CA-CB	-17.70	78.73	110.60
1	C	125	HIS	N-CA-CB	16.30	139.93	110.60
1	C	86	LEU	C-N-CA	-15.02	84.16	121.70
1	A	182	ARG	CD-NE-CZ	14.16	143.43	123.60
1	D	324	ARG	CD-NE-CZ	14.04	143.25	123.60
1	B	135	SER	N-CA-CB	12.78	129.67	110.50
1	C	86	LEU	N-CA-C	-11.22	80.71	111.00
1	B	325	GLN	C-N-CA	-11.01	94.17	121.70
1	D	325	GLN	C-N-CA	-10.19	96.23	121.70
1	C	125	HIS	N-CA-C	-9.94	84.15	111.00
1	C	87	TYR	N-CA-CB	-9.87	92.83	110.60
1	D	326	ASN	N-CA-C	9.83	137.54	111.00
1	A	326	ASN	N-CA-C	9.65	137.06	111.00
1	C	182	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	326	ASN	N-CA-C	9.48	136.59	111.00
1	D	182	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	325	GLN	C-N-CA	-9.32	98.41	121.70
1	B	182	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	D	182	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	C	182	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	B	182	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	324	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	B	324	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	324	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	324	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	B	134	LEU	CB-CA-C	-7.56	95.83	110.20
1	B	135	SER	N-CA-C	-7.35	91.16	111.00
1	A	107	LYS	N-CA-C	-7.32	91.24	111.00
1	A	107	LYS	N-CA-CB	6.78	122.80	110.60
1	C	87	TYR	N-CA-C	6.41	128.30	111.00
1	C	124	ALA	C-N-CA	-5.82	107.16	121.70
1	B	182	ARG	CD-NE-CZ	5.51	131.32	123.60
1	D	182	ARG	CD-NE-CZ	5.48	131.27	123.60
1	C	182	ARG	CD-NE-CZ	5.47	131.25	123.60
1	C	80	VAL	N-CA-C	-5.28	96.76	111.00
1	A	61	PHE	N-CA-CB	-5.05	101.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	PHE	N-CA-CB	-5.03	101.54	110.60
1	B	150	ALA	N-CA-C	-5.02	97.45	111.00
1	D	61	PHE	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	GLN	Peptide
1	B	134	LEU	Peptide
1	B	325	GLN	Peptide
1	C	85	ALA	Peptide
1	D	325	GLN	Peptide

## 5.2 Too-close contacts

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	2882	0	2946	241	2
1	B	2893	0	2956	208	3
1	C	2800	0	2868	237	1
1	D	2318	0	2350	152	2
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	2	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
All	All	11005	0	11168	819	4

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 37.

All (819) 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:326:ASN:CA	1:A:326:ASN:N	1.89	1.36
1:D:326:ASN:N	1:D:326:ASN:CA	1.96	1.28
1:C:87:TYR:CA	1:C:87:TYR:N	1.98	1.26
1:B:326:ASN:N	1:B:326:ASN:CA	2.06	1.18
1:B:326:ASN:N	1:B:326:ASN:HB2	1.62	1.13
1:B:323:ILE:CG2	1:B:325:GLN:HE21	1.61	1.13
1:B:26:ILE:HD12	1:B:32:VAL:HG21	1.27	1.13
1:A:120:VAL:HG12	1:A:182:ARG:HH11	0.99	1.12
1:C:86:LEU:CA	1:C:86:LEU:N	2.13	1.11
1:D:26:ILE:HD12	1:D:32:VAL:HG21	1.26	1.11
1:C:120:VAL:HG13	1:C:182:ARG:NH2	1.66	1.09
1:B:286:ARG:HB2	1:B:289:HIS:HD2	1.18	1.09
1:B:326:ASN:CB	1:B:326:ASN:N	2.17	1.08
1:D:326:ASN:N	1:D:326:ASN:CB	2.17	1.07
1:D:326:ASN:N	1:D:326:ASN:HB2	1.69	1.07
1:A:120:VAL:HG12	1:A:182:ARG:NH1	1.69	1.07
1:A:326:ASN:N	1:A:326:ASN:CB	2.19	1.06
1:B:260:MET:HA	1:B:322:SER:HB3	1.38	1.04
1:D:286:ARG:HB2	1:D:289:HIS:HD2	1.23	1.03
1:B:135:SER:O	1:B:137:GLY:N	1.89	1.03
1:A:260:MET:HA	1:A:322:SER:HB3	1.38	1.03
1:A:286:ARG:HB2	1:A:289:HIS:HD2	1.18	1.03
1:C:260:MET:HA	1:C:322:SER:HB3	1.39	1.03
1:D:260:MET:HA	1:D:322:SER:HB3	1.39	1.03
1:C:86:LEU:C	1:C:87:TYR:CA	2.27	1.02
1:C:120:VAL:HG13	1:C:182:ARG:HH22	1.19	1.02
1:C:86:LEU:O	1:C:87:TYR:CA	2.08	1.02
1:C:286:ARG:HB2	1:C:289:HIS:HD2	1.19	1.01
1:B:323:ILE:HD12	1:B:324:ARG:NH1	1.78	0.99
1:B:323:ILE:HG22	1:B:325:GLN:HE21	1.25	0.97
1:A:240:ASN:HD21	1:A:328:VAL:H	1.12	0.96
1:A:326:ASN:N	1:A:326:ASN:HB2	1.76	0.96
1:A:236:SER:HB2	1:A:237:PRO:HD3	1.47	0.95
1:A:120:VAL:HA	1:C:324:ARG:HH21	1.27	0.95
1:B:236:SER:HB2	1:B:237:PRO:HD3	1.47	0.95
1:C:236:SER:HB2	1:C:237:PRO:HD3	1.49	0.94
1:D:240:ASN:HD21	1:D:328:VAL:H	1.14	0.94
1:D:236:SER:HB2	1:D:237:PRO:HD3	1.47	0.93
1:B:240:ASN:HD21	1:B:328:VAL:H	1.15	0.92
1:A:286:ARG:HB2	1:A:289:HIS:CD2	2.04	0.92
1:C:240:ASN:HD21	1:C:328:VAL:H	1.13	0.91
1:D:191:THR:HG22	1:D:193:ASP:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ARG:HB2	1:C:289:HIS:CD2	2.05	0.91
1:B:80:VAL:HG21	1:B:144:ILE:HD13	1.52	0.90
1:B:286:ARG:HB2	1:B:289:HIS:CD2	2.05	0.90
1:A:90:LEU:HB3	1:A:131:PRO:HD2	1.53	0.90
1:C:259:PRO:HB2	1:C:323:ILE:HD12	1.53	0.89
1:D:48:MET:HB3	1:D:55:ILE:HD11	1.55	0.89
1:A:120:VAL:HG13	1:C:324:ARG:NH2	1.87	0.89
1:C:191:THR:HG22	1:C:193:ASP:H	1.38	0.88
1:D:286:ARG:HB2	1:D:289:HIS:CD2	2.09	0.87
1:C:20:LYS:HE2	1:C:209:ALA:O	1.73	0.87
1:D:260:MET:HE1	1:D:300:LEU:HD22	1.57	0.87
1:B:323:ILE:HD12	1:B:324:ARG:HH12	1.39	0.86
1:B:191:THR:HG22	1:B:193:ASP:H	1.40	0.86
1:A:138:GLN:HA	1:A:141:ARG:HE	1.39	0.86
1:D:152:PRO:HG2	1:D:153:SER:H	1.39	0.85
1:D:2:ALA:HB2	1:D:153:SER:HB2	1.58	0.85
1:A:197:ALA:HB1	1:A:204:ILE:HD12	1.59	0.85
1:C:197:ALA:HB1	1:C:204:ILE:HD12	1.60	0.84
1:D:48:MET:HB3	1:D:55:ILE:CD1	2.07	0.84
1:A:191:THR:HG22	1:A:193:ASP:H	1.41	0.84
1:C:236:SER:CB	1:C:237:PRO:HD3	2.08	0.84
1:A:325:GLN:C	1:A:326:ASN:CA	2.46	0.84
1:A:236:SER:CB	1:A:237:PRO:HD3	2.07	0.83
1:B:236:SER:CB	1:B:237:PRO:HD3	2.07	0.83
1:D:151:GLU:HB2	1:D:185:ARG:NH2	1.94	0.83
1:D:236:SER:CB	1:D:237:PRO:HD3	2.09	0.82
1:D:301:GLU:O	1:D:320:ILE:HD13	1.79	0.82
1:D:2:ALA:N	1:D:186:THR:HG1	1.78	0.81
1:D:260:MET:HA	1:D:322:SER:CB	2.10	0.81
1:A:260:MET:HA	1:A:322:SER:CB	2.10	0.81
1:B:134:LEU:C	1:B:136:GLY:H	1.71	0.81
1:B:323:ILE:CG2	1:B:325:GLN:NE2	2.43	0.81
1:D:325:GLN:C	1:D:326:ASN:CA	2.49	0.81
1:C:324:ARG:HD3	1:C:324:ARG:H	1.46	0.81
1:A:138:GLN:HG2	1:A:141:ARG:HH21	1.43	0.81
1:B:260:MET:HA	1:B:322:SER:CB	2.11	0.81
1:C:260:MET:HA	1:C:322:SER:CB	2.10	0.80
1:C:2:ALA:HB2	1:C:153:SER:HB3	1.63	0.80
1:A:292:PRO:O	1:A:293:SER:HB3	1.81	0.79
1:D:292:PRO:O	1:D:293:SER:HB3	1.83	0.79
1:A:2:ALA:CB	1:A:153:SER:HB2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:PRO:O	1:C:293:SER:HB3	1.83	0.78
1:B:292:PRO:O	1:B:293:SER:HB3	1.83	0.78
1:A:155:PHE:HB3	1:A:187:MET:HG2	1.65	0.78
1:B:119:GLU:O	1:B:120:VAL:HG23	1.84	0.78
1:B:374:ALA:O	1:B:375:SER:HB2	1.84	0.78
1:D:4:VAL:HG22	1:D:62:ILE:HD12	1.64	0.78
1:B:134:LEU:O	1:B:136:GLY:N	2.17	0.77
1:C:87:TYR:CG	1:C:87:TYR:N	2.53	0.77
1:B:87:TYR:H	1:B:95:ASN:HD21	1.28	0.77
1:D:42:LYS:HD2	1:D:190:VAL:HG13	1.66	0.77
1:D:33:VAL:HG22	1:D:189:TYR:HB3	1.68	0.76
1:A:33:VAL:HB	1:A:204:ILE:HD13	1.68	0.76
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.50	0.76
1:B:325:GLN:C	1:B:326:ASN:CA	2.54	0.75
1:D:6:LEU:HD23	1:D:22:ILE:HD11	1.67	0.75
1:C:33:VAL:HB	1:C:204:ILE:HD13	1.67	0.75
1:C:97:SER:HB3	1:C:110:ILE:HD11	1.67	0.75
1:A:6:LEU:HD23	1:A:22:ILE:HD11	1.69	0.75
1:A:236:SER:HB2	1:A:237:PRO:CD	2.17	0.75
1:B:236:SER:HB2	1:B:237:PRO:CD	2.15	0.75
1:A:2:ALA:N	1:A:186:THR:HG1	1.84	0.75
1:D:80:VAL:HG23	1:D:157:LEU:HG	1.68	0.75
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.52	0.75
1:D:236:SER:HB2	1:D:237:PRO:CD	2.16	0.74
1:A:61:PHE:CZ	1:A:64:GLU:HA	2.22	0.74
1:C:34:PHE:HB2	1:C:190:VAL:HG22	1.69	0.74
1:B:80:VAL:HG21	1:B:144:ILE:CD1	2.16	0.74
1:D:61:PHE:CZ	1:D:64:GLU:HA	2.22	0.74
1:C:157:LEU:HD12	1:C:157:LEU:N	2.03	0.74
1:C:6:LEU:HD23	1:C:22:ILE:HD11	1.70	0.74
1:C:86:LEU:C	1:C:86:LEU:N	2.41	0.74
1:C:87:TYR:N	1:C:87:TYR:CD1	2.54	0.74
1:A:116:GLN:O	1:A:120:VAL:HB	1.87	0.73
1:A:140:GLN:O	1:A:144:ILE:HG12	1.89	0.73
1:A:92:VAL:HG23	1:A:129:ARG:O	1.86	0.73
1:A:42:LYS:HD2	1:A:190:VAL:HG13	1.71	0.73
1:C:236:SER:HB2	1:C:237:PRO:CD	2.17	0.73
1:B:148:LEU:HD13	1:B:179:LEU:CD1	2.18	0.73
1:C:9:VAL:HB	1:C:22:ILE:HD13	1.71	0.72
1:A:33:VAL:HG22	1:A:189:TYR:HB3	1.71	0.72
1:D:4:VAL:HG22	1:D:62:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD12	1:A:67:MET:HG3	1.70	0.72
1:B:253:GLN:HG2	1:B:267:TRP:CE3	2.25	0.72
1:C:120:VAL:CG1	1:C:182:ARG:HH22	2.02	0.72
1:C:61:PHE:CZ	1:C:64:GLU:HA	2.24	0.72
1:A:191:THR:HG22	1:A:192:HIS:H	1.55	0.71
1:B:61:PHE:CZ	1:B:64:GLU:HA	2.24	0.71
1:C:253:GLN:HG2	1:C:267:TRP:CE3	2.25	0.71
1:D:9:VAL:HB	1:D:22:ILE:HD13	1.72	0.71
1:C:120:VAL:HG22	1:C:182:ARG:HH12	1.56	0.71
1:A:119:GLU:N	1:A:124:ALA:HB2	2.06	0.71
1:C:33:VAL:HG22	1:C:189:TYR:HB3	1.72	0.71
1:A:120:VAL:O	1:A:121:LEU:HB2	1.91	0.71
1:C:228:ARG:HH11	1:C:228:ARG:HG3	1.55	0.71
1:D:228:ARG:HH11	1:D:228:ARG:HG3	1.54	0.71
1:D:191:THR:HG22	1:D:192:HIS:H	1.56	0.70
1:A:253:GLN:HG2	1:A:267:TRP:CE3	2.26	0.70
1:B:26:ILE:HG21	1:B:188:ILE:HD11	1.71	0.70
1:C:191:THR:HG22	1:C:192:HIS:H	1.56	0.70
1:C:86:LEU:O	1:C:87:TYR:HA	1.91	0.70
1:A:34:PHE:HB2	1:A:190:VAL:HG22	1.74	0.70
1:A:9:VAL:HB	1:A:22:ILE:HD13	1.72	0.70
1:D:323:ILE:CG2	1:D:325:GLN:HE21	2.04	0.70
1:D:22:ILE:HD12	1:D:45:LEU:HD21	1.74	0.69
1:B:62:ILE:HD12	1:B:67:MET:HG3	1.73	0.69
1:D:253:GLN:HG2	1:D:267:TRP:CE3	2.27	0.69
1:B:191:THR:HG22	1:B:192:HIS:H	1.56	0.69
1:A:22:ILE:HD12	1:A:45:LEU:HD21	1.74	0.69
1:A:323:ILE:HG22	1:A:325:GLN:HG2	1.75	0.69
1:B:6:LEU:HD22	1:B:22:ILE:HD11	1.75	0.69
1:C:87:TYR:N	1:C:87:TYR:CB	2.56	0.69
1:B:2:ALA:N	1:B:186:THR:HG1	1.91	0.69
1:C:6:LEU:HD21	1:C:49:ILE:HD11	1.74	0.69
1:C:323:ILE:HG22	1:C:325:GLN:HG2	1.75	0.68
1:A:2:ALA:HB3	1:A:153:SER:HB2	1.74	0.68
1:C:22:ILE:HD12	1:C:45:LEU:HD21	1.74	0.68
1:A:260:MET:C	1:A:262:ASN:H	1.97	0.68
1:A:96:MET:O	1:A:149:VAL:HG21	1.94	0.68
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.08	0.68
1:A:125:HIS:O	1:A:126:LEU:HD23	1.95	0.67
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.09	0.67
1:C:101:LYS:HZ3	1:C:101:LYS:HB2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ALA:H	1:B:56:THR:HG21	1.60	0.67
1:C:45:LEU:HD12	1:C:207:LEU:HD11	1.76	0.67
1:A:12:ALA:H	1:A:56:THR:HG21	1.60	0.67
1:D:12:ALA:H	1:D:56:THR:HG21	1.60	0.66
1:A:120:VAL:CG1	1:A:182:ARG:HH11	1.93	0.66
1:A:240:ASN:ND2	1:A:328:VAL:H	1.91	0.66
1:A:6:LEU:HD21	1:A:49:ILE:HD11	1.76	0.66
1:C:113:ARG:HB3	1:C:149:VAL:HG13	1.77	0.66
1:C:113:ARG:O	1:C:117:VAL:HG22	1.95	0.66
1:C:9:VAL:HB	1:C:22:ILE:CD1	2.26	0.66
1:A:324:ARG:HD3	1:A:324:ARG:H	1.60	0.66
1:A:9:VAL:HB	1:A:22:ILE:CD1	2.26	0.66
1:C:228:ARG:HG3	1:C:228:ARG:NH1	2.11	0.66
1:A:100:LEU:HD13	1:A:110:ILE:HA	1.78	0.66
1:B:183:LEU:O	1:B:183:LEU:HD12	1.96	0.66
1:B:323:ILE:HG22	1:B:325:GLN:NE2	2.04	0.66
1:B:43:SER:O	1:B:47:ARG:HG3	1.96	0.66
1:C:260:MET:C	1:C:262:ASN:H	1.98	0.66
1:D:323:ILE:HG22	1:D:325:GLN:HE21	1.61	0.66
1:B:324:ARG:HD3	1:B:324:ARG:H	1.61	0.65
1:C:120:VAL:HG22	1:C:182:ARG:NH1	2.11	0.65
1:C:240:ASN:ND2	1:C:328:VAL:H	1.92	0.65
1:C:155:PHE:C	1:C:156:LEU:HD12	2.17	0.65
1:A:87:TYR:O	1:A:90:LEU:HD13	1.96	0.65
1:D:345:ILE:N	1:D:345:ILE:HD13	2.11	0.65
1:A:112:GLN:O	1:A:116:GLN:HB2	1.97	0.65
1:B:307:VAL:HG13	1:B:316:ILE:CD1	2.26	0.65
1:D:9:VAL:HB	1:D:22:ILE:CD1	2.27	0.65
1:B:260:MET:C	1:B:262:ASN:H	1.97	0.65
1:B:345:ILE:N	1:B:345:ILE:HD13	2.12	0.65
1:B:6:LEU:HD21	1:B:49:ILE:HD11	1.77	0.65
1:C:2:ALA:CB	1:C:153:SER:HB3	2.26	0.65
1:D:251:ILE:H	1:D:251:ILE:HD12	1.61	0.65
1:A:292:PRO:O	1:A:293:SER:CB	2.45	0.65
1:D:183:LEU:HD12	1:D:183:LEU:O	1.95	0.65
1:A:251:ILE:H	1:A:251:ILE:HD12	1.61	0.65
1:D:260:MET:C	1:D:262:ASN:H	1.97	0.65
1:A:111:ASN:O	1:A:115:ASN:HB2	1.97	0.64
1:B:128:ASP:O	1:B:129:ARG:HB2	1.96	0.64
1:C:43:SER:O	1:C:47:ARG:HG3	1.98	0.64
1:D:48:MET:SD	1:D:55:ILE:HD13	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:O	1:B:272:SER:HB3	1.96	0.64
1:C:2:ALA:HA	1:C:28:GLU:OE1	1.98	0.64
1:C:307:VAL:HG13	1:C:316:ILE:CD1	2.28	0.64
1:A:183:LEU:O	1:A:183:LEU:HD12	1.97	0.64
1:C:137:GLY:HA2	1:C:172:MET:CE	2.27	0.64
1:C:271:GLU:O	1:C:272:SER:HB3	1.97	0.64
1:C:62:ILE:HD12	1:C:67:MET:HG3	1.77	0.64
1:C:98:PHE:O	1:C:99:GLY:O	2.16	0.64
1:D:43:SER:O	1:D:47:ARG:HG3	1.97	0.64
1:D:2:ALA:HA	1:D:28:GLU:OE1	1.98	0.64
1:D:228:ARG:NH1	1:D:228:ARG:HG3	2.11	0.63
1:A:90:LEU:HD12	1:A:131:PRO:CG	2.28	0.63
1:C:183:LEU:HD12	1:C:183:LEU:O	1.98	0.63
1:A:271:GLU:O	1:A:272:SER:HB3	1.97	0.63
1:A:43:SER:O	1:A:47:ARG:HG3	1.99	0.63
1:C:146:ARG:HG2	1:C:146:ARG:HH11	1.64	0.63
1:B:147:THR:O	1:B:150:ALA:O	2.16	0.63
1:A:288:GLU:HG2	1:B:312:ASN:HB2	1.81	0.63
1:B:300:LEU:HB3	1:B:320:ILE:HD11	1.80	0.63
1:C:86:LEU:O	1:C:87:TYR:C	2.36	0.63
1:C:130:LYS:O	1:C:132:LYS:N	2.26	0.63
1:A:147:THR:O	1:A:150:ALA:HB3	1.98	0.63
1:A:88:PRO:O	1:A:90:LEU:HD22	1.99	0.62
1:A:120:VAL:HG13	1:C:324:ARG:HH22	1.63	0.62
1:A:2:ALA:HA	1:A:28:GLU:OE1	1.99	0.62
1:D:292:PRO:O	1:D:293:SER:CB	2.47	0.62
1:D:307:VAL:HG13	1:D:316:ILE:CD1	2.29	0.62
1:D:323:ILE:HG22	1:D:325:GLN:HG2	1.79	0.62
1:A:26:ILE:HG21	1:A:188:ILE:HD11	1.82	0.62
1:B:135:SER:C	1:B:137:GLY:H	1.95	0.62
1:A:138:GLN:HA	1:A:141:ARG:NE	2.13	0.61
1:A:300:LEU:HB2	1:A:345:ILE:HD11	1.82	0.61
1:D:271:GLU:O	1:D:272:SER:HB3	2.00	0.61
1:A:109:VAL:HG22	1:C:357:GLU:HG2	1.83	0.61
1:B:236:SER:CB	1:B:237:PRO:CD	2.77	0.61
1:D:273:ARG:O	1:D:275:VAL:HG12	1.99	0.61
1:A:240:ASN:HD21	1:A:328:VAL:N	1.93	0.61
1:A:118:ALA:HB1	1:A:124:ALA:HA	1.83	0.61
1:C:300:LEU:HB2	1:C:345:ILE:HD11	1.83	0.61
1:B:34:PHE:HB2	1:B:190:VAL:HG22	1.81	0.61
1:B:273:ARG:O	1:B:275:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASN:HB2	1:B:288:GLU:HG2	1.83	0.61
1:B:89:HIS:NE2	1:B:90:LEU:HD13	2.15	0.61
1:C:97:SER:CB	1:C:110:ILE:HD11	2.31	0.60
1:A:119:GLU:H	1:A:124:ALA:HB2	1.66	0.60
1:D:155:PHE:HE1	1:D:185:ARG:HD3	1.65	0.60
1:B:2:ALA:HA	1:B:28:GLU:OE1	2.02	0.60
1:C:108:GLU:HG3	1:C:109:VAL:N	2.16	0.60
1:C:42:LYS:HD2	1:C:190:VAL:HG13	1.82	0.60
1:C:40:CYS:SG	1:C:42:LYS:HG3	2.42	0.60
1:A:166:ALA:H	1:B:192:HIS:CD2	2.19	0.60
1:B:2:ALA:N	1:B:186:THR:HB	2.17	0.60
1:B:240:ASN:ND2	1:B:328:VAL:H	1.94	0.60
1:B:105:ALA:HB3	1:B:110:ILE:HD11	1.83	0.60
1:C:273:ARG:O	1:C:275:VAL:HG12	2.02	0.60
1:C:292:PRO:O	1:C:293:SER:CB	2.48	0.60
1:A:273:ARG:O	1:A:275:VAL:HG12	2.02	0.59
1:A:296:ALA:HA	1:A:299:ILE:HD11	1.84	0.59
1:C:108:GLU:HG3	1:C:109:VAL:H	1.66	0.59
1:A:300:LEU:HB2	1:A:345:ILE:CD1	2.32	0.59
1:C:123:LEU:O	1:C:124:ALA:HB3	2.02	0.59
1:D:191:THR:HG22	1:D:192:HIS:N	2.17	0.59
1:B:120:VAL:HG13	1:B:175:GLU:HG3	1.84	0.59
1:A:26:ILE:HD13	1:A:188:ILE:HD11	1.84	0.59
1:A:260:MET:C	1:A:262:ASN:N	2.56	0.59
1:C:312:ASN:HB2	1:D:288:GLU:HG2	1.83	0.59
1:B:138:GLN:O	1:B:142:VAL:HG23	2.02	0.59
1:B:260:MET:C	1:B:262:ASN:N	2.56	0.59
1:B:300:LEU:HB3	1:B:320:ILE:CD1	2.32	0.59
1:B:292:PRO:O	1:B:293:SER:CB	2.48	0.59
1:D:240:ASN:ND2	1:D:328:VAL:H	1.93	0.59
1:C:41:GLY:HA2	3:C:403:ADP:O2A	2.02	0.59
1:B:155:PHE:HB2	1:B:187:MET:HG2	1.84	0.58
1:B:6:LEU:CD2	1:B:22:ILE:HD11	2.33	0.58
1:C:291:LEU:HB3	1:C:292:PRO:HD2	1.84	0.58
1:C:300:LEU:HB2	1:C:345:ILE:CD1	2.32	0.58
1:B:260:MET:HE1	1:B:300:LEU:HD22	1.85	0.58
1:B:46:LEU:HB3	1:B:79:MET:HE3	1.85	0.58
1:B:80:VAL:HG11	1:B:144:ILE:HD13	1.85	0.58
1:A:109:VAL:HG13	1:C:357:GLU:CD	2.24	0.58
1:D:260:MET:C	1:D:262:ASN:N	2.56	0.58
1:A:98:PHE:HB2	1:A:146:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:HG22	1:B:192:HIS:N	2.17	0.58
1:D:316:ILE:CG2	1:D:318:ILE:HD11	2.33	0.58
1:A:119:GLU:HB2	1:A:124:ALA:CB	2.33	0.58
1:B:135:SER:C	1:B:137:GLY:N	2.52	0.58
1:B:144:ILE:HD11	1:B:160:PRO:CB	2.33	0.58
1:A:26:ILE:HD13	1:A:188:ILE:CD1	2.33	0.58
1:C:101:LYS:HB2	1:C:101:LYS:NZ	2.19	0.58
1:B:40:CYS:SG	1:B:42:LYS:HG3	2.44	0.58
1:B:273:ARG:O	1:B:275:VAL:N	2.37	0.58
1:C:273:ARG:O	1:C:275:VAL:N	2.37	0.58
1:D:40:CYS:SG	1:D:42:LYS:HG3	2.43	0.58
1:A:119:GLU:HB2	1:A:124:ALA:HB2	1.85	0.57
1:B:89:HIS:CD2	1:B:90:LEU:HD13	2.39	0.57
1:C:253:GLN:HG2	1:C:267:TRP:HE3	1.69	0.57
1:B:148:LEU:HD13	1:B:179:LEU:HD11	1.85	0.57
1:B:86:LEU:O	1:B:88:PRO:HD3	2.04	0.57
1:C:92:VAL:HG23	1:C:129:ARG:O	2.04	0.57
1:B:100:LEU:HD23	1:B:110:ILE:HD13	1.87	0.57
1:B:35:VAL:HG23	1:B:204:ILE:HG23	1.86	0.57
1:B:253:GLN:HG2	1:B:267:TRP:HE3	1.69	0.57
1:C:9:VAL:HG13	1:C:55:ILE:HG23	1.85	0.57
1:A:100:LEU:HB3	1:A:110:ILE:HG22	1.85	0.57
1:C:191:THR:HG22	1:C:192:HIS:N	2.18	0.57
1:C:296:ALA:HA	1:C:299:ILE:HD11	1.85	0.57
1:D:291:LEU:HB3	1:D:292:PRO:HD2	1.87	0.57
1:A:150:ALA:HB3	1:A:152:PRO:HD3	1.86	0.57
1:B:240:ASN:HD21	1:B:328:VAL:N	1.95	0.57
1:C:89:HIS:CD2	1:C:90:LEU:HD13	2.40	0.57
1:D:9:VAL:HG13	1:D:55:ILE:HG23	1.86	0.57
1:B:86:LEU:HD12	1:B:131:PRO:HB3	1.87	0.57
1:B:323:ILE:HG22	1:B:325:GLN:HG2	1.87	0.57
1:C:107:LYS:HA	1:C:110:ILE:CG2	2.35	0.57
1:A:22:ILE:HG12	1:A:22:ILE:O	2.05	0.56
1:A:46:LEU:HB3	1:A:79:MET:HE3	1.86	0.56
1:C:103:ALA:C	1:C:105:ALA:H	2.08	0.56
1:A:105:ALA:O	1:A:109:VAL:HB	2.05	0.56
1:A:98:PHE:CB	1:A:146:ARG:HD2	2.35	0.56
1:B:258:LEU:HB2	1:B:260:MET:HG2	1.87	0.56
1:A:110:ILE:O	1:A:114:VAL:HG23	2.05	0.56
1:B:80:VAL:CG2	1:B:144:ILE:HD13	2.29	0.56
1:C:2:ALA:N	1:C:186:THR:HG1	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LYS:HB3	1:C:190:VAL:CG1	2.35	0.56
1:B:100:LEU:CD2	1:B:110:ILE:HD13	2.35	0.56
1:B:315:GLN:HG2	1:B:330:ARG:HG2	1.87	0.56
1:B:90:LEU:HG	1:B:94:GLU:HB3	1.88	0.56
1:D:34:PHE:CD2	1:D:205:VAL:CG1	2.88	0.56
1:B:316:ILE:CG2	1:B:318:ILE:HD11	2.36	0.56
1:C:92:VAL:O	1:C:96:MET:HG3	2.06	0.56
1:A:120:VAL:HA	1:C:324:ARG:NH2	2.10	0.56
1:B:9:VAL:HG13	1:B:55:ILE:HG23	1.87	0.56
1:C:197:ALA:HB1	1:C:204:ILE:CD1	2.34	0.56
1:C:236:SER:CB	1:C:237:PRO:CD	2.78	0.56
1:D:324:ARG:CG	1:D:325:GLN:H	2.18	0.56
1:A:40:CYS:SG	1:A:42:LYS:HG3	2.46	0.56
1:C:140:GLN:HE21	1:C:144:ILE:HG12	1.69	0.56
1:C:260:MET:C	1:C:262:ASN:N	2.56	0.56
1:A:9:VAL:HG13	1:A:55:ILE:HG23	1.87	0.56
1:C:137:GLY:HA2	1:C:172:MET:HE1	1.87	0.56
1:A:273:ARG:O	1:A:275:VAL:N	2.39	0.56
1:C:2:ALA:HA	1:C:28:GLU:CD	2.26	0.56
1:C:46:LEU:HB3	1:C:79:MET:CE	2.36	0.55
1:D:2:ALA:HA	1:D:28:GLU:CD	2.26	0.55
1:C:258:LEU:HB2	1:C:260:MET:HG2	1.88	0.55
1:A:130:LYS:HE3	1:A:130:LYS:H	1.70	0.55
1:B:35:VAL:HG12	1:B:233:PHE:HE2	1.70	0.55
1:C:315:GLN:HG2	1:C:330:ARG:HG2	1.89	0.55
1:A:253:GLN:HG2	1:A:267:TRP:HE3	1.70	0.55
1:D:273:ARG:O	1:D:275:VAL:N	2.39	0.55
1:A:197:ALA:HB1	1:A:204:ILE:CD1	2.33	0.55
1:C:157:LEU:N	1:C:157:LEU:CD1	2.69	0.55
1:C:252:ASP:HB3	1:C:365:LEU:HD13	1.89	0.55
1:C:98:PHE:O	1:C:99:GLY:C	2.44	0.55
1:D:300:LEU:HB3	1:D:320:ILE:HD11	1.89	0.55
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.87	0.55
1:B:32:VAL:HB	1:B:188:ILE:HD13	1.88	0.55
1:C:260:MET:HE1	1:C:300:LEU:HD22	1.89	0.55
1:A:120:VAL:O	1:A:182:ARG:NH1	2.40	0.55
1:B:258:LEU:CB	1:B:260:MET:HG2	2.37	0.55
1:C:22:ILE:O	1:C:22:ILE:HG12	2.07	0.55
1:A:2:ALA:HA	1:A:28:GLU:CD	2.27	0.55
1:A:315:GLN:HG2	1:A:330:ARG:HG2	1.89	0.55
1:D:152:PRO:HG2	1:D:153:SER:N	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASN:HD21	1:D:328:VAL:N	1.95	0.54
1:D:300:LEU:HB3	1:D:320:ILE:CD1	2.36	0.54
1:A:148:LEU:HD13	1:A:183:LEU:HD21	1.89	0.54
1:B:131:PRO:O	1:B:139:ARG:HD3	2.07	0.54
1:B:260:MET:CE	1:B:300:LEU:HD22	2.38	0.54
1:D:236:SER:CB	1:D:237:PRO:CD	2.79	0.54
1:A:191:THR:HG22	1:A:192:HIS:N	2.19	0.54
1:C:110:ILE:O	1:C:114:VAL:HG12	2.08	0.54
1:C:121:LEU:O	1:C:122:GLN:HB2	2.07	0.54
1:C:112:GLN:O	1:C:116:GLN:HG3	2.07	0.54
1:C:36:GLY:O	1:C:192:HIS:HA	2.07	0.54
1:A:120:VAL:O	1:A:182:ARG:CZ	2.56	0.54
1:A:46:LEU:HB3	1:A:79:MET:CE	2.38	0.54
1:A:91:SER:HB3	1:A:94:GLU:HB2	1.89	0.54
1:B:35:VAL:HG12	1:B:233:PHE:CE2	2.43	0.54
1:B:252:ASP:HB3	1:B:365:LEU:HD13	1.89	0.54
1:C:134:LEU:HB2	1:C:139:ARG:NH1	2.23	0.54
1:A:258:LEU:HB2	1:A:260:MET:HG2	1.89	0.54
1:D:155:PHE:HB2	1:D:187:MET:HG2	1.88	0.54
1:B:148:LEU:HD22	1:B:179:LEU:HD11	1.89	0.54
1:C:258:LEU:CB	1:C:260:MET:HG2	2.38	0.54
1:A:252:ASP:HB3	1:A:365:LEU:HD13	1.89	0.54
1:A:291:LEU:HB3	1:A:292:PRO:HD2	1.89	0.53
1:A:90:LEU:O	1:A:91:SER:HB3	2.08	0.53
1:A:98:PHE:H	1:A:146:ARG:HD2	1.73	0.53
1:B:123:LEU:O	1:B:126:LEU:HD12	2.08	0.53
1:D:323:ILE:CG2	1:D:325:GLN:NE2	2.71	0.53
1:D:34:PHE:HD2	1:D:205:VAL:HG13	1.72	0.53
1:A:114:VAL:HG12	1:A:127:LEU:HD11	1.90	0.53
1:B:140:GLN:OE1	1:B:140:GLN:HA	2.08	0.53
1:D:252:ASP:HB3	1:D:365:LEU:HD13	1.89	0.53
1:B:2:ALA:HA	1:B:28:GLU:CD	2.29	0.53
1:C:86:LEU:CD1	1:C:131:PRO:HB3	2.38	0.53
1:C:33:VAL:HB	1:C:204:ILE:CD1	2.37	0.53
1:D:221:LEU:HB3	1:D:234:ILE:HD13	1.90	0.53
1:B:67:MET:O	1:B:68:ASN:C	2.46	0.53
1:C:106:LYS:C	1:C:108:GLU:H	2.10	0.53
1:D:283:LEU:C	1:D:283:LEU:HD23	2.29	0.53
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.23	0.53
1:D:315:GLN:HG2	1:D:330:ARG:HG2	1.90	0.53
1:B:304:VAL:HG22	1:B:318:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:PHE:CD2	1:D:205:VAL:HG11	2.44	0.53
1:B:46:LEU:HB3	1:B:79:MET:CE	2.39	0.53
1:C:26:ILE:HD12	1:C:26:ILE:N	2.24	0.53
1:C:324:ARG:N	1:C:324:ARG:HD3	2.19	0.53
1:D:48:MET:HB3	1:D:55:ILE:HD13	1.87	0.53
1:A:55:ILE:N	1:A:55:ILE:HD12	2.23	0.53
1:B:150:ALA:O	1:B:152:PRO:HD3	2.08	0.53
1:B:33:VAL:HG22	1:B:189:TYR:HB3	1.91	0.53
1:B:22:ILE:HD13	1:B:45:LEU:HD21	1.90	0.53
1:C:246:VAL:HG12	1:C:279:ALA:O	2.07	0.53
1:B:323:ILE:HG21	1:B:325:GLN:HE21	1.65	0.53
1:B:157:LEU:HD13	1:B:189:TYR:HD1	1.74	0.52
1:A:258:LEU:CB	1:A:260:MET:HG2	2.38	0.52
1:D:258:LEU:HB2	1:D:260:MET:HG2	1.90	0.52
1:B:198:MET:HE2	1:B:218:PRO:HB3	1.89	0.52
1:A:120:VAL:CG1	1:C:324:ARG:NH2	2.68	0.52
1:A:295:ILE:N	1:A:295:ILE:HD12	2.24	0.52
1:C:255:GLN:HB2	1:C:267:TRP:CD2	2.45	0.52
1:D:350:GLU:CD	1:D:350:GLU:H	2.12	0.52
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.75	0.52
1:A:316:ILE:HD12	1:A:316:ILE:N	2.24	0.52
1:A:292:PRO:HG2	1:A:295:ILE:HD13	1.90	0.52
1:A:55:ILE:H	1:A:55:ILE:HD12	1.74	0.52
1:D:251:ILE:N	1:D:251:ILE:HD12	2.25	0.52
1:D:258:LEU:CB	1:D:260:MET:HG2	2.39	0.52
1:D:67:MET:O	1:D:68:ASN:C	2.48	0.52
1:B:255:GLN:HB2	1:B:267:TRP:CD2	2.45	0.52
1:B:350:GLU:CD	1:B:350:GLU:H	2.13	0.52
1:A:113:ARG:NE	1:C:357:GLU:OE2	2.42	0.52
1:D:46:LEU:HB3	1:D:79:MET:CE	2.39	0.52
1:A:135:SER:O	1:A:137:GLY:N	2.43	0.52
1:C:260:MET:CE	1:C:300:LEU:HD22	2.39	0.52
1:D:301:GLU:N	1:D:320:ILE:HD11	2.25	0.52
1:A:96:MET:HE1	1:A:117:VAL:HG23	1.92	0.52
1:A:260:MET:CE	1:A:300:LEU:HD22	2.40	0.52
1:A:67:MET:O	1:A:68:ASN:C	2.48	0.52
1:A:65:LYS:HD3	1:A:65:LYS:N	2.25	0.51
1:D:304:VAL:HG22	1:D:318:ILE:CD1	2.40	0.51
1:A:33:VAL:HG12	1:A:35:VAL:HG22	1.92	0.51
1:C:33:VAL:HG12	1:C:35:VAL:HG22	1.92	0.51
1:D:299:ILE:N	1:D:299:ILE:HD12	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:HB2	1:A:267:TRP:CD2	2.46	0.51
1:A:251:ILE:HD12	1:A:251:ILE:N	2.25	0.51
1:B:191:THR:CG2	1:B:193:ASP:H	2.17	0.51
1:B:35:VAL:CG1	1:B:233:PHE:HE2	2.24	0.51
1:D:272:SER:O	1:D:273:ARG:O	2.29	0.51
1:A:154:VAL:HG13	1:A:186:THR:HG22	1.93	0.51
1:C:283:LEU:HD23	1:C:283:LEU:C	2.31	0.51
1:A:11:LYS:HD2	1:A:56:THR:HG23	1.93	0.51
1:B:307:VAL:HG13	1:B:316:ILE:HD13	1.91	0.51
1:C:33:VAL:HA	1:C:189:TYR:O	2.11	0.51
1:D:33:VAL:HG12	1:D:35:VAL:HG22	1.92	0.51
1:A:86:LEU:N	1:A:86:LEU:HD12	2.26	0.51
1:C:110:ILE:HG23	1:C:111:ASN:ND2	2.25	0.51
1:B:283:LEU:HD23	1:B:283:LEU:C	2.31	0.51
1:C:307:VAL:HG13	1:C:316:ILE:HD13	1.92	0.51
1:C:65:LYS:HD3	1:C:65:LYS:N	2.26	0.51
1:A:33:VAL:HB	1:A:204:ILE:CD1	2.39	0.51
1:A:288:GLU:HG3	1:A:330:ARG:HD3	1.93	0.50
1:C:350:GLU:H	1:C:350:GLU:CD	2.13	0.50
1:C:91:SER:O	1:C:95:ASN:HB2	2.11	0.50
1:D:34:PHE:HB2	1:D:190:VAL:HG22	1.91	0.50
1:D:22:ILE:HG12	1:D:22:ILE:O	2.09	0.50
1:D:307:VAL:HG13	1:D:316:ILE:HD13	1.93	0.50
1:B:233:PHE:HB3	1:B:234:ILE:HD12	1.93	0.50
1:D:34:PHE:HD2	1:D:205:VAL:CG1	2.24	0.50
1:A:123:LEU:HD11	1:A:141:ARG:HB3	1.93	0.50
1:A:151:GLU:N	1:A:152:PRO:CD	2.74	0.50
1:B:323:ILE:HG21	1:B:325:GLN:NE2	2.24	0.50
1:B:35:VAL:CG2	1:B:204:ILE:HG23	2.40	0.50
1:C:191:THR:CG2	1:C:193:ASP:H	2.17	0.50
1:C:325:GLN:O	1:C:326:ASN:O	2.29	0.50
1:D:316:ILE:HG22	1:D:318:ILE:HD11	1.93	0.50
1:A:151:GLU:HG3	1:A:185:ARG:NH2	2.27	0.50
1:D:11:LYS:HD2	1:D:56:THR:HG23	1.94	0.50
1:A:283:LEU:HD23	1:A:283:LEU:C	2.32	0.50
1:B:246:VAL:HG12	1:B:279:ALA:O	2.12	0.50
1:C:42:LYS:HB3	1:C:190:VAL:HG13	1.93	0.50
1:D:253:GLN:HG2	1:D:267:TRP:HE3	1.72	0.50
1:D:151:GLU:HB2	1:D:185:ARG:HH21	1.72	0.50
1:D:155:PHE:HE1	1:D:185:ARG:CD	2.23	0.50
1:D:255:GLN:HB2	1:D:267:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:HD22	1:B:146:ARG:HH21	1.58	0.50
1:C:67:MET:O	1:C:68:ASN:C	2.48	0.50
1:C:137:GLY:HA2	1:C:172:MET:HE3	1.94	0.50
1:A:133:ALA:O	1:A:135:SER:OG	2.21	0.49
1:A:325:GLN:O	1:A:326:ASN:CA	2.60	0.49
1:A:90:LEU:HD12	1:A:131:PRO:HG3	1.93	0.49
1:C:134:LEU:HA	1:C:138:GLN:NE2	2.27	0.49
1:C:120:VAL:HG12	1:C:121:LEU:N	2.26	0.49
1:C:123:LEU:HD21	1:C:142:VAL:HG22	1.94	0.49
1:B:29:GLY:O	1:B:180:HIS:CE1	2.65	0.49
1:A:246:VAL:HG12	1:A:279:ALA:O	2.11	0.49
1:B:271:GLU:HG2	1:B:273:ARG:HB2	1.95	0.49
1:B:42:LYS:HB3	1:B:190:VAL:CG1	2.42	0.49
1:C:140:GLN:NE2	1:C:144:ILE:HG12	2.27	0.49
1:D:65:LYS:HD3	1:D:65:LYS:N	2.26	0.49
1:B:272:SER:O	1:B:273:ARG:O	2.31	0.49
1:B:288:GLU:HG3	1:B:330:ARG:HD3	1.95	0.49
1:C:146:ARG:HG2	1:C:146:ARG:NH1	2.25	0.49
1:A:350:GLU:CD	1:A:350:GLU:H	2.14	0.49
1:C:240:ASN:HD21	1:C:328:VAL:N	1.94	0.49
1:C:6:LEU:HD11	1:C:49:ILE:CD1	2.42	0.49
1:A:90:LEU:O	1:A:91:SER:CB	2.61	0.49
1:B:65:LYS:HD3	1:B:65:LYS:N	2.27	0.49
1:C:288:GLU:HG2	1:D:312:ASN:HB2	1.95	0.49
1:D:272:SER:HA	1:D:275:VAL:HG11	1.95	0.49
1:A:191:THR:CG2	1:A:193:ASP:H	2.19	0.49
1:A:130:LYS:C	1:A:132:LYS:H	2.14	0.49
1:C:271:GLU:HG2	1:C:273:ARG:HB2	1.94	0.49
1:B:11:LYS:HD2	1:B:56:THR:HG23	1.94	0.48
1:A:133:ALA:O	1:A:135:SER:N	2.47	0.48
1:A:146:ARG:O	1:A:149:VAL:HG22	2.14	0.48
1:B:234:ILE:HD12	1:B:234:ILE:N	2.29	0.48
1:D:271:GLU:HG2	1:D:273:ARG:HB2	1.95	0.48
1:C:107:LYS:HA	1:C:110:ILE:HG21	1.95	0.48
1:A:318:ILE:N	1:A:318:ILE:HD12	2.28	0.48
1:C:45:LEU:CD1	1:C:207:LEU:HD11	2.41	0.48
1:C:257:GLU:OE1	1:C:263:ARG:HB3	2.13	0.48
1:C:318:ILE:HD12	1:C:318:ILE:N	2.29	0.48
1:D:34:PHE:CE2	1:D:205:VAL:HG11	2.49	0.48
1:B:374:ALA:O	1:B:375:SER:CB	2.60	0.48
1:C:370:GLY:HA2	1:D:336:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:PHE:CD2	1:D:205:VAL:HG13	2.48	0.48
1:A:6:LEU:HD11	1:A:49:ILE:CD1	2.43	0.48
1:B:257:GLU:OE1	1:B:263:ARG:HB3	2.14	0.48
1:B:320:ILE:HD12	1:B:327:LEU:HD22	1.96	0.48
1:B:33:VAL:HG12	1:B:35:VAL:HG22	1.95	0.48
1:B:324:ARG:CG	1:B:325:GLN:H	2.27	0.48
1:C:198:MET:HE2	1:C:218:PRO:HB3	1.95	0.48
1:C:97:SER:O	1:C:98:PHE:CB	2.60	0.48
1:A:257:GLU:OE1	1:A:263:ARG:HB3	2.13	0.48
1:A:82:GLN:O	1:A:82:GLN:HG2	2.14	0.48
1:B:260:MET:O	1:B:263:ARG:N	2.35	0.48
1:C:37:PRO:O	1:C:38:SER:C	2.52	0.48
1:C:117:VAL:HG21	1:C:149:VAL:HG22	1.96	0.48
1:C:149:VAL:C	1:C:151:GLU:H	2.17	0.48
1:A:32:VAL:HB	1:A:188:ILE:CD1	2.44	0.47
1:D:288:GLU:HG3	1:D:330:ARG:HD3	1.96	0.47
1:A:272:SER:O	1:A:273:ARG:O	2.32	0.47
1:C:46:LEU:HB3	1:C:79:MET:HE3	1.95	0.47
1:D:257:GLU:OE1	1:D:263:ARG:HB3	2.14	0.47
1:B:6:LEU:HD11	1:B:49:ILE:CD1	2.44	0.47
1:D:325:GLN:O	1:D:326:ASN:CA	2.61	0.47
1:A:134:LEU:O	1:A:139:ARG:NE	2.47	0.47
1:A:324:ARG:CG	1:A:325:GLN:H	2.26	0.47
1:A:192:HIS:CD2	1:B:165:ASP:HA	2.49	0.47
1:B:42:LYS:HB3	1:B:190:VAL:HG13	1.95	0.47
1:D:172:MET:O	1:D:176:ILE:HG12	2.15	0.47
1:A:92:VAL:HB	1:A:127:LEU:O	2.15	0.47
1:B:316:ILE:HG22	1:B:318:ILE:HD11	1.96	0.47
1:C:323:ILE:HG22	1:C:325:GLN:CG	2.45	0.47
1:C:6:LEU:HD11	1:C:49:ILE:HD11	1.95	0.47
1:B:232:GLY:O	1:B:238:LYS:HE2	2.13	0.47
1:C:135:SER:OG	1:C:138:GLN:HG3	2.15	0.47
1:C:232:GLY:O	1:C:238:LYS:HE2	2.15	0.47
1:C:95:ASN:O	1:C:146:ARG:HD2	2.15	0.47
1:A:6:LEU:HD11	1:A:49:ILE:HD11	1.96	0.47
1:B:42:LYS:HD2	1:B:190:VAL:HG13	1.96	0.47
1:B:22:ILE:HD12	1:B:24:LEU:HD22	1.97	0.47
1:C:114:VAL:HG22	1:C:127:LEU:HD21	1.97	0.47
1:C:141:ARG:HG3	1:C:141:ARG:HH11	1.80	0.47
1:C:288:GLU:HG3	1:C:330:ARG:HD3	1.96	0.47
1:A:109:VAL:HG13	1:C:357:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LYS:HA	1:C:110:ILE:HG22	1.97	0.47
1:C:272:SER:HA	1:C:275:VAL:HG11	1.97	0.47
1:C:272:SER:O	1:C:273:ARG:O	2.32	0.47
1:A:108:GLU:N	1:A:108:GLU:OE1	2.47	0.47
1:A:148:LEU:C	1:A:150:ALA:N	2.68	0.47
1:C:103:ALA:O	1:C:105:ALA:N	2.46	0.47
1:C:80:VAL:HG21	1:C:144:ILE:HD13	1.97	0.47
1:A:194:GLN:HB2	1:A:234:ILE:HD13	1.96	0.47
1:B:2:ALA:N	1:B:186:THR:CB	2.78	0.47
1:B:272:SER:HA	1:B:275:VAL:HG11	1.96	0.47
1:D:246:VAL:HG12	1:D:279:ALA:O	2.14	0.47
1:A:271:GLU:HG2	1:A:273:ARG:HB2	1.96	0.47
1:C:367:LYS:HD2	1:C:373:SER:OG	2.15	0.47
1:A:37:PRO:O	1:A:38:SER:C	2.53	0.46
1:C:134:LEU:HB2	1:C:139:ARG:HD3	1.96	0.46
1:C:172:MET:O	1:C:176:ILE:HG12	2.15	0.46
1:C:247:THR:O	1:C:248:ALA:HB2	2.15	0.46
1:C:30:GLU:OE1	1:C:203:LYS:HE3	2.15	0.46
1:D:221:LEU:HB3	1:D:234:ILE:CD1	2.45	0.46
1:A:2:ALA:HB2	1:A:153:SER:HB2	1.93	0.46
1:C:86:LEU:HD13	1:C:131:PRO:HB3	1.97	0.46
1:A:192:HIS:CD2	1:B:166:ALA:H	2.33	0.46
1:B:106:LYS:HB2	1:B:109:VAL:HG23	1.97	0.46
1:B:144:ILE:HD11	1:B:160:PRO:HB3	1.97	0.46
1:B:22:ILE:O	1:B:22:ILE:HG13	2.13	0.46
1:C:79:MET:HG3	1:C:156:LEU:O	2.15	0.46
1:A:172:MET:O	1:A:176:ILE:HG12	2.15	0.46
1:A:293:SER:C	1:A:295:ILE:N	2.68	0.46
1:D:198:MET:HE2	1:D:218:PRO:HB3	1.98	0.46
1:D:37:PRO:O	1:D:38:SER:C	2.53	0.46
1:B:6:LEU:HD11	1:B:49:ILE:HD11	1.96	0.46
1:C:101:LYS:CB	1:C:101:LYS:NZ	2.79	0.46
1:A:272:SER:HA	1:A:275:VAL:HG11	1.97	0.46
1:B:45:LEU:HD12	1:B:207:LEU:HD11	1.98	0.46
1:B:37:PRO:O	1:B:38:SER:C	2.54	0.46
1:B:88:PRO:HA	1:B:131:PRO:HG3	1.97	0.46
1:D:197:ALA:HB1	1:D:204:ILE:HD13	1.97	0.46
1:A:96:MET:CE	1:A:117:VAL:HG23	2.46	0.45
1:B:86:LEU:HB3	1:B:95:ASN:ND2	2.30	0.45
1:D:155:PHE:N	1:D:186:THR:O	2.42	0.45
1:B:122:GLN:HB2	1:B:141:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLY:O	1:A:141:ARG:HD3	2.17	0.45
1:A:148:LEU:C	1:A:150:ALA:H	2.20	0.45
1:A:129:ARG:HH11	1:A:129:ARG:HG2	1.80	0.45
1:B:34:PHE:HD2	1:B:205:VAL:HG13	1.82	0.45
1:B:323:ILE:HD12	1:B:324:ARG:HH11	1.75	0.45
1:C:194:GLN:HB2	1:C:234:ILE:HD13	1.97	0.45
1:D:198:MET:CE	1:D:204:ILE:HD12	2.46	0.45
1:C:318:ILE:O	1:C:326:ASN:HA	2.16	0.45
1:C:42:LYS:HB3	1:C:190:VAL:HG11	1.99	0.45
1:B:100:LEU:HG	1:B:110:ILE:HD13	1.98	0.45
1:D:323:ILE:HG22	1:D:325:GLN:NE2	2.29	0.45
1:B:173:ARG:NE	1:B:196:GLU:HG2	2.32	0.45
1:B:320:ILE:CD1	1:B:327:LEU:HD22	2.47	0.45
1:C:134:LEU:HB2	1:C:139:ARG:HH11	1.80	0.45
1:D:46:LEU:HB3	1:D:79:MET:HE3	1.99	0.45
1:A:76:GLY:O	1:A:153:SER:N	2.50	0.45
1:B:29:GLY:O	1:B:180:HIS:HE1	1.98	0.45
1:C:34:PHE:HD2	1:C:205:VAL:HG13	1.82	0.45
1:C:293:SER:C	1:C:295:ILE:N	2.68	0.45
1:D:191:THR:CG2	1:D:193:ASP:H	2.16	0.45
1:D:260:MET:CE	1:D:300:LEU:HD22	2.39	0.45
1:A:42:LYS:HB3	1:A:190:VAL:CG1	2.47	0.45
1:A:109:VAL:HG13	1:C:357:GLU:CG	2.47	0.45
1:D:198:MET:HE2	1:D:204:ILE:HD12	1.99	0.44
1:A:268:LEU:O	1:A:270:VAL:N	2.49	0.44
1:B:2:ALA:O	1:B:3:SER:HB3	2.17	0.44
1:C:173:ARG:NE	1:C:196:GLU:HG2	2.32	0.44
1:D:268:LEU:O	1:D:270:VAL:N	2.49	0.44
1:D:316:ILE:HG21	1:D:318:ILE:HD11	2.00	0.44
1:A:90:LEU:HD12	1:A:131:PRO:HG2	1.99	0.44
1:C:155:PHE:CD1	1:C:155:PHE:N	2.84	0.44
1:D:301:GLU:O	1:D:320:ILE:CD1	2.60	0.44
1:B:71:PRO:HA	1:B:72:PRO:HD3	1.87	0.44
1:C:141:ARG:O	1:C:145:GLY:N	2.48	0.44
1:C:374:ALA:O	1:C:375:SER:CB	2.65	0.44
1:B:247:THR:O	1:B:248:ALA:HB2	2.18	0.44
1:C:87:TYR:HA	1:C:88:PRO:HD3	1.61	0.44
1:C:140:GLN:HE21	1:C:144:ILE:CG1	2.31	0.44
1:C:237:PRO:HD2	1:C:330:ARG:HH11	1.83	0.44
1:D:25:ASP:O	1:D:203:LYS:NZ	2.50	0.44
1:A:117:VAL:HG21	1:A:149:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:HIS:NE2	1:C:90:LEU:HD13	2.32	0.44
1:A:198:MET:HE2	1:A:218:PRO:HB3	1.99	0.44
1:B:27:HIS:O	1:B:30:GLU:HB2	2.18	0.44
1:B:293:SER:C	1:B:295:ILE:N	2.68	0.44
1:C:106:LYS:C	1:C:108:GLU:N	2.70	0.44
1:C:86:LEU:HA	1:C:86:LEU:HD23	1.80	0.44
1:B:100:LEU:HG	1:B:110:ILE:CD1	2.48	0.43
1:B:12:ALA:H	1:B:56:THR:CG2	2.29	0.43
1:B:144:ILE:HD11	1:B:160:PRO:HB2	1.99	0.43
1:C:135:SER:H	1:C:138:GLN:NE2	2.16	0.43
1:C:2:ALA:O	1:C:3:SER:HB3	2.18	0.43
1:D:345:ILE:CD1	1:D:345:ILE:N	2.78	0.43
1:D:2:ALA:O	1:D:3:SER:HB3	2.18	0.43
1:C:37:PRO:HD3	1:C:233:PHE:CE1	2.53	0.43
1:D:323:ILE:N	1:D:323:ILE:HD12	2.33	0.43
1:A:12:ALA:H	1:A:56:THR:CG2	2.31	0.43
1:A:154:VAL:HG12	1:A:155:PHE:N	2.33	0.43
1:A:46:LEU:HD13	1:A:79:MET:CE	2.48	0.43
1:B:71:PRO:HG2	1:B:74:GLU:CD	2.39	0.43
1:A:33:VAL:HA	1:A:189:TYR:O	2.18	0.43
1:A:79:MET:HG2	1:A:81:PHE:CE2	2.52	0.43
1:B:34:PHE:CD2	1:B:205:VAL:HG13	2.52	0.43
1:B:34:PHE:CD2	1:B:205:VAL:CG1	3.01	0.43
1:C:108:GLU:HG3	1:C:109:VAL:HG23	2.01	0.43
1:C:163:ASN:N	1:C:163:ASN:ND2	2.67	0.43
1:A:20:LYS:HE2	1:A:209:ALA:O	2.18	0.43
1:A:34:PHE:HD2	1:A:205:VAL:HG13	1.84	0.43
1:A:356:ARG:HB2	1:A:358:ASP:OD1	2.18	0.43
1:B:134:LEU:CA	1:B:139:ARG:HH12	2.31	0.43
1:A:32:VAL:HB	1:A:188:ILE:HD13	2.00	0.43
1:A:323:ILE:N	1:A:323:ILE:HD12	2.33	0.43
1:B:83:SER:HA	1:B:163:ASN:OD1	2.19	0.43
1:C:108:GLU:CG	1:C:109:VAL:H	2.31	0.43
1:A:118:ALA:C	1:A:120:VAL:N	2.72	0.43
1:A:11:LYS:HB2	1:A:48:MET:SD	2.59	0.43
1:A:39:GLY:HA2	3:A:401:ADP:O3B	2.19	0.43
1:C:112:GLN:OE1	1:C:112:GLN:HA	2.18	0.43
1:A:106:LYS:O	1:A:110:ILE:HG23	2.19	0.42
1:A:93:ALA:HB2	1:A:127:LEU:HG	2.00	0.42
1:A:163:ASN:N	1:A:163:ASN:ND2	2.66	0.42
1:B:62:ILE:CD1	1:B:67:MET:HG3	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:CG	1:B:110:ILE:HD13	2.48	0.42
1:D:260:MET:O	1:D:263:ARG:N	2.35	0.42
1:A:173:ARG:NE	1:A:196:GLU:HG2	2.34	0.42
1:B:63:GLY:O	1:B:64:GLU:HG2	2.20	0.42
1:A:119:GLU:CA	1:A:124:ALA:HB2	2.49	0.42
1:A:247:THR:O	1:A:248:ALA:HB2	2.18	0.42
1:A:260:MET:HE1	1:A:300:LEU:HD22	2.00	0.42
1:B:235:GLY:O	1:B:236:SER:C	2.57	0.42
1:C:79:MET:CE	1:C:156:LEU:HB3	2.50	0.42
1:C:27:HIS:O	1:C:30:GLU:HB2	2.20	0.42
1:D:12:ALA:H	1:D:56:THR:CG2	2.30	0.42
1:D:175:GLU:HA	1:D:175:GLU:OE1	2.20	0.42
1:D:247:THR:O	1:D:248:ALA:HB2	2.19	0.42
1:A:172:MET:HB2	1:A:172:MET:HE2	1.97	0.42
1:C:120:VAL:HG12	1:C:121:LEU:HD23	2.00	0.42
1:D:173:ARG:NE	1:D:196:GLU:HG2	2.34	0.42
1:D:27:HIS:O	1:D:30:GLU:HB2	2.19	0.42
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.87	0.42
1:B:2:ALA:HB2	1:B:153:SER:HB2	2.02	0.42
1:B:157:LEU:HD13	1:B:189:TYR:CD1	2.53	0.42
1:C:227:ASP:HB2	1:C:359:GLY:O	2.20	0.42
1:A:148:LEU:O	1:A:150:ALA:N	2.53	0.42
1:A:288:GLU:HG2	1:B:312:ASN:CB	2.47	0.42
1:A:94:GLU:C	1:A:95:ASN:O	2.58	0.42
1:B:198:MET:CE	1:B:204:ILE:HD12	2.49	0.42
1:C:71:PRO:HG2	1:C:74:GLU:CD	2.40	0.42
1:D:293:SER:C	1:D:295:ILE:N	2.68	0.42
1:A:137:GLY:O	1:A:140:GLN:HB3	2.19	0.42
1:A:324:ARG:HG2	1:A:325:GLN:H	1.85	0.42
1:A:71:PRO:HG2	1:A:74:GLU:CD	2.40	0.42
1:C:288:GLU:H	1:C:288:GLU:CD	2.22	0.42
1:D:316:ILE:HG22	1:D:318:ILE:CD1	2.48	0.42
1:A:27:HIS:O	1:A:30:GLU:HB2	2.20	0.42
1:B:107:LYS:HG2	1:B:111:ASN:OD1	2.19	0.42
1:A:117:VAL:O	1:A:121:LEU:HB2	2.19	0.42
1:B:288:GLU:H	1:B:288:GLU:CD	2.23	0.42
1:B:304:VAL:HA	1:B:318:ILE:HD13	2.01	0.42
1:C:108:GLU:CG	1:C:109:VAL:N	2.82	0.42
1:C:110:ILE:HG23	1:C:111:ASN:N	2.35	0.42
1:C:117:VAL:HG21	1:C:149:VAL:CG2	2.50	0.42
1:D:219:LEU:HA	1:D:219:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:HA	1:D:290:LEU:HD23	1.93	0.42
1:C:356:ARG:HB2	1:C:358:ASP:OD1	2.19	0.41
1:A:141:ARG:NH1	1:A:141:ARG:HG2	2.34	0.41
1:A:320:ILE:O	1:A:320:ILE:HG22	2.21	0.41
1:B:316:ILE:HG22	1:B:318:ILE:CD1	2.51	0.41
1:B:300:LEU:HD13	1:B:320:ILE:HD13	2.01	0.41
1:B:324:ARG:HG2	1:B:325:GLN:H	1.85	0.41
1:C:107:LYS:O	1:C:111:ASN:OD1	2.38	0.41
1:A:175:GLU:HA	1:A:175:GLU:OE1	2.20	0.41
1:A:2:ALA:O	1:A:3:SER:HB3	2.20	0.41
1:B:325:GLN:O	1:B:326:ASN:CA	2.68	0.41
1:B:46:LEU:HD13	1:B:79:MET:CE	2.49	0.41
1:C:103:ALA:HB2	1:C:110:ILE:HD13	2.01	0.41
1:C:109:VAL:HG13	1:C:113:ARG:NH1	2.36	0.41
1:C:323:ILE:O	1:C:324:ARG:O	2.38	0.41
1:C:42:LYS:CD	1:C:191:THR:O	2.68	0.41
1:D:71:PRO:HG2	1:D:74:GLU:CD	2.40	0.41
1:A:90:LEU:CB	1:A:131:PRO:HD2	2.37	0.41
1:A:235:GLY:O	1:A:236:SER:C	2.59	0.41
1:A:84:TYR:O	1:A:84:TYR:CD2	2.73	0.41
1:B:131:PRO:C	1:B:133:ALA:H	2.24	0.41
1:B:356:ARG:HB2	1:B:358:ASP:OD1	2.20	0.41
1:C:46:LEU:HD13	1:C:79:MET:CE	2.50	0.41
1:C:92:VAL:HB	1:C:127:LEU:HA	2.02	0.41
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.86	0.41
1:B:291:LEU:HD11	1:B:348:PRO:HB3	2.02	0.41
1:A:62:ILE:HB	1:A:67:MET:HG3	2.03	0.41
1:A:241:PHE:C	1:A:242:LEU:HD23	2.41	0.41
1:A:309:GLN:O	1:A:310:LEU:HD23	2.21	0.41
1:B:316:ILE:HG21	1:B:318:ILE:HD11	2.01	0.41
1:C:93:ALA:HB2	1:C:127:LEU:HB3	2.03	0.41
1:C:64:GLU:C	1:C:65:LYS:HD3	2.41	0.41
1:C:63:GLY:O	1:C:64:GLU:HG2	2.20	0.41
1:A:45:LEU:HD12	1:A:207:LEU:HD11	2.02	0.41
1:A:64:GLU:C	1:A:65:LYS:HD3	2.40	0.41
1:B:163:ASN:ND2	1:B:163:ASN:N	2.68	0.41
1:B:324:ARG:O	1:B:325:GLN:HB2	2.19	0.41
1:D:9:VAL:CB	1:D:22:ILE:HD13	2.47	0.41
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.87	0.41
1:A:258:LEU:C	1:A:260:MET:H	2.23	0.41
1:A:95:ASN:C	1:A:97:SER:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CB	1:A:187:MET:HG2	2.44	0.41
1:A:237:PRO:HD2	1:A:330:ARG:HH11	1.86	0.41
1:B:198:MET:HE2	1:B:204:ILE:HD12	2.03	0.41
1:B:241:PHE:C	1:B:242:LEU:HD23	2.40	0.41
1:B:258:LEU:C	1:B:260:MET:H	2.25	0.41
1:C:34:PHE:CD2	1:C:205:VAL:HG13	2.56	0.41
1:D:291:LEU:HD11	1:D:348:PRO:HB3	2.02	0.41
1:D:46:LEU:HD13	1:D:79:MET:CE	2.51	0.41
1:A:34:PHE:CD2	1:A:205:VAL:CG1	3.03	0.41
1:C:179:LEU:HD23	1:C:179:LEU:C	2.41	0.41
1:C:241:PHE:C	1:C:242:LEU:HD23	2.42	0.41
1:D:34:PHE:HA	1:D:205:VAL:HG13	2.04	0.41
1:D:304:VAL:HA	1:D:318:ILE:HD13	2.03	0.41
1:D:300:LEU:C	1:D:320:ILE:HD11	2.40	0.41
1:A:41:GLY:HA2	3:A:401:ADP:O2A	2.22	0.40
1:B:88:PRO:HA	1:B:131:PRO:CG	2.51	0.40
1:C:138:GLN:O	1:C:139:ARG:C	2.58	0.40
1:C:92:VAL:HG13	1:C:142:VAL:HG13	2.03	0.40
1:A:62:ILE:CD1	1:A:67:MET:HG3	2.44	0.40
1:B:135:SER:CB	1:B:138:GLN:HE21	2.35	0.40
1:D:45:LEU:HD12	1:D:207:LEU:HD11	2.03	0.40
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.92	0.40
1:C:36:GLY:HA3	1:C:40:CYS:SG	2.62	0.40
1:C:60:LEU:HD12	1:C:61:PHE:H	1.85	0.40
1:C:71:PRO:HA	1:C:72:PRO:HD3	1.87	0.40
1:D:179:LEU:C	1:D:179:LEU:HD23	2.42	0.40
1:A:130:LYS:N	1:A:130:LYS:CD	2.85	0.40
1:A:145:GLY:O	1:A:149:VAL:HG13	2.22	0.40
1:A:201:ALA:HB3	1:A:204:ILE:HD11	2.03	0.40
1:A:34:PHE:CD2	1:A:205:VAL:HG13	2.57	0.40
1:A:322:SER:O	1:A:323:ILE:HB	2.21	0.40
1:B:46:LEU:HD22	1:B:156:LEU:HB3	2.02	0.40
1:B:84:TYR:HB3	1:B:143:ALA:CB	2.51	0.40
1:C:104:GLY:O	1:C:105:ALA:HB2	2.22	0.40
1:C:86:LEU:HD12	1:C:131:PRO:HB3	2.03	0.40
1:C:175:GLU:OE1	1:C:175:GLU:HA	2.21	0.40
1:C:268:LEU:O	1:C:270:VAL:N	2.52	0.40
1:D:11:LYS:HB2	1:D:48:MET:SD	2.62	0.40
1:D:237:PRO:HD2	1:D:330:ARG:HH11	1.85	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CE2	1:B:374:ALA:CB[1_655]	1.76	0.44
1:A:61:PHE:CZ	1:B:374:ALA:CB[1_655]	1.86	0.34
1:B:102:LEU:CD2	1:D:367:LYS:NZ[1_545]	2.04	0.16
1:C:374:ALA:CB	1:D:61:PHE:CE2[1_655]	2.17	0.03

## 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	370/381 (97%)	309 (84%)	35 (10%)	26 (7%)	<b>1</b>	<b>3</b>
1	B	372/381 (98%)	319 (86%)	29 (8%)	24 (6%)	<b>1</b>	<b>3</b>
1	C	357/381 (94%)	297 (83%)	34 (10%)	26 (7%)	<b>1</b>	<b>2</b>
1	D	293/381 (77%)	256 (87%)	19 (6%)	18 (6%)	<b>1</b>	<b>4</b>
All	All	1392/1524 (91%)	1181 (85%)	117 (8%)	94 (7%)	<b>1</b>	<b>3</b>

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	121	LEU
1	A	134	LEU
1	A	136	GLY
1	A	273	ARG
1	A	274	ASP
1	A	296	ALA
1	A	324	ARG
1	A	326	ASN
1	B	38	SER
1	B	82	GLN
1	B	96	MET
1	B	120	VAL
1	B	236	SER

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Mol	Chain	Res	Type
1	B	273	ARG
1	B	274	ASP
1	B	296	ALA
1	B	324	ARG
1	B	326	ASN
1	C	38	SER
1	C	86	LEU
1	C	98	PHE
1	C	99	GLY
1	C	236	SER
1	C	273	ARG
1	C	274	ASP
1	C	296	ALA
1	C	324	ARG
1	D	38	SER
1	D	152	PRO
1	D	153	SER
1	D	273	ARG
1	D	274	ASP
1	D	296	ALA
1	D	324	ARG
1	D	326	ASN
1	A	82	GLN
1	A	135	SER
1	A	182	ARG
1	A	236	SER
1	A	293	SER
1	B	104	GLY
1	B	134	LEU
1	B	136	GLY
1	B	182	ARG
1	B	293	SER
1	C	150	ALA
1	C	182	ARG
1	C	293	SER
1	C	326	ASN
1	D	182	ARG
1	D	236	SER
1	D	293	SER
1	A	90	LEU
1	A	91	SER
1	A	95	ASN

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Mol	Chain	Res	Type
1	A	104	GLY
1	A	271	GLU
1	A	322	SER
1	B	129	ARG
1	B	271	GLU
1	B	322	SER
1	C	105	ALA
1	C	131	PRO
1	C	271	GLU
1	C	297	ASP
1	C	322	SER
1	D	271	GLU
1	D	322	SER
1	A	297	ASP
1	A	323	ILE
1	B	297	ASP
1	B	323	ILE
1	C	120	VAL
1	C	125	HIS
1	C	152	PRO
1	C	323	ILE
1	D	297	ASP
1	D	323	ILE
1	A	3	SER
1	A	151	GLU
1	B	3	SER
1	C	3	SER
1	C	101	LYS
1	C	298	VAL
1	D	3	SER
1	D	64	GLU
1	A	64	GLU
1	A	298	VAL
1	B	64	GLU
1	B	298	VAL
1	C	64	GLU
1	D	298	VAL
1	B	151	GLU

### 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	315/323 (98%)	295 (94%)	20 (6%)	18	46
1	B	316/323 (98%)	295 (93%)	21 (7%)	16	44
1	C	307/323 (95%)	289 (94%)	18 (6%)	19	49
1	D	256/323 (79%)	241 (94%)	15 (6%)	19	49
All	All	1194/1292 (92%)	1120 (94%)	74 (6%)	18	47

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	24	LEU
1	A	31	PHE
1	A	57	SER
1	A	65	LYS
1	A	81	PHE
1	A	84	TYR
1	A	90	LEU
1	A	115	ASN
1	A	130	LYS
1	A	141	ARG
1	A	157	LEU
1	A	175	GLU
1	A	205	VAL
1	A	228	ARG
1	A	324	ARG
1	A	326	ASN
1	A	347	LEU
1	A	350	GLU
1	A	351	ARG
1	B	22	ILE
1	B	24	LEU
1	B	30	GLU
1	B	31	PHE

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Mol	Chain	Res	Type
1	B	57	SER
1	B	65	LYS
1	B	90	LEU
1	B	116	GLN
1	B	126	LEU
1	B	146	ARG
1	B	157	LEU
1	B	175	GLU
1	B	205	VAL
1	B	228	ARG
1	B	320	ILE
1	B	324	ARG
1	B	326	ASN
1	B	345	ILE
1	B	347	LEU
1	B	350	GLU
1	B	351	ARG
1	C	22	ILE
1	C	24	LEU
1	C	31	PHE
1	C	57	SER
1	C	65	LYS
1	C	95	ASN
1	C	97	SER
1	C	98	PHE
1	C	101	LYS
1	C	123	LEU
1	C	132	LYS
1	C	175	GLU
1	C	205	VAL
1	C	228	ARG
1	C	324	ARG
1	C	347	LEU
1	C	350	GLU
1	C	351	ARG
1	D	22	ILE
1	D	24	LEU
1	D	31	PHE
1	D	57	SER
1	D	65	LYS
1	D	175	GLU
1	D	205	VAL

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Mol	Chain	Res	Type
1	D	228	ARG
1	D	320	ILE
1	D	324	ARG
1	D	326	ASN
1	D	345	ILE
1	D	347	LEU
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	82	GLN
1	A	111	ASN
1	A	115	ASN
1	A	116	GLN
1	A	122	GLN
1	A	140	GLN
1	A	163	ASN
1	A	171	GLN
1	A	192	HIS
1	A	240	ASN
1	A	264	GLN
1	A	265	GLN
1	A	325	GLN
1	A	331	GLN
1	B	82	GLN
1	B	95	ASN
1	B	116	GLN
1	B	138	GLN
1	B	171	GLN
1	B	180	HIS
1	B	192	HIS
1	B	240	ASN
1	B	255	GLN
1	B	264	GLN
1	B	265	GLN
1	B	289	HIS
1	B	325	GLN
1	B	331	GLN
1	C	111	ASN
1	C	115	ASN

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Mol	Chain	Res	Type
1	C	138	GLN
1	C	140	GLN
1	C	163	ASN
1	C	171	GLN
1	C	240	ASN
1	C	264	GLN
1	C	265	GLN
1	C	289	HIS
1	C	331	GLN
1	D	171	GLN
1	D	240	ASN
1	D	264	GLN
1	D	265	GLN
1	D	325	GLN
1	D	331	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	1.05	1 (4%)	29,45,45	2.45	9 (31%)
3	ADP	D	404	2	24,29,29	1.04	1 (4%)	29,45,45	2.28	9 (31%)
3	ADP	C	403	-	24,29,29	1.06	1 (4%)	29,45,45	2.33	8 (27%)
3	ADP	B	402	2	24,29,29	1.05	2 (8%)	29,45,45	2.42	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	-	2/12/32/32	0/3/3/3
3	ADP	D	404	2	-	2/12/32/32	0/3/3/3
3	ADP	C	403	-	-	2/12/32/32	0/3/3/3
3	ADP	B	402	2	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C2-N1	3.23	1.39	1.33
3	C	403	ADP	C2-N1	3.16	1.39	1.33
3	D	404	ADP	C2-N1	2.99	1.39	1.33
3	B	402	ADP	C2-N1	2.86	1.39	1.33
3	B	402	ADP	PB-O3B	-2.18	1.46	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	O5'-PA-O1A	-8.52	75.78	109.07
3	C	403	ADP	O5'-PA-O1A	-8.41	76.22	109.07
3	B	402	ADP	O5'-PA-O1A	-8.19	77.05	109.07
3	D	404	ADP	O5'-PA-O1A	-7.93	78.09	109.07
3	B	402	ADP	O2A-PA-O5'	-4.10	88.71	107.75
3	B	402	ADP	C5-C6-N6	4.00	126.43	120.35
3	D	404	ADP	C5-C6-N6	3.86	126.22	120.35
3	C	403	ADP	C5-C6-N6	3.74	126.03	120.35
3	A	401	ADP	C5-C6-N6	3.72	126.01	120.35
3	C	403	ADP	O2A-PA-O5'	-3.66	90.74	107.75
3	A	401	ADP	C3'-C2'-C1'	3.65	106.48	100.98
3	D	404	ADP	O2A-PA-O5'	-3.64	90.82	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	ADP	N3-C2-N1	-3.61	123.04	128.68
3	B	402	ADP	O2A-PA-O1A	3.54	129.73	112.24
3	A	401	ADP	O2A-PA-O5'	-3.52	91.42	107.75
3	A	401	ADP	N3-C2-N1	-3.50	123.21	128.68
3	D	404	ADP	N3-C2-N1	-3.36	123.43	128.68
3	A	401	ADP	O2A-PA-O1A	3.34	128.77	112.24
3	B	402	ADP	N3-C2-N1	-3.28	123.55	128.68
3	B	402	ADP	C3'-C2'-C1'	3.26	105.89	100.98
3	D	404	ADP	C3'-C2'-C1'	3.11	105.67	100.98
3	C	403	ADP	O2A-PA-O1A	3.08	127.46	112.24
3	A	401	ADP	C5-C6-N1	-2.88	113.81	120.35
3	C	403	ADP	C2-N1-C6	2.84	123.61	118.75
3	B	402	ADP	C5-C6-N1	-2.81	113.98	120.35
3	A	401	ADP	C2-N1-C6	2.80	123.55	118.75
3	D	404	ADP	O2A-PA-O1A	2.79	126.05	112.24
3	D	404	ADP	C5-C6-N1	-2.78	114.04	120.35
3	C	403	ADP	C5-C6-N1	-2.78	114.05	120.35
3	D	404	ADP	C2-N1-C6	2.76	123.48	118.75
3	B	402	ADP	C2-N1-C6	2.71	123.39	118.75
3	C	403	ADP	C3'-C2'-C1'	2.37	104.54	100.98
3	A	401	ADP	O5'-C5'-C4'	2.24	116.70	108.99
3	D	404	ADP	O5'-C5'-C4'	2.23	116.68	108.99
3	B	402	ADP	O5'-C5'-C4'	2.21	116.61	108.99

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ADP	PA-O3A-PB-O2B
3	B	402	ADP	PA-O3A-PB-O2B
3	C	403	ADP	PA-O3A-PB-O2B
3	D	404	ADP	PA-O3A-PB-O2B
3	A	401	ADP	PA-O3A-PB-O3B
3	B	402	ADP	PA-O3A-PB-O3B
3	C	403	ADP	PA-O3A-PB-O3B
3	D	404	ADP	PA-O3A-PB-O3B

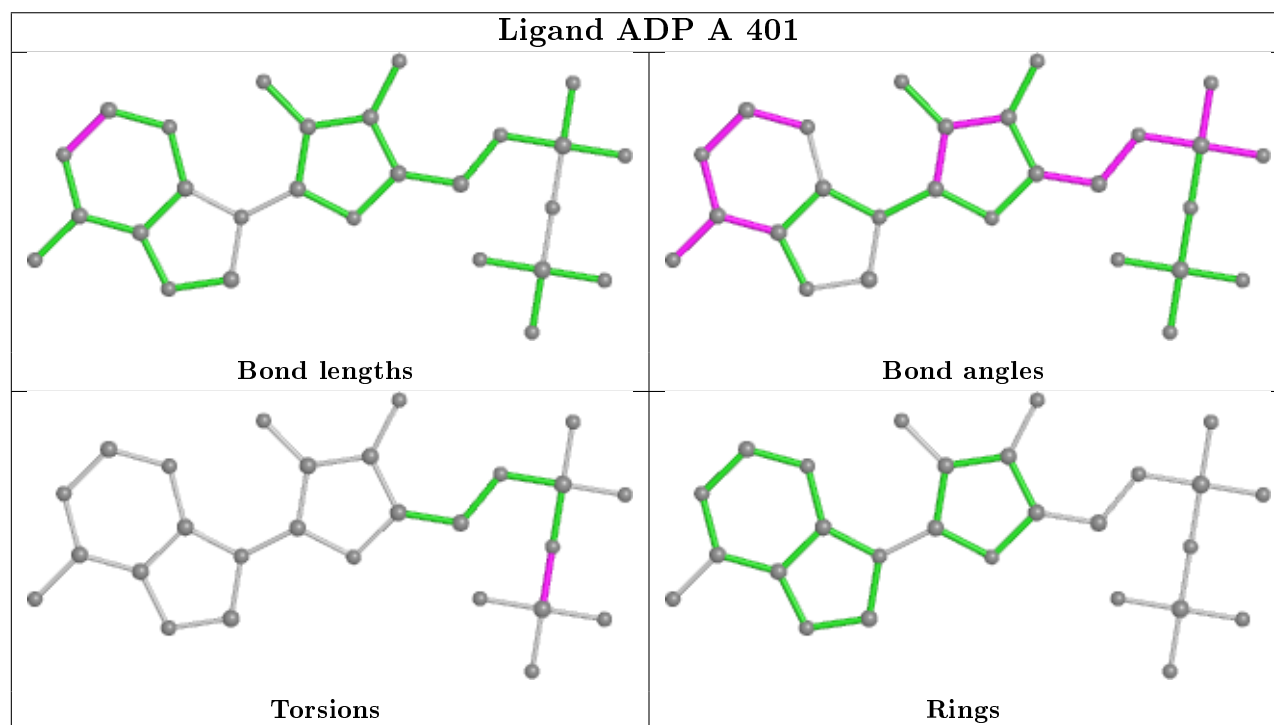
There are no ring outliers.

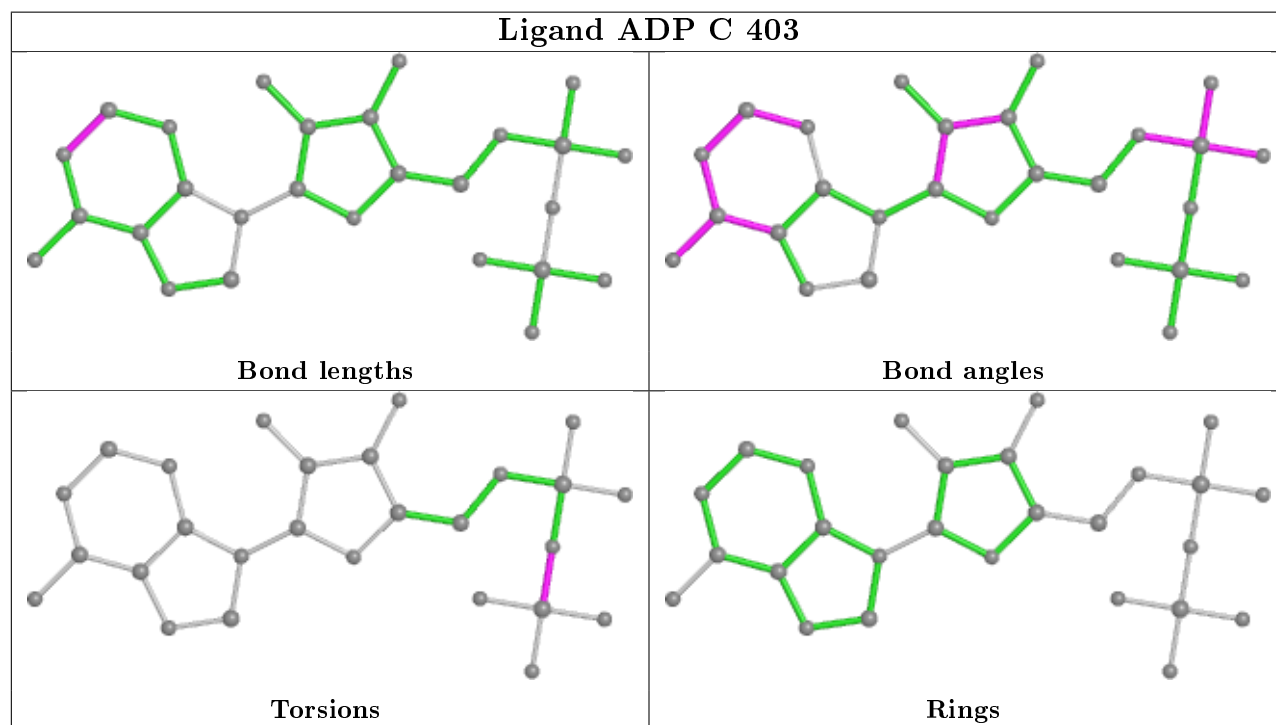
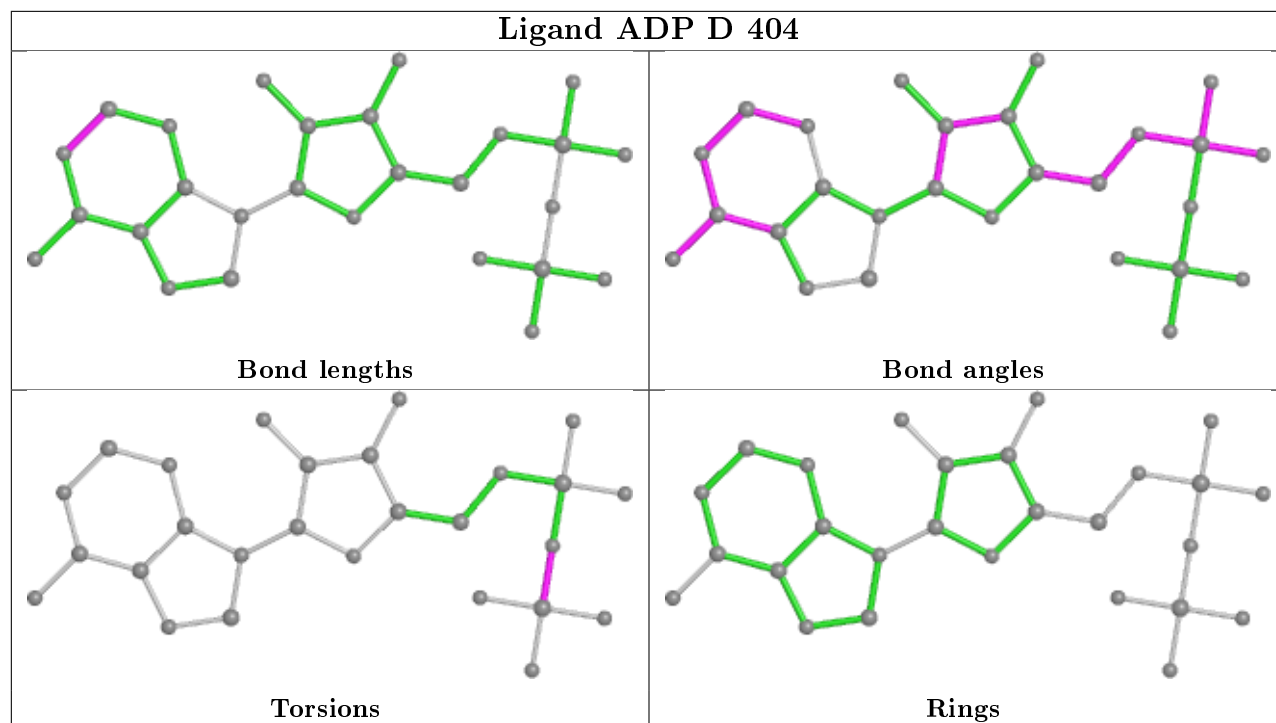
2 monomers are involved in 3 short contacts:

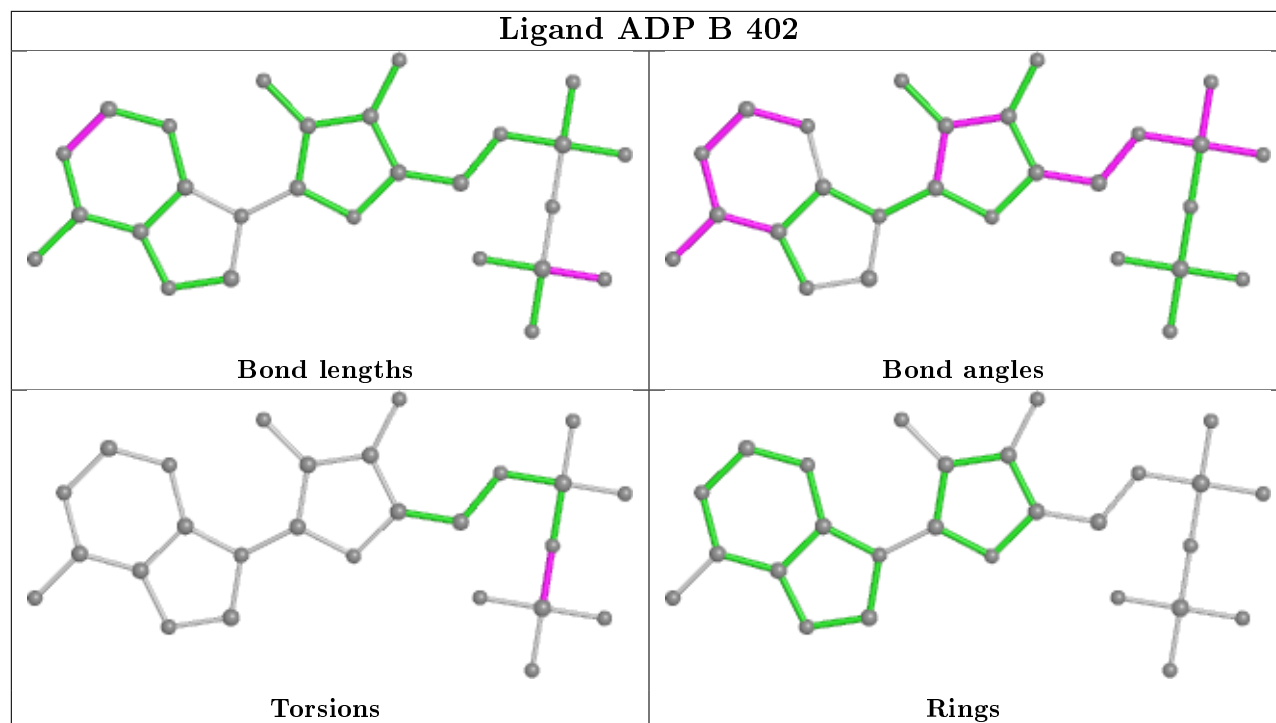


Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	2	0
3	C	403	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	372/381 (97%)	0.21	28 (7%) 14 8	18, 57, 133, 168	0
1	B	374/381 (98%)	-0.21	11 (2%) 51 41	16, 38, 91, 168	0
1	C	363/381 (95%)	0.22	23 (6%) 20 12	22, 71, 137, 172	0
1	D	299/381 (78%)	0.10	16 (5%) 25 17	18, 51, 129, 175	0
All	All	1408/1524 (92%)	0.08	78 (5%) 25 16	16, 52, 131, 175	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ALA	6.9
1	A	83	SER	6.0
1	D	373	SER	5.3
1	B	324	ARG	5.1
1	A	134	LEU	4.8
1	A	105	ALA	4.3
1	B	326	ASN	4.0
1	A	122	GLN	4.0
1	D	80	VAL	4.0
1	B	325	GLN	3.9
1	B	295	ILE	3.9
1	A	373	SER	3.8
1	A	163	ASN	3.7
1	D	168	LEU	3.6
1	C	125	HIS	3.6
1	C	73	ALA	3.6
1	A	15	GLU	3.5
1	A	87	TYR	3.5
1	D	178	ARG	3.5
1	A	86	LEU	3.4
1	A	119	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	3.3
1	B	375	SER	3.3
1	A	85	ALA	3.3
1	A	81	PHE	3.2
1	C	261	PRO	3.2
1	A	129	ARG	3.1
1	A	125	HIS	3.1
1	C	20	LYS	3.1
1	A	132	LYS	3.1
1	D	324	ARG	3.1
1	C	102	LEU	3.0
1	A	88	PRO	3.0
1	A	108	GLU	3.0
1	C	103	ALA	2.9
1	C	2	ALA	2.9
1	C	18	VAL	2.8
1	A	324	ARG	2.8
1	B	260	MET	2.8
1	C	23	ASN	2.8
1	A	61	PHE	2.7
1	C	60	LEU	2.7
1	B	135	SER	2.6
1	A	128	ASP	2.6
1	C	71	PRO	2.6
1	D	61	PHE	2.6
1	B	336	LEU	2.5
1	C	80	VAL	2.5
1	A	297	ASP	2.5
1	D	160	PRO	2.4
1	C	26	ILE	2.4
1	D	171	GLN	2.4
1	C	86	LEU	2.4
1	C	182	ARG	2.4
1	C	19	SER	2.4
1	D	261	PRO	2.4
1	C	100	LEU	2.3
1	C	324	ARG	2.3
1	D	251	ILE	2.3
1	B	374	ALA	2.3
1	C	168	LEU	2.3
1	A	135	SER	2.2
1	D	172	MET	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	372	ALA	2.2
1	B	236	SER	2.2
1	C	295	ILE	2.1
1	C	85	ALA	2.1
1	D	69	ASP	2.1
1	B	337	VAL	2.1
1	D	263	ARG	2.1
1	C	104	GLY	2.1
1	D	174	ILE	2.0
1	D	14	GLY	2.0
1	A	252	ASP	2.0
1	A	274	ASP	2.0
1	A	296	ALA	2.0
1	A	137	GLY	2.0
1	C	62	ILE	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](#)

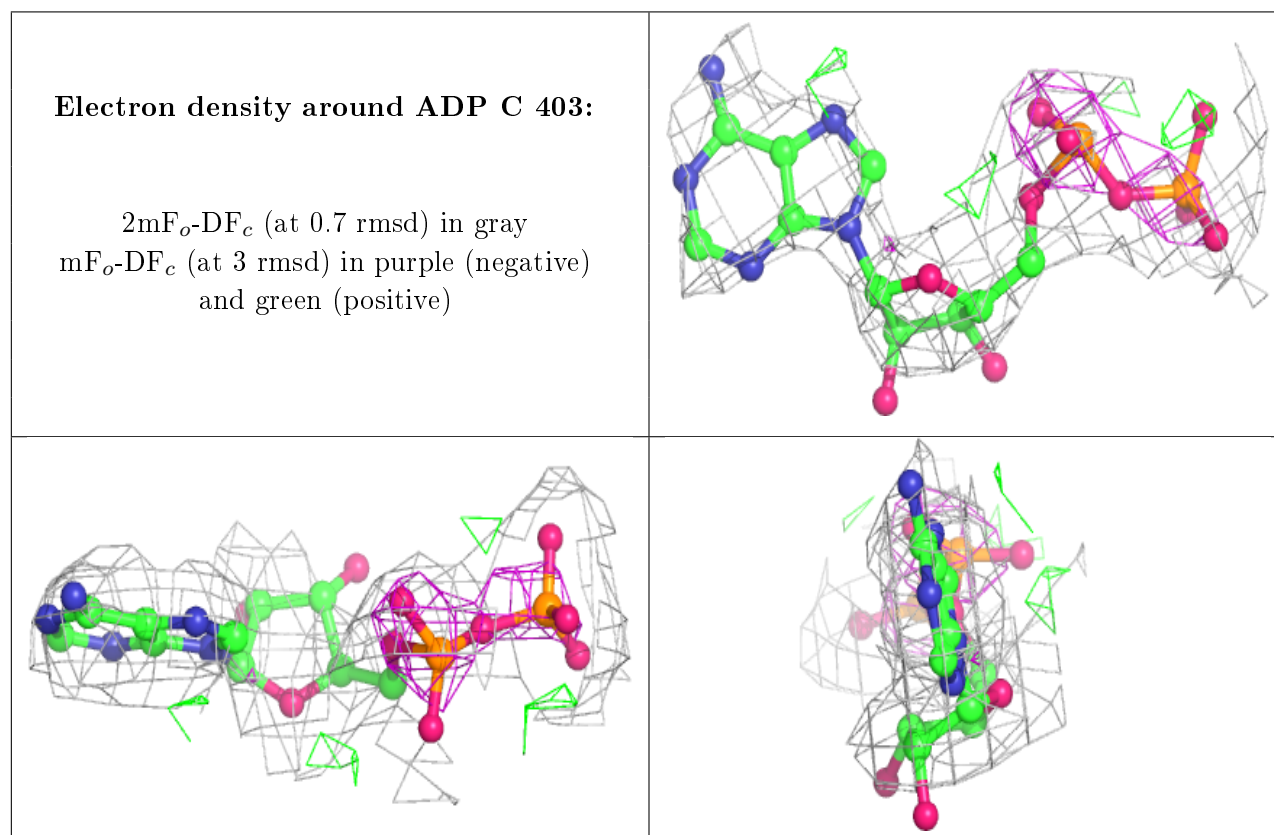
There are no carbohydrates in this entry.

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

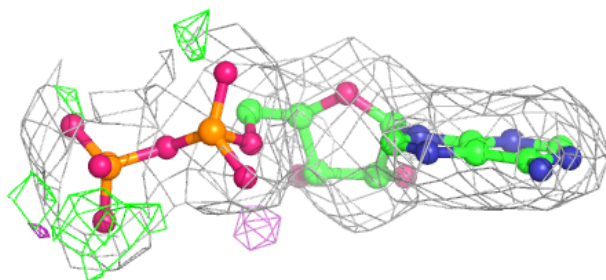
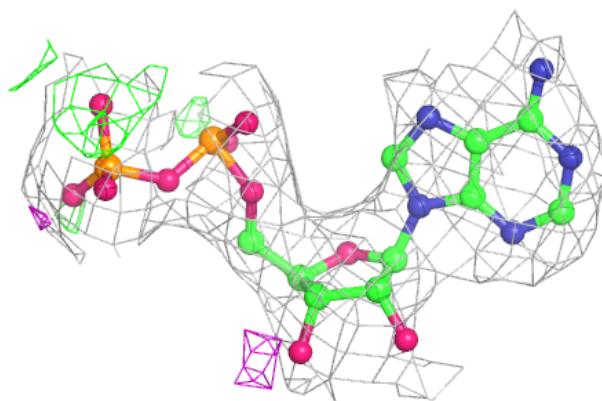
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	502	1/1	0.79	0.21	29,29,29,29	0
3	ADP	C	403	27/27	0.86	0.36	44,86,93,93	0
2	MG	D	504	1/1	0.87	0.16	33,33,33,33	0
2	MG	B	501	1/1	0.92	0.29	29,29,29,29	0
3	ADP	A	401	27/27	0.94	0.18	38,77,83,84	0
3	ADP	D	404	27/27	0.94	0.16	44,79,83,84	0
2	MG	C	503	1/1	0.96	0.12	28,28,28,28	0
3	ADP	B	402	27/27	0.96	0.16	33,70,79,80	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.

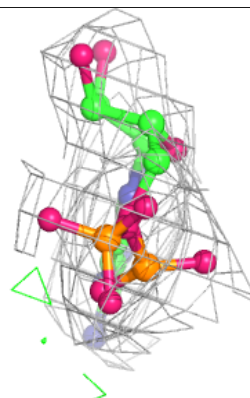
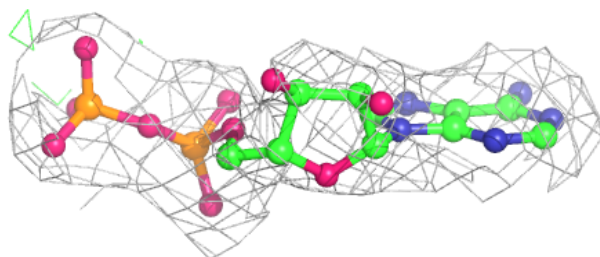
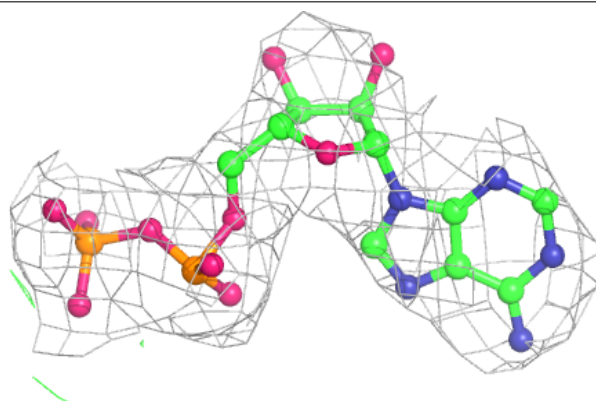


**Electron density around ADP A 401:**

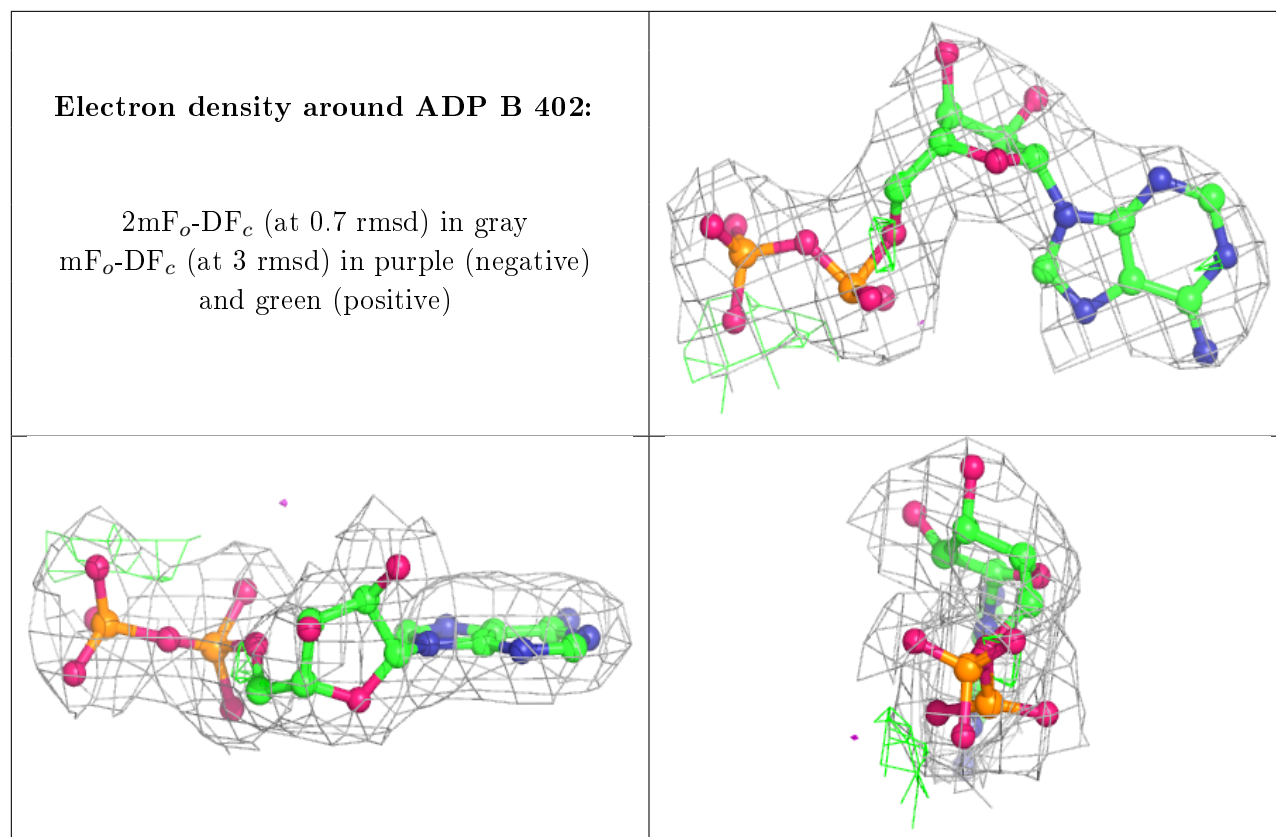
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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 [i](#)

There are no such residues in this entry.