



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:00 am BST

PDB ID : 3LY6  
Title : Crystal structure of human transglutaminase 2 complex with adenosine 5' Triphosphate  
Authors : Han, B.G.; Lee, B.I.  
Deposited on : 2010-02-26  
Resolution : 3.14 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

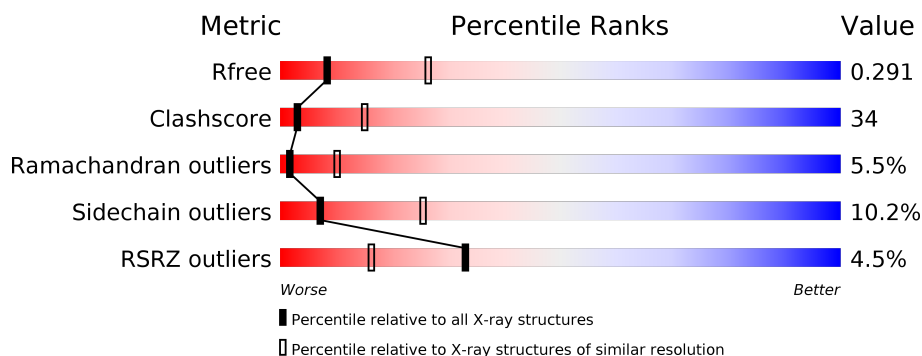
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	697	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>44%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	697	<div> <div>4%</div> <div> <div></div> <div>44%</div> <div>44%</div> <div>9%</div> <div>..</div> </div> </div>
1	C	697	<div> <div>7%</div> <div> <div></div> <div>46%</div> <div>42%</div> <div>9%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16296 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein-glutamine gamma-glutamyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	683	Total	C	N	O	S	0	0	0
			5401	3414	931	1026	30			
1	B	683	Total	C	N	O	S	0	0	0
			5401	3414	931	1026	30			
1	C	683	Total	C	N	O	S	0	0	0
			5401	3414	931	1026	30			

There are 33 discrepancies between the modelled and reference sequences:

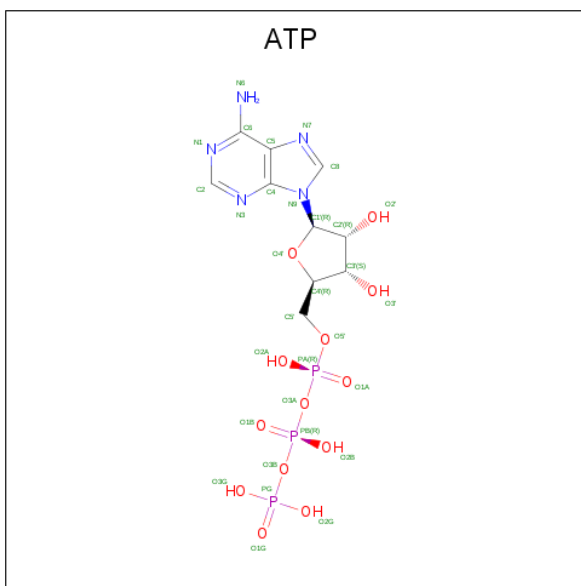
Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLY	VAL	SEE REMARK 999	UNP P21980
A	688	LEU	-	EXPRESSION TAG	UNP P21980
A	689	GLU	-	EXPRESSION TAG	UNP P21980
A	690	HIS	-	EXPRESSION TAG	UNP P21980
A	691	HIS	-	EXPRESSION TAG	UNP P21980
A	692	HIS	-	EXPRESSION TAG	UNP P21980
A	693	HIS	-	EXPRESSION TAG	UNP P21980
A	694	HIS	-	EXPRESSION TAG	UNP P21980
A	695	HIS	-	EXPRESSION TAG	UNP P21980
A	696	HIS	-	EXPRESSION TAG	UNP P21980
A	697	HIS	-	EXPRESSION TAG	UNP P21980
B	224	GLY	VAL	SEE REMARK 999	UNP P21980
B	688	LEU	-	EXPRESSION TAG	UNP P21980
B	689	GLU	-	EXPRESSION TAG	UNP P21980
B	690	HIS	-	EXPRESSION TAG	UNP P21980
B	691	HIS	-	EXPRESSION TAG	UNP P21980
B	692	HIS	-	EXPRESSION TAG	UNP P21980
B	693	HIS	-	EXPRESSION TAG	UNP P21980
B	694	HIS	-	EXPRESSION TAG	UNP P21980
B	695	HIS	-	EXPRESSION TAG	UNP P21980
B	696	HIS	-	EXPRESSION TAG	UNP P21980
B	697	HIS	-	EXPRESSION TAG	UNP P21980
C	224	GLY	VAL	SEE REMARK 999	UNP P21980

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Chain	Residue	Modelled	Actual	Comment	Reference
C	688	LEU	-	EXPRESSION TAG	UNP P21980
C	689	GLU	-	EXPRESSION TAG	UNP P21980
C	690	HIS	-	EXPRESSION TAG	UNP P21980
C	691	HIS	-	EXPRESSION TAG	UNP P21980
C	692	HIS	-	EXPRESSION TAG	UNP P21980
C	693	HIS	-	EXPRESSION TAG	UNP P21980
C	694	HIS	-	EXPRESSION TAG	UNP P21980
C	695	HIS	-	EXPRESSION TAG	UNP P21980
C	696	HIS	-	EXPRESSION TAG	UNP P21980
C	697	HIS	-	EXPRESSION TAG	UNP P21980

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

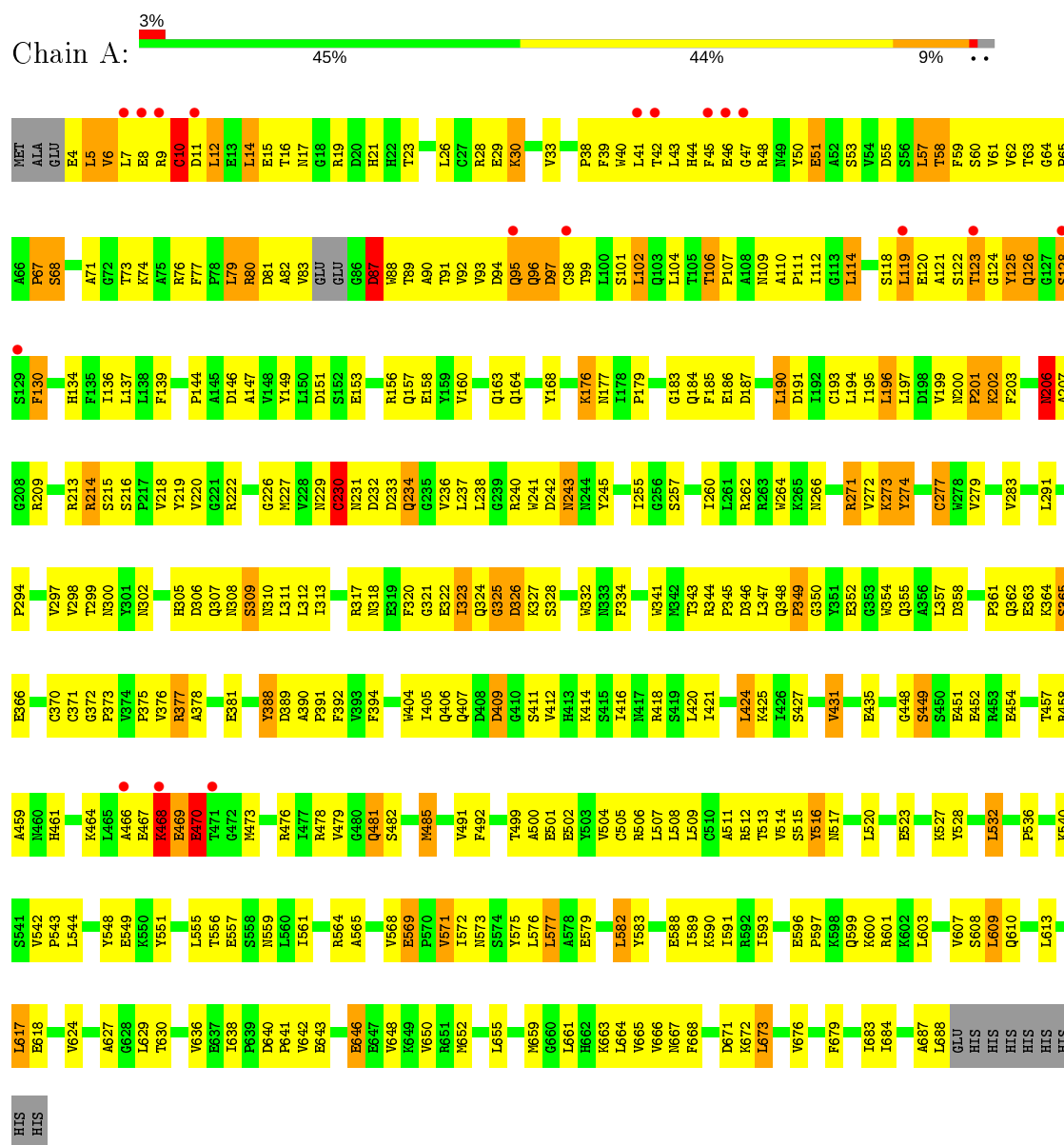


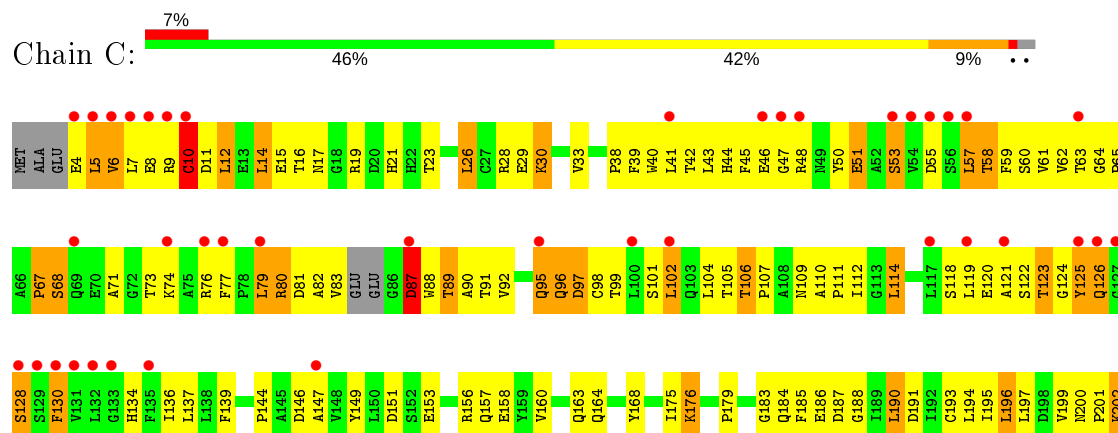
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

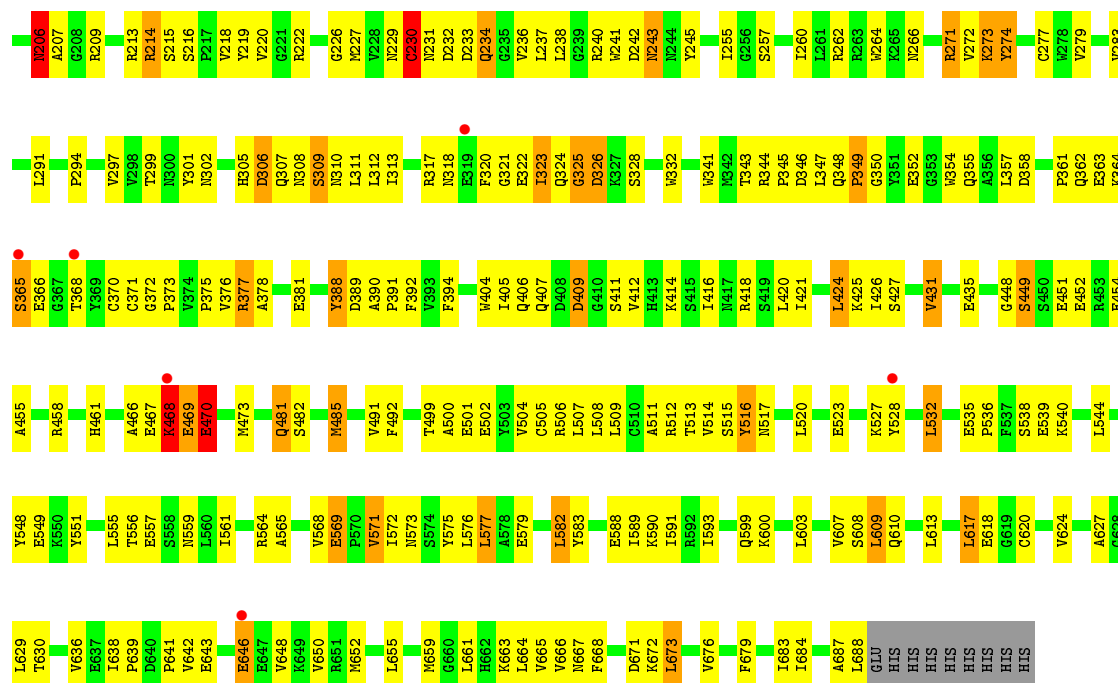
### 3 Residue-property plots

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: Protein-glutamine gamma-glutamyltransferase 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.18 Å   215.76 Å   165.96 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 3.14 49.76 – 3.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.14) 92.0 (49.76-3.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 3.12 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.233   ,   0.297 0.232   ,   0.291	Depositor DCC
$R_{free}$ test set	4227 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 73.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	1/5518 (0.0%)	0.66	1/7488 (0.0%)
1	B	0.40	0/5518	0.66	1/7488 (0.0%)
1	C	0.40	0/5518	0.65	1/7488 (0.0%)
All	All	0.40	1/16554 (0.0%)	0.66	3/22464 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	CYS	CB-SG	-5.31	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	ASP	N-CA-C	6.47	128.47	111.00
1	A	87	ASP	N-CA-C	6.17	127.66	111.00
1	B	87	ASP	N-CA-C	6.01	127.24	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5401	0	5301	364	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5401	0	5301	379	0
1	C	5401	0	5301	365	0
2	A	31	0	12	4	0
2	B	31	0	12	7	0
2	C	31	0	12	6	0
All	All	16296	0	15939	1097	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1097) 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:5:LEU:HA	1:C:123:THR:HG21	1.33	1.06
1:A:5:LEU:HA	1:A:123:THR:HG21	1.36	1.03
1:B:5:LEU:HA	1:B:123:THR:HG21	1.36	1.01
1:A:87:ASP:HB3	1:A:107:PRO:HG3	1.44	1.00
1:B:87:ASP:HB3	1:B:107:PRO:HG3	1.42	1.00
1:C:499:THR:HG22	1:C:501:GLU:H	1.28	0.98
1:C:636:VAL:HG11	1:C:650:VAL:HG21	1.44	0.98
1:C:87:ASP:HB3	1:C:107:PRO:HG3	1.46	0.98
1:A:271:ARG:HD2	1:A:271:ARG:H	1.26	0.97
1:C:583:TYR:H	2:C:702:ATP:HN62	1.05	0.97
1:B:271:ARG:HD2	1:B:271:ARG:H	1.26	0.97
1:B:499:THR:HG22	1:B:501:GLU:H	1.32	0.95
1:A:636:VAL:HG11	1:A:650:VAL:HG21	1.46	0.95
1:C:271:ARG:HD2	1:C:271:ARG:H	1.27	0.93
1:A:499:THR:HG22	1:A:501:GLU:H	1.32	0.93
1:B:636:VAL:HG11	1:B:650:VAL:HG21	1.51	0.91
1:B:583:TYR:H	2:B:701:ATP:HN62	1.16	0.91
1:C:163:GLN:HG2	1:C:184:GLN:NE2	1.87	0.89
1:A:583:TYR:H	2:A:700:ATP:HN62	1.21	0.88
1:B:163:GLN:HG2	1:B:184:GLN:NE2	1.88	0.88
1:B:17:ASN:ND2	1:B:39:PHE:HB2	1.91	0.86
1:A:163:GLN:HG2	1:A:184:GLN:NE2	1.90	0.85
1:C:17:ASN:HD22	1:C:39:PHE:HB2	1.41	0.85
1:B:17:ASN:HD22	1:B:39:PHE:HB2	1.41	0.85
1:B:271:ARG:N	1:B:271:ARG:HD2	1.91	0.85
1:A:271:ARG:HD2	1:A:271:ARG:N	1.91	0.84
1:A:147:ALA:HB1	1:A:343:THR:HG22	1.58	0.84
1:A:17:ASN:HD22	1:A:39:PHE:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HG3	1:A:46:GLU:HB2	1.60	0.84
1:C:17:ASN:ND2	1:C:39:PHE:HB2	1.92	0.84
1:A:17:ASN:ND2	1:A:39:PHE:HB2	1.92	0.83
1:C:9:ARG:HG3	1:C:46:GLU:HB2	1.60	0.83
1:C:271:ARG:HD2	1:C:271:ARG:N	1.91	0.83
1:B:9:ARG:HG3	1:B:46:GLU:HB2	1.61	0.83
1:B:618:GLU:HG3	1:B:641:PRO:HB3	1.61	0.81
1:B:538:SER:HB3	1:C:538:SER:HB3	1.61	0.81
1:C:618:GLU:HG3	1:C:641:PRO:HB3	1.61	0.81
1:C:14:LEU:HD22	1:C:40:TRP:HE3	1.45	0.81
1:A:618:GLU:HG3	1:A:641:PRO:HB3	1.63	0.80
1:B:147:ALA:HB1	1:B:343:THR:HG22	1.63	0.80
1:C:62:VAL:HG12	1:C:74:LYS:HG3	1.63	0.80
1:A:14:LEU:HD22	1:A:40:TRP:HE3	1.48	0.79
1:C:643:GLU:HB2	1:C:646:GLU:HG2	1.64	0.79
1:B:643:GLU:HB2	1:B:646:GLU:HG2	1.64	0.79
1:A:491:VAL:HG11	1:A:582:LEU:HD21	1.64	0.79
1:A:67:PRO:HB3	1:A:74:LYS:HB2	1.65	0.79
1:C:418:ARG:NH2	1:C:470:GLU:HB3	1.99	0.78
1:A:62:VAL:HG12	1:A:74:LYS:HG3	1.65	0.78
1:A:7:LEU:HD22	1:A:46:GLU:O	1.83	0.78
1:B:14:LEU:HD22	1:B:40:TRP:HE3	1.49	0.78
1:A:418:ARG:NH2	1:A:470:GLU:HB3	2.00	0.77
1:B:62:VAL:HG12	1:B:74:LYS:HG3	1.64	0.77
1:C:67:PRO:HB3	1:C:74:LYS:HB2	1.66	0.77
1:C:147:ALA:HB1	1:C:343:THR:HG22	1.66	0.77
1:C:491:VAL:HG11	1:C:582:LEU:HD21	1.67	0.77
1:B:418:ARG:NH2	1:B:470:GLU:HB3	2.00	0.76
1:B:491:VAL:HG11	1:B:582:LEU:HD21	1.66	0.76
1:B:7:LEU:HD22	1:B:46:GLU:O	1.84	0.76
1:A:241:TRP:HD1	1:A:517:ASN:ND2	1.83	0.76
1:B:67:PRO:HB3	1:B:74:LYS:HB2	1.67	0.76
1:B:668:PHE:HB3	1:B:676:VAL:CG2	2.15	0.76
1:B:326:ASP:C	1:B:328:SER:H	1.90	0.75
1:A:81:ASP:HB2	1:B:600:LYS:NZ	2.00	0.75
1:A:643:GLU:HB2	1:A:646:GLU:HG2	1.68	0.75
1:A:668:PHE:HB3	1:A:676:VAL:CG2	2.17	0.74
1:C:344:ARG:HD2	1:C:355:GLN:OE1	1.87	0.74
1:C:241:TRP:HD1	1:C:517:ASN:ND2	1.85	0.74
1:B:344:ARG:HD3	1:B:347:LEU:HD12	1.69	0.74
1:B:416:ILE:HB	1:B:576:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HD2	1:A:355:GLN:OE1	1.88	0.74
1:C:416:ILE:HB	1:C:576:LEU:HD12	1.68	0.74
1:B:243:ASN:ND2	1:B:556:THR:HG22	2.03	0.73
1:C:9:ARG:CG	1:C:46:GLU:HB2	2.18	0.73
1:C:7:LEU:HD22	1:C:46:GLU:O	1.87	0.73
1:C:318:ASN:HB3	1:C:324:GLN:NE2	2.03	0.73
1:B:9:ARG:CG	1:B:46:GLU:HB2	2.18	0.73
1:B:469:GLU:O	1:B:470:GLU:HG3	1.88	0.73
1:B:63:THR:HG23	1:B:64:GLY:H	1.54	0.73
1:C:499:THR:HG22	1:C:501:GLU:N	2.04	0.73
1:A:318:ASN:HB3	1:A:324:GLN:NE2	2.04	0.73
1:A:469:GLU:O	1:A:470:GLU:HG3	1.88	0.73
1:A:9:ARG:CG	1:A:46:GLU:HB2	2.18	0.73
1:A:50:TYR:HB3	1:A:95:GLN:NE2	2.03	0.73
1:C:344:ARG:HD3	1:C:347:LEU:HD12	1.71	0.73
1:C:668:PHE:HB3	1:C:676:VAL:CG2	2.18	0.72
1:A:326:ASP:C	1:A:328:SER:H	1.91	0.72
1:A:344:ARG:HD3	1:A:347:LEU:HD12	1.70	0.72
1:A:302:ASN:HD22	1:A:424:LEU:HD22	1.55	0.72
1:A:50:TYR:HB3	1:A:95:GLN:HE21	1.54	0.72
1:A:668:PHE:HB3	1:A:676:VAL:HG22	1.69	0.72
1:B:10:CYS:HB2	1:B:44:HIS:HB2	1.72	0.72
1:C:317:ARG:HD3	1:C:321:GLY:O	1.89	0.72
1:C:469:GLU:O	1:C:470:GLU:HG3	1.89	0.72
1:C:326:ASP:C	1:C:328:SER:H	1.91	0.72
1:B:668:PHE:HB3	1:B:676:VAL:HG22	1.70	0.72
1:B:48:ARG:HH12	1:B:51:GLU:HB2	1.55	0.72
1:C:222:ARG:HD3	1:C:372:GLY:O	1.89	0.72
1:A:222:ARG:HD3	1:A:372:GLY:O	1.90	0.72
1:A:271:ARG:H	1:A:271:ARG:CD	1.94	0.72
1:B:241:TRP:HD1	1:B:517:ASN:ND2	1.87	0.72
1:B:48:ARG:NH1	1:B:51:GLU:HB2	2.05	0.71
1:C:10:CYS:HB2	1:C:44:HIS:HB2	1.73	0.71
1:C:418:ARG:HH22	1:C:470:GLU:HB3	1.55	0.71
1:C:50:TYR:HB3	1:C:95:GLN:NE2	2.04	0.71
1:A:418:ARG:HH22	1:A:470:GLU:HB3	1.56	0.71
1:B:28:ARG:HH21	1:B:187:ASP:HA	1.55	0.71
1:B:222:ARG:HD3	1:B:372:GLY:O	1.91	0.70
1:C:311:LEU:HD11	1:C:394:PHE:HD2	1.56	0.70
1:A:164:GLN:HG3	1:A:663:LYS:H	1.57	0.70
1:B:418:ARG:HH22	1:B:470:GLU:HB3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ASN:ND2	1:C:556:THR:HG22	2.06	0.70
1:C:63:THR:HG23	1:C:64:GLY:H	1.54	0.70
1:C:642:VAL:HG21	1:C:648:VAL:HG22	1.73	0.70
1:C:668:PHE:HB3	1:C:676:VAL:HG22	1.71	0.70
1:B:58:THR:HG23	1:B:120:GLU:HB2	1.71	0.70
1:C:14:LEU:HD22	1:C:40:TRP:CE3	2.27	0.70
1:C:50:TYR:HB3	1:C:95:GLN:HE21	1.55	0.70
1:A:512:ARG:HG2	1:A:523:GLU:HA	1.73	0.70
1:C:58:THR:HG23	1:C:120:GLU:HB2	1.72	0.70
1:A:407:GLN:HB2	1:A:411:SER:O	1.92	0.69
1:A:4:GLU:HG3	1:A:5:LEU:H	1.57	0.69
1:B:407:GLN:HB2	1:B:411:SER:O	1.91	0.69
1:B:406:GLN:HA	1:B:412:VAL:HG12	1.75	0.69
1:A:81:ASP:HB2	1:B:600:LYS:HZ2	1.56	0.69
1:B:179:PRO:HB2	1:B:665:VAL:HG12	1.75	0.69
1:C:179:PRO:HB2	1:C:665:VAL:HG12	1.74	0.69
1:B:317:ARG:HD3	1:B:321:GLY:O	1.92	0.69
1:B:50:TYR:HB3	1:B:95:GLN:NE2	2.06	0.69
1:B:164:GLN:HG3	1:B:663:LYS:H	1.58	0.69
1:B:318:ASN:HB3	1:B:324:GLN:NE2	2.08	0.69
1:B:344:ARG:HD2	1:B:355:GLN:OE1	1.92	0.69
1:C:406:GLN:HA	1:C:412:VAL:HG12	1.74	0.69
1:A:420:LEU:HD23	1:A:421:ILE:N	2.07	0.69
1:A:311:LEU:HD11	1:A:394:PHE:HD2	1.57	0.69
1:A:416:ILE:HB	1:A:576:LEU:HD12	1.72	0.69
1:C:29:GLU:O	1:C:30:LYS:HB2	1.92	0.69
1:C:420:LEU:HD23	1:C:421:ILE:N	2.08	0.69
1:C:512:ARG:HG2	1:C:523:GLU:HA	1.74	0.69
1:B:163:GLN:HG2	1:B:184:GLN:HE22	1.58	0.69
1:B:9:ARG:HE	1:B:46:GLU:CB	2.06	0.69
1:B:499:THR:HG22	1:B:501:GLU:N	2.07	0.69
1:B:63:THR:HG23	1:B:64:GLY:N	2.08	0.68
1:C:28:ARG:HH21	1:C:187:ASP:HA	1.57	0.68
1:A:163:GLN:HG2	1:A:184:GLN:HE22	1.58	0.68
1:C:48:ARG:HH12	1:C:51:GLU:HB2	1.58	0.68
1:A:9:ARG:HE	1:A:46:GLU:CB	2.07	0.68
1:B:512:ARG:HG2	1:B:523:GLU:HA	1.75	0.68
1:B:624:VAL:CG1	1:B:664:LEU:HD11	2.23	0.68
1:A:243:ASN:ND2	1:A:556:THR:HG22	2.08	0.68
1:B:50:TYR:HB3	1:B:95:GLN:HE21	1.59	0.68
1:A:48:ARG:NH1	1:A:51:GLU:HB2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:O	1:B:600:LYS:HD3	1.94	0.68
1:A:317:ARG:CZ	1:A:323:ILE:HD11	2.24	0.68
1:A:10:CYS:HB2	1:A:44:HIS:HB2	1.76	0.68
1:A:317:ARG:HD3	1:A:321:GLY:O	1.94	0.68
1:A:48:ARG:HH12	1:A:51:GLU:HB2	1.59	0.68
1:C:4:GLU:HG3	1:C:5:LEU:H	1.59	0.68
1:A:642:VAL:HG21	1:A:648:VAL:HG22	1.76	0.68
1:C:407:GLN:HB2	1:C:411:SER:O	1.93	0.68
1:C:48:ARG:NH1	1:C:51:GLU:HB2	2.09	0.68
1:A:179:PRO:HB2	1:A:665:VAL:HG12	1.76	0.67
1:B:4:GLU:HG3	1:B:5:LEU:H	1.58	0.67
1:A:29:GLU:O	1:A:30:LYS:HB2	1.93	0.67
1:B:643:GLU:HB2	1:B:646:GLU:CG	2.25	0.67
1:C:63:THR:HG23	1:C:64:GLY:N	2.09	0.67
1:C:9:ARG:HE	1:C:46:GLU:CB	2.07	0.67
1:B:29:GLU:O	1:B:30:LYS:HB2	1.95	0.67
1:B:362:GLN:O	1:B:364:LYS:HG3	1.95	0.67
1:B:683:ILE:HD12	1:C:683:ILE:HD12	1.76	0.67
1:C:164:GLN:HG3	1:C:663:LYS:H	1.59	0.67
1:C:232:ASP:OD2	1:C:271:ARG:HG2	1.94	0.67
1:A:14:LEU:HD22	1:A:40:TRP:CE3	2.29	0.67
1:C:107:PRO:HD2	1:C:110:ALA:HB2	1.76	0.67
1:A:28:ARG:HH21	1:A:187:ASP:HA	1.59	0.67
1:B:14:LEU:HD22	1:B:40:TRP:CE3	2.30	0.67
1:A:406:GLN:HA	1:A:412:VAL:HG12	1.77	0.67
1:B:294:PRO:HB2	1:B:341:TRP:HB3	1.76	0.67
1:A:232:ASP:OD2	1:A:271:ARG:HG2	1.95	0.66
1:A:63:THR:HG23	1:A:64:GLY:H	1.59	0.66
1:A:241:TRP:HD1	1:A:517:ASN:HD21	1.42	0.66
1:B:71:ALA:O	1:B:73:THR:HG23	1.96	0.66
1:C:163:GLN:HG2	1:C:184:GLN:HE22	1.58	0.66
1:A:62:VAL:HB	1:A:67:PRO:CG	2.26	0.66
1:B:232:ASP:OD2	1:B:271:ARG:HG2	1.96	0.66
1:A:318:ASN:OD1	1:A:322:GLU:HB3	1.95	0.66
1:C:302:ASN:HD22	1:C:424:LEU:HD22	1.61	0.66
1:A:624:VAL:CG1	1:A:664:LEU:HD11	2.25	0.66
1:C:163:GLN:HA	1:C:184:GLN:HE22	1.60	0.66
1:C:241:TRP:CD1	1:C:517:ASN:ND2	2.64	0.66
1:A:499:THR:HG22	1:A:501:GLU:N	2.07	0.66
1:B:112:ILE:HD13	1:B:139:PHE:CE2	2.31	0.66
1:C:241:TRP:HD1	1:C:517:ASN:HD21	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:TRP:HD1	1:B:517:ASN:HD21	1.45	0.66
1:C:404:TRP:CZ3	1:C:414:LYS:HB2	2.30	0.66
1:C:564:ARG:HG3	1:C:579:GLU:HG2	1.77	0.66
1:A:343:THR:HG23	1:A:345:PRO:HD3	1.76	0.65
1:B:311:LEU:HD11	1:B:394:PHE:HD2	1.60	0.65
1:C:112:ILE:HD13	1:C:139:PHE:CE2	2.31	0.65
1:A:107:PRO:HD2	1:A:110:ALA:HB2	1.78	0.65
1:B:107:PRO:HD2	1:B:110:ALA:HB2	1.79	0.65
1:C:294:PRO:HB2	1:C:341:TRP:HB3	1.76	0.65
1:C:583:TYR:N	2:C:702:ATP:HN62	1.88	0.65
1:B:405:ILE:HD12	1:B:575:TYR:HB3	1.79	0.65
1:C:643:GLU:HB2	1:C:646:GLU:CG	2.27	0.65
1:C:362:GLN:O	1:C:364:LYS:HG3	1.97	0.65
1:B:229:ASN:HD22	1:B:361:PRO:CD	2.10	0.65
1:C:62:VAL:HB	1:C:67:PRO:CG	2.27	0.65
1:A:564:ARG:HG3	1:A:579:GLU:HG2	1.78	0.65
1:B:163:GLN:HA	1:B:184:GLN:HE22	1.61	0.65
1:C:354:TRP:O	1:C:376:VAL:HG23	1.97	0.65
1:B:318:ASN:OD1	1:B:322:GLU:HB3	1.96	0.65
1:C:71:ALA:O	1:C:73:THR:HG23	1.96	0.64
1:B:82:ALA:O	1:B:83:VAL:HB	1.98	0.64
1:A:294:PRO:HB2	1:A:341:TRP:HB3	1.78	0.64
1:A:112:ILE:HD13	1:A:139:PHE:CE2	2.33	0.64
1:A:357:LEU:HD21	1:A:373:PRO:HD3	1.80	0.64
1:C:33:VAL:HG23	1:C:137:LEU:HD12	1.79	0.64
1:A:241:TRP:CD1	1:A:517:ASN:ND2	2.63	0.64
1:B:302:ASN:HD22	1:B:424:LEU:HD22	1.61	0.64
1:B:420:LEU:HD23	1:B:421:ILE:N	2.11	0.64
1:C:624:VAL:CG1	1:C:664:LEU:HD11	2.27	0.64
1:A:60:SER:HA	1:A:76:ARG:HA	1.79	0.64
1:B:564:ARG:HG3	1:B:579:GLU:HG2	1.80	0.64
1:C:42:THR:HG22	1:C:101:SER:HB3	1.80	0.64
1:A:58:THR:HG23	1:A:120:GLU:HB2	1.78	0.64
1:C:318:ASN:OD1	1:C:322:GLU:HB3	1.97	0.64
1:A:514:VAL:HG12	1:A:515:SER:N	2.13	0.63
1:B:241:TRP:CD1	1:B:517:ASN:ND2	2.66	0.63
1:B:60:SER:HA	1:B:76:ARG:HA	1.79	0.63
1:A:404:TRP:CZ3	1:A:414:LYS:HB2	2.33	0.63
1:A:63:THR:HG23	1:A:64:GLY:N	2.12	0.63
1:B:317:ARG:CZ	1:B:323:ILE:HD11	2.28	0.63
1:C:405:ILE:HD12	1:C:575:TYR:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HG23	1:B:137:LEU:HD12	1.80	0.63
1:B:507:LEU:HG	1:B:509:LEU:HD13	1.80	0.63
1:B:642:VAL:HG21	1:B:648:VAL:HG22	1.80	0.63
1:B:62:VAL:HB	1:B:67:PRO:CG	2.27	0.63
1:A:405:ILE:HD12	1:A:575:TYR:HB3	1.80	0.63
1:B:308:ASN:O	1:B:309:SER:CB	2.47	0.63
1:C:60:SER:HA	1:C:76:ARG:HA	1.80	0.63
1:A:308:ASN:O	1:A:309:SER:CB	2.47	0.63
1:A:362:GLN:O	1:A:364:LYS:HG3	1.98	0.63
1:C:308:ASN:O	1:C:309:SER:CB	2.46	0.63
1:A:323:ILE:H	1:A:323:ILE:HD12	1.63	0.63
1:A:643:GLU:HB2	1:A:646:GLU:CG	2.29	0.63
1:A:229:ASN:HD22	1:A:361:PRO:CD	2.12	0.62
1:A:71:ALA:O	1:A:73:THR:HG23	1.99	0.62
1:A:33:VAL:HG23	1:A:137:LEU:HD12	1.81	0.62
1:B:6:VAL:HG22	1:B:123:THR:HB	1.79	0.62
1:B:81:ASP:HB3	1:B:92:VAL:HG13	1.82	0.62
1:C:243:ASN:HA	1:C:245:TYR:CZ	2.34	0.62
1:C:229:ASN:HD22	1:C:361:PRO:CD	2.11	0.62
1:B:65:PRO:HG3	1:B:207:ALA:HB1	1.82	0.62
1:C:82:ALA:O	1:C:83:VAL:HB	1.99	0.62
1:B:57:LEU:CD2	1:B:57:LEU:H	2.12	0.62
1:C:222:ARG:HG2	1:C:373:PRO:CD	2.29	0.62
1:B:481:GLN:HG2	1:B:482:SER:N	2.15	0.62
1:C:6:VAL:HG22	1:C:123:THR:HB	1.80	0.62
1:C:323:ILE:HD12	1:C:323:ILE:H	1.65	0.62
1:C:68:SER:HB3	1:C:71:ALA:HB3	1.82	0.62
1:C:468:LYS:O	1:C:468:LYS:HD2	2.00	0.61
1:A:42:THR:HG22	1:A:101:SER:HB3	1.81	0.61
1:B:537:PHE:HB3	1:C:540:LYS:NZ	2.15	0.61
1:B:671:ASP:CG	1:B:672:LYS:HD2	2.20	0.61
1:B:42:THR:HG22	1:B:101:SER:HB3	1.81	0.61
1:B:404:TRP:CZ3	1:B:414:LYS:HB2	2.35	0.61
1:C:343:THR:HG23	1:C:345:PRO:HD3	1.80	0.61
1:A:502:GLU:HG3	1:A:502:GLU:O	2.00	0.61
1:B:12:LEU:HD22	1:B:14:LEU:H	1.65	0.61
1:C:357:LEU:HD21	1:C:373:PRO:HD3	1.83	0.61
1:C:5:LEU:HD22	1:C:123:THR:CG2	2.31	0.61
1:C:371:CYS:HB3	1:C:389:ASP:HB2	1.83	0.61
1:A:569:GLU:OE2	1:A:571:VAL:HB	1.99	0.61
1:B:468:LYS:O	1:B:468:LYS:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HG21	1:A:667:ASN:HB2	1.83	0.61
1:A:371:CYS:HB3	1:A:389:ASP:HB2	1.83	0.61
1:A:57:LEU:H	1:A:57:LEU:CD2	2.13	0.61
1:A:325:GLY:O	1:A:326:ASP:HB3	2.01	0.61
1:A:507:LEU:HG	1:A:509:LEU:HD13	1.83	0.61
1:B:371:CYS:HB3	1:B:389:ASP:HB2	1.83	0.61
1:C:12:LEU:HD22	1:C:14:LEU:H	1.64	0.61
1:C:317:ARG:CZ	1:C:577:LEU:HD11	2.30	0.61
1:C:671:ASP:CG	1:C:672:LYS:HD2	2.20	0.61
1:A:302:ASN:ND2	1:A:424:LEU:HD22	2.14	0.60
1:C:481:GLN:HG2	1:C:482:SER:N	2.16	0.60
1:C:65:PRO:HG3	1:C:207:ALA:HB1	1.83	0.60
1:C:317:ARG:CZ	1:C:323:ILE:HD11	2.31	0.60
1:C:507:LEU:HG	1:C:509:LEU:HD13	1.84	0.60
1:A:12:LEU:HD22	1:A:14:LEU:H	1.66	0.60
1:A:163:GLN:HA	1:A:184:GLN:HE22	1.65	0.60
1:B:357:LEU:HD21	1:B:373:PRO:HD3	1.83	0.60
1:B:255:ILE:HG21	1:B:667:ASN:HB2	1.83	0.60
1:A:158:GLU:HG2	1:A:431:VAL:HA	1.82	0.60
1:C:636:VAL:HG11	1:C:650:VAL:CG2	2.27	0.60
1:A:109:ASN:O	1:A:215:SER:HB2	2.01	0.60
1:C:514:VAL:HG12	1:C:515:SER:N	2.16	0.60
1:A:468:LYS:HD2	1:A:468:LYS:O	2.02	0.60
1:B:317:ARG:CZ	1:B:577:LEU:HD11	2.31	0.60
1:C:325:GLY:O	1:C:326:ASP:HB3	2.02	0.60
1:A:222:ARG:HG2	1:A:373:PRO:CD	2.31	0.60
1:B:323:ILE:H	1:B:323:ILE:HD12	1.66	0.60
1:B:222:ARG:HG2	1:B:373:PRO:CD	2.32	0.60
1:B:8:GLU:HA	1:B:45:PHE:HA	1.83	0.60
1:B:5:LEU:HD22	1:B:123:THR:CG2	2.32	0.60
1:B:343:THR:HG23	1:B:345:PRO:HD3	1.84	0.59
1:B:514:VAL:HG12	1:B:515:SER:N	2.16	0.59
1:A:481:GLN:HG2	1:A:482:SER:N	2.17	0.59
1:A:325:GLY:O	1:A:326:ASP:CB	2.51	0.59
1:B:158:GLU:HG2	1:B:431:VAL:HA	1.83	0.59
1:A:57:LEU:HB2	1:A:119:LEU:HD21	1.85	0.59
1:A:6:VAL:HG22	1:A:123:THR:HB	1.82	0.59
1:B:45:PHE:O	1:B:98:CYS:HB3	2.03	0.59
1:C:81:ASP:HB3	1:C:92:VAL:HG13	1.84	0.59
1:A:671:ASP:CG	1:A:672:LYS:HD2	2.22	0.59
1:C:163:GLN:HG2	1:C:184:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:GLU:HG3	1:C:502:GLU:O	2.03	0.59
1:A:317:ARG:CZ	1:A:577:LEU:HD11	2.33	0.59
1:B:271:ARG:CD	1:B:271:ARG:H	1.93	0.59
1:B:325:GLY:O	1:B:326:ASP:HB3	2.01	0.59
1:C:344:ARG:HH11	1:C:375:PRO:HD3	1.68	0.59
1:A:514:VAL:HG12	1:A:515:SER:O	2.02	0.59
1:C:109:ASN:O	1:C:215:SER:HB2	2.02	0.59
1:C:5:LEU:HD22	1:C:123:THR:HG21	1.83	0.59
1:A:136:ILE:HD13	1:A:194:LEU:HD11	1.84	0.59
1:A:81:ASP:HB3	1:A:92:VAL:HG13	1.85	0.59
1:A:191:ASP:O	1:A:195:ILE:HG13	2.03	0.59
1:B:9:ARG:HE	1:B:46:GLU:HB3	1.68	0.59
1:C:96:GLN:O	1:C:97:ASP:HB3	2.03	0.59
1:B:325:GLY:O	1:B:326:ASP:CB	2.51	0.59
1:A:65:PRO:HG3	1:A:207:ALA:HB1	1.85	0.58
1:A:82:ALA:O	1:A:83:VAL:HB	2.03	0.58
1:C:325:GLY:O	1:C:326:ASP:CB	2.51	0.58
1:C:569:GLU:OE2	1:C:571:VAL:HB	2.01	0.58
1:B:569:GLU:OE2	1:B:571:VAL:HB	2.03	0.58
1:B:5:LEU:HD22	1:B:123:THR:HG21	1.84	0.58
1:C:418:ARG:HH22	1:C:470:GLU:CB	2.16	0.58
1:A:243:ASN:HA	1:A:245:TYR:CZ	2.37	0.58
1:C:57:LEU:HB2	1:C:119:LEU:HD21	1.86	0.58
1:B:232:ASP:CG	1:B:271:ARG:HG2	2.24	0.58
1:B:502:GLU:O	1:B:502:GLU:HG3	2.04	0.58
1:C:8:GLU:HA	1:C:45:PHE:HA	1.84	0.58
1:C:527:LYS:O	1:C:528:TYR:HD2	1.86	0.58
1:B:136:ILE:HD13	1:B:194:LEU:HD11	1.85	0.58
1:B:206:ASN:HD22	1:B:206:ASN:C	2.07	0.58
1:C:57:LEU:CD2	1:C:57:LEU:H	2.16	0.58
1:C:514:VAL:HG12	1:C:515:SER:O	2.04	0.58
1:A:590:LYS:HB2	1:A:608:SER:OG	2.04	0.58
1:B:344:ARG:HH11	1:B:375:PRO:HD3	1.68	0.58
1:B:514:VAL:HG12	1:B:515:SER:O	2.03	0.58
1:C:9:ARG:HE	1:C:46:GLU:HB3	1.69	0.58
1:A:5:LEU:HD22	1:A:123:THR:CG2	2.34	0.58
1:B:600:LYS:O	1:B:600:LYS:HD2	2.04	0.58
1:A:8:GLU:HA	1:A:45:PHE:HA	1.85	0.57
1:A:569:GLU:OE2	1:A:572:ILE:HG12	2.05	0.57
1:A:4:GLU:HG3	1:A:5:LEU:N	2.18	0.57
1:B:68:SER:HB3	1:B:71:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ILE:HG21	1:C:667:ASN:HB2	1.86	0.57
1:A:418:ARG:HH22	1:A:470:GLU:CB	2.17	0.57
1:A:491:VAL:HG23	1:A:544:LEU:HB3	1.85	0.57
1:B:111:PRO:HG3	1:B:215:SER:HB3	1.85	0.57
1:B:373:PRO:O	1:B:388:TYR:HB2	2.05	0.57
1:C:218:VAL:HG21	1:C:344:ARG:HH21	1.70	0.57
1:C:491:VAL:HG23	1:C:544:LEU:HB3	1.86	0.57
1:A:9:ARG:HE	1:A:46:GLU:HB3	1.69	0.57
1:C:569:GLU:OE2	1:C:572:ILE:HG12	2.04	0.57
1:C:609:LEU:HD13	1:C:610:GLN:N	2.19	0.57
1:B:26:LEU:HD13	1:B:185:PHE:CD1	2.40	0.57
1:B:19:ARG:CB	1:B:19:ARG:HH11	2.18	0.57
1:C:271:ARG:CD	1:C:271:ARG:H	1.95	0.57
1:A:26:LEU:HD13	1:A:185:PHE:CD1	2.40	0.57
1:A:344:ARG:HH11	1:A:375:PRO:HD3	1.69	0.57
1:B:112:ILE:HG12	1:B:214:ARG:O	2.05	0.57
1:B:57:LEU:HB2	1:B:119:LEU:HD21	1.87	0.57
1:A:365:SER:C	1:A:366:GLU:HG3	2.25	0.57
1:C:309:SER:O	1:C:311:LEU:HD22	2.05	0.57
1:A:114:LEU:HD21	1:A:134:HIS:HB3	1.87	0.57
1:A:68:SER:HB3	1:A:71:ALA:HB3	1.87	0.57
1:A:51:GLU:O	1:A:55:ASP:HB2	2.05	0.56
1:A:96:GLN:O	1:A:97:ASP:HB3	2.05	0.56
1:B:418:ARG:HH22	1:B:470:GLU:CB	2.18	0.56
1:B:4:GLU:HG3	1:B:5:LEU:N	2.20	0.56
1:C:467:GLU:HG2	1:C:469:GLU:OE2	2.05	0.56
1:B:19:ARG:HB3	1:B:19:ARG:HH11	1.70	0.56
1:C:365:SER:C	1:C:366:GLU:HG3	2.26	0.56
1:A:609:LEU:HD13	1:A:610:GLN:N	2.21	0.56
1:B:190:LEU:O	1:B:193:CYS:HB2	2.05	0.56
1:C:277:CYS:SG	1:C:516:TYR:OH	2.63	0.56
1:C:527:LYS:O	1:C:528:TYR:CD2	2.58	0.56
1:C:51:GLU:O	1:C:55:ASP:HB2	2.06	0.56
1:A:600:LYS:HD2	1:A:600:LYS:O	2.06	0.56
1:B:163:GLN:HG2	1:B:184:GLN:HE21	1.71	0.56
1:C:7:LEU:O	1:C:8:GLU:HB3	2.05	0.56
1:C:136:ILE:HD13	1:C:194:LEU:HD11	1.86	0.56
1:C:45:PHE:O	1:C:98:CYS:HB3	2.05	0.56
1:A:371:CYS:HB3	1:A:389:ASP:CB	2.35	0.56
1:B:365:SER:C	1:B:366:GLU:HG3	2.26	0.56
1:C:111:PRO:HG3	1:C:215:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LEU:HD11	1:C:394:PHE:CD2	2.39	0.56
1:A:373:PRO:O	1:A:388:TYR:HB2	2.05	0.56
1:B:583:TYR:N	2:B:701:ATP:HN62	1.97	0.56
1:C:326:ASP:C	1:C:328:SER:N	2.59	0.56
1:A:476:ARG:NH1	2:A:700:ATP:O1G	2.39	0.56
1:B:326:ASP:C	1:B:328:SER:N	2.58	0.56
1:A:232:ASP:CG	1:A:271:ARG:HG2	2.26	0.56
1:C:57:LEU:HA	1:C:120:GLU:O	2.05	0.56
1:C:4:GLU:HG3	1:C:5:LEU:N	2.21	0.56
1:A:190:LEU:O	1:A:193:CYS:HB2	2.06	0.56
1:A:485:MET:CE	1:A:551:TYR:HE1	2.19	0.55
1:A:7:LEU:O	1:A:8:GLU:HB3	2.06	0.55
1:B:122:SER:C	1:B:124:GLY:H	2.10	0.55
1:B:42:THR:HA	1:B:101:SER:HA	1.87	0.55
1:B:9:ARG:HE	1:B:46:GLU:HB2	1.70	0.55
1:C:119:LEU:HD23	1:C:120:GLU:N	2.21	0.55
1:C:232:ASP:CG	1:C:271:ARG:HG2	2.25	0.55
1:C:158:GLU:HG2	1:C:431:VAL:HA	1.87	0.55
1:A:119:LEU:HD23	1:A:120:GLU:N	2.21	0.55
1:A:5:LEU:HD22	1:A:123:THR:HG21	1.87	0.55
1:C:482:SER:HA	2:C:702:ATP:N3	2.22	0.55
1:B:191:ASP:O	1:B:195:ILE:HG13	2.06	0.55
1:B:569:GLU:OE2	1:B:572:ILE:HG12	2.05	0.55
1:C:59:PHE:CE2	1:C:119:LEU:HG	2.41	0.55
1:B:16:THR:HG22	1:B:19:ARG:NH2	2.21	0.55
1:A:19:ARG:CB	1:A:19:ARG:HH11	2.19	0.55
1:A:326:ASP:C	1:A:328:SER:N	2.59	0.55
1:B:96:GLN:O	1:B:97:ASP:HB3	2.06	0.55
1:A:45:PHE:O	1:A:98:CYS:HB3	2.07	0.55
1:B:5:LEU:HD13	1:B:6:VAL:N	2.22	0.55
1:A:226:GLY:HA2	1:A:230:CYS:SG	2.46	0.55
1:A:311:LEU:HD11	1:A:394:PHE:CD2	2.39	0.55
1:A:344:ARG:HD3	1:A:347:LEU:CD1	2.37	0.55
1:B:309:SER:O	1:B:311:LEU:HD22	2.07	0.55
1:C:229:ASN:HD22	1:C:361:PRO:CG	2.20	0.55
1:A:16:THR:HG22	1:A:19:ARG:NH2	2.21	0.55
1:B:354:TRP:O	1:B:376:VAL:HG23	2.07	0.55
1:C:343:THR:C	1:C:345:PRO:HD3	2.27	0.55
1:C:548:TYR:HA	1:C:551:TYR:CE2	2.41	0.55
1:A:42:THR:HA	1:A:101:SER:HA	1.87	0.55
1:C:122:SER:C	1:C:124:GLY:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:HD22	1:C:361:PRO:HG2	1.72	0.55
1:B:302:ASN:ND2	1:B:424:LEU:HD22	2.21	0.55
1:B:687:ALA:O	1:B:688:LEU:HB2	2.07	0.55
1:C:114:LEU:HD21	1:C:134:HIS:HB3	1.89	0.55
1:C:19:ARG:CB	1:C:19:ARG:HH11	2.20	0.55
1:C:371:CYS:HB3	1:C:389:ASP:CB	2.36	0.55
1:C:485:MET:CE	1:C:551:TYR:HE1	2.19	0.55
1:A:354:TRP:O	1:A:376:VAL:HG23	2.08	0.54
1:B:375:PRO:O	1:B:378:ALA:HB3	2.07	0.54
1:B:661:LEU:HD13	1:B:683:ILE:CD1	2.37	0.54
1:B:51:GLU:O	1:B:55:ASP:HB2	2.08	0.54
1:A:57:LEU:HA	1:A:120:GLU:O	2.07	0.54
1:A:358:ASP:O	1:A:370:CYS:HB2	2.06	0.54
1:C:206:ASN:C	1:C:206:ASN:HD22	2.09	0.54
1:C:373:PRO:O	1:C:388:TYR:HB2	2.07	0.54
1:C:513:THR:HG22	1:C:561:ILE:HG12	1.89	0.54
1:A:449:SER:HB2	1:A:451:GLU:OE1	2.07	0.54
1:A:687:ALA:O	1:A:688:LEU:HB2	2.08	0.54
1:A:9:ARG:HE	1:A:46:GLU:HB2	1.71	0.54
1:C:42:THR:HA	1:C:101:SER:HA	1.89	0.54
1:A:588:GLU:HG2	1:A:589:ILE:N	2.23	0.54
1:B:119:LEU:HD23	1:B:120:GLU:N	2.22	0.54
1:B:243:ASN:HA	1:B:245:TYR:CZ	2.43	0.54
1:C:112:ILE:HG12	1:C:214:ARG:O	2.07	0.54
1:C:642:VAL:HG21	1:C:648:VAL:CG2	2.35	0.54
1:A:19:ARG:HB3	1:A:19:ARG:HH11	1.72	0.54
1:B:109:ASN:O	1:B:215:SER:HB2	2.07	0.54
1:B:539:GLU:N	1:C:539:GLU:O	2.40	0.54
1:C:26:LEU:HD13	1:C:185:PHE:CD1	2.43	0.54
1:C:222:ARG:HG2	1:C:373:PRO:HD3	1.87	0.54
1:B:65:PRO:CG	1:B:207:ALA:HB1	2.37	0.54
1:B:218:VAL:HG21	1:B:344:ARG:HH21	1.73	0.54
1:C:583:TYR:H	2:C:702:ATP:N6	1.90	0.54
1:B:609:LEU:HD13	1:B:610:GLN:N	2.23	0.54
1:A:671:ASP:OD2	1:A:672:LYS:HD2	2.08	0.54
1:B:590:LYS:HB2	1:B:608:SER:OG	2.08	0.54
1:C:16:THR:HG22	1:C:19:ARG:NH2	2.23	0.54
1:C:302:ASN:ND2	1:C:424:LEU:HD22	2.21	0.54
1:C:358:ASP:O	1:C:370:CYS:HB2	2.08	0.54
1:A:229:ASN:HD22	1:A:361:PRO:CG	2.21	0.53
1:B:344:ARG:HD3	1:B:347:LEU:CD1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:CD2	1:C:134:HIS:HB3	2.38	0.53
1:C:191:ASP:O	1:C:195:ILE:HG13	2.08	0.53
1:C:344:ARG:HD3	1:C:347:LEU:CD1	2.38	0.53
1:C:590:LYS:HB2	1:C:608:SER:OG	2.08	0.53
1:B:343:THR:C	1:B:345:PRO:HD3	2.28	0.53
1:B:491:VAL:HG23	1:B:544:LEU:HB3	1.90	0.53
1:C:190:LEU:O	1:C:193:CYS:HB2	2.09	0.53
1:A:222:ARG:HG2	1:A:373:PRO:HD2	1.90	0.53
1:B:57:LEU:HA	1:B:120:GLU:O	2.09	0.53
1:B:7:LEU:O	1:B:8:GLU:HB3	2.08	0.53
1:C:226:GLY:HA2	1:C:230:CYS:SG	2.48	0.53
1:C:324:GLN:O	1:C:325:GLY:O	2.26	0.53
1:C:664:LEU:O	1:C:679:PHE:HA	2.09	0.53
1:C:687:ALA:O	1:C:688:LEU:HB2	2.08	0.53
1:A:59:PHE:CE2	1:A:119:LEU:HG	2.43	0.53
1:A:111:PRO:HG3	1:A:215:SER:HB3	1.91	0.53
1:A:309:SER:O	1:A:311:LEU:HD22	2.09	0.53
1:A:114:LEU:CD2	1:A:134:HIS:HB3	2.39	0.53
1:B:371:CYS:HB3	1:B:389:ASP:CB	2.38	0.53
1:C:514:VAL:HG22	1:C:520:LEU:HD23	1.91	0.53
1:B:147:ALA:CB	1:B:343:THR:HG22	2.38	0.53
1:B:499:THR:HG22	1:B:500:ALA:N	2.23	0.53
1:C:19:ARG:HH11	1:C:19:ARG:HB3	1.73	0.53
1:C:600:LYS:O	1:C:600:LYS:HD2	2.09	0.53
1:A:343:THR:C	1:A:345:PRO:HD3	2.28	0.53
1:B:222:ARG:HG2	1:B:373:PRO:HD2	1.91	0.53
1:B:548:TYR:HA	1:B:551:TYR:CE2	2.44	0.53
1:B:485:MET:CE	1:B:551:TYR:HE1	2.22	0.53
1:C:222:ARG:HG2	1:C:373:PRO:HD2	1.90	0.53
1:B:229:ASN:HD22	1:B:361:PRO:CG	2.21	0.52
1:B:358:ASP:O	1:B:370:CYS:HB2	2.08	0.52
1:B:92:VAL:HA	1:B:102:LEU:HD12	1.91	0.52
1:C:65:PRO:CG	1:C:207:ALA:HB1	2.39	0.52
1:A:222:ARG:HG2	1:A:373:PRO:HD3	1.90	0.52
1:A:322:GLU:O	1:A:324:GLN:N	2.42	0.52
1:A:68:SER:H	1:A:74:LYS:HB3	1.73	0.52
1:A:206:ASN:C	1:A:206:ASN:HD22	2.13	0.52
1:A:636:VAL:HG11	1:A:650:VAL:CG2	2.31	0.52
1:A:196:LEU:CD2	1:A:227:MET:HB3	2.40	0.52
1:B:153:GLU:OE2	1:B:156:ARG:NH1	2.42	0.52
1:B:229:ASN:HD22	1:B:361:PRO:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:SER:H	1:B:74:LYS:CB	2.23	0.52
1:C:153:GLU:OE2	1:C:156:ARG:NH1	2.43	0.52
1:A:81:ASP:HB3	1:A:92:VAL:CG1	2.40	0.52
1:B:114:LEU:HD21	1:B:134:HIS:HB3	1.92	0.52
1:B:324:GLN:O	1:B:325:GLY:O	2.28	0.52
1:B:405:ILE:HD12	1:B:575:TYR:CB	2.39	0.52
1:B:513:THR:HG22	1:B:561:ILE:HG12	1.91	0.52
1:B:59:PHE:CE2	1:B:119:LEU:HG	2.44	0.52
1:A:112:ILE:HG12	1:A:214:ARG:O	2.10	0.52
1:A:121:ALA:HB3	1:A:128:SER:O	2.09	0.52
1:A:7:LEU:H	1:A:7:LEU:HD12	1.75	0.52
1:B:104:LEU:N	1:B:104:LEU:HD12	2.25	0.52
1:A:467:GLU:HG2	1:A:469:GLU:OE2	2.10	0.52
1:B:222:ARG:HG2	1:B:373:PRO:HD3	1.91	0.52
1:C:322:GLU:O	1:C:324:GLN:N	2.43	0.52
1:C:499:THR:HG22	1:C:500:ALA:N	2.24	0.52
1:A:229:ASN:HD22	1:A:361:PRO:HG2	1.73	0.52
1:A:548:TYR:HA	1:A:551:TYR:CE2	2.43	0.52
1:A:664:LEU:O	1:A:679:PHE:HA	2.10	0.52
1:B:322:GLU:O	1:B:324:GLN:N	2.42	0.52
1:C:467:GLU:HB3	1:C:469:GLU:OE1	2.09	0.52
1:C:77:PHE:HE1	1:C:90:ALA:HB2	1.75	0.52
1:A:57:LEU:H	1:A:57:LEU:HD22	1.75	0.52
1:A:57:LEU:O	1:A:57:LEU:HD23	2.10	0.52
1:B:68:SER:H	1:B:74:LYS:HB3	1.74	0.52
1:C:77:PHE:CE1	1:C:90:ALA:HB2	2.45	0.52
1:A:307:GLN:NE2	1:A:307:GLN:HA	2.25	0.51
1:A:324:GLN:O	1:A:325:GLY:O	2.28	0.51
1:A:506:ARG:HB2	1:A:568:VAL:HB	1.92	0.51
1:B:514:VAL:HG22	1:B:520:LEU:HD23	1.92	0.51
1:B:308:ASN:O	1:B:309:SER:HB3	2.10	0.51
1:B:661:LEU:HD13	1:B:683:ILE:HD13	1.91	0.51
1:C:80:ARG:O	1:C:91:THR:HA	2.10	0.51
1:B:226:GLY:HA2	1:B:230:CYS:SG	2.50	0.51
1:B:664:LEU:O	1:B:679:PHE:HA	2.10	0.51
1:C:125:TYR:CD1	1:C:126:GLN:HG3	2.46	0.51
1:A:104:LEU:HD12	1:A:104:LEU:N	2.26	0.51
1:B:114:LEU:CD2	1:B:134:HIS:HB3	2.40	0.51
1:B:125:TYR:CD1	1:B:126:GLN:HG3	2.45	0.51
1:B:121:ALA:HB3	1:B:128:SER:O	2.10	0.51
1:C:307:GLN:HA	1:C:307:GLN:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:C	1:A:124:GLY:H	2.14	0.51
1:A:375:PRO:O	1:A:378:ALA:HB3	2.11	0.51
1:B:277:CYS:SG	1:B:516:TYR:OH	2.65	0.51
1:C:9:ARG:HE	1:C:46:GLU:HB2	1.73	0.51
1:A:125:TYR:CD1	1:A:126:GLN:HG3	2.46	0.51
1:A:271:ARG:N	1:A:271:ARG:CD	2.62	0.51
1:A:505:CYS:HB3	1:A:568:VAL:O	2.10	0.51
1:A:92:VAL:HA	1:A:102:LEU:HD12	1.92	0.51
1:B:88:TRP:CH2	1:B:106:THR:HG22	2.46	0.51
1:C:121:ALA:HB3	1:C:128:SER:O	2.10	0.51
1:C:92:VAL:HA	1:C:102:LEU:HD12	1.92	0.51
1:B:196:LEU:CD2	1:B:227:MET:HB3	2.41	0.51
1:B:673:LEU:HD22	1:B:676:VAL:CG1	2.41	0.51
1:C:405:ILE:HD12	1:C:575:TYR:CB	2.40	0.51
1:B:57:LEU:HD22	1:B:57:LEU:H	1.75	0.51
1:B:671:ASP:OD2	1:B:672:LYS:HD2	2.11	0.51
1:C:671:ASP:OD2	1:C:672:LYS:HD2	2.11	0.51
1:A:153:GLU:OE2	1:A:156:ARG:NH1	2.44	0.50
1:C:449:SER:HB2	1:C:451:GLU:OE1	2.11	0.50
1:C:661:LEU:HD13	1:C:683:ILE:HD13	1.93	0.50
1:A:636:VAL:HG23	1:A:652:MET:CE	2.40	0.50
1:C:88:TRP:CH2	1:C:106:THR:HG22	2.46	0.50
1:A:146:ASP:OD1	1:A:147:ALA:N	2.44	0.50
1:A:377:ARG:O	1:A:381:GLU:HG2	2.11	0.50
1:A:642:VAL:HG21	1:A:648:VAL:CG2	2.39	0.50
1:A:514:VAL:HG22	1:A:520:LEU:HD23	1.92	0.50
1:B:326:ASP:O	1:B:328:SER:N	2.45	0.50
1:B:38:PRO:HA	1:B:104:LEU:O	2.12	0.50
1:B:588:GLU:HG2	1:B:589:ILE:N	2.26	0.50
1:C:216:SER:O	1:C:220:VAL:HG23	2.11	0.50
1:C:636:VAL:HG23	1:C:652:MET:CE	2.41	0.50
1:A:68:SER:H	1:A:74:LYS:CB	2.25	0.50
1:B:311:LEU:HD11	1:B:394:PHE:CD2	2.44	0.50
1:B:467:GLU:HG2	1:B:469:GLU:OE2	2.11	0.50
1:B:482:SER:HA	2:B:701:ATP:N3	2.27	0.50
1:B:63:THR:CG2	1:B:64:GLY:H	2.24	0.50
1:C:240:ARG:HB2	1:C:274:TYR:CD1	2.46	0.50
1:A:405:ILE:HD12	1:A:575:TYR:CB	2.41	0.50
1:C:68:SER:H	1:C:74:LYS:CB	2.25	0.50
1:C:104:LEU:N	1:C:104:LEU:HD12	2.26	0.50
1:C:61:VAL:HG21	1:C:88:TRP:CZ3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:O	1:A:23:THR:HG23	2.11	0.49
1:A:467:GLU:HB3	1:A:469:GLU:OE1	2.11	0.49
1:A:499:THR:HG22	1:A:500:ALA:N	2.26	0.49
1:A:4:GLU:OE2	1:A:4:GLU:HA	2.12	0.49
1:B:240:ARG:HB2	1:B:274:TYR:CD1	2.47	0.49
1:B:377:ARG:O	1:B:381:GLU:HG2	2.11	0.49
1:B:449:SER:HB2	1:B:451:GLU:OE1	2.12	0.49
1:B:79:LEU:HD13	1:B:79:LEU:O	2.11	0.49
1:C:511:ALA:C	1:C:512:ARG:HG3	2.32	0.49
1:C:81:ASP:HB3	1:C:92:VAL:CG1	2.42	0.49
1:A:38:PRO:HA	1:A:104:LEU:O	2.12	0.49
1:C:588:GLU:HG2	1:C:589:ILE:N	2.27	0.49
1:C:661:LEU:HD13	1:C:683:ILE:CD1	2.42	0.49
1:A:65:PRO:CG	1:A:207:ALA:HB1	2.42	0.49
1:B:77:PHE:HE1	1:B:90:ALA:HB2	1.77	0.49
1:A:307:GLN:HG3	1:A:313:ILE:HD11	1.93	0.49
1:B:307:GLN:NE2	1:B:307:GLN:HA	2.27	0.49
1:C:163:GLN:CA	1:C:184:GLN:HE22	2.25	0.49
1:C:68:SER:H	1:C:74:LYS:HB3	1.76	0.49
1:A:237:LEU:HD21	1:A:260:ILE:HG21	1.93	0.49
1:B:216:SER:O	1:B:220:VAL:HG23	2.13	0.49
1:A:81:ASP:O	1:B:600:LYS:CD	2.60	0.49
1:A:390:ALA:HB3	1:A:391:PRO:HD3	1.95	0.49
1:A:673:LEU:HD22	1:A:676:VAL:CG1	2.42	0.49
1:C:673:LEU:HD22	1:C:676:VAL:CG1	2.42	0.49
1:A:218:VAL:HG21	1:A:344:ARG:HH21	1.77	0.49
1:B:613:LEU:CD1	1:B:672:LYS:HB3	2.42	0.49
1:B:81:ASP:HB3	1:B:92:VAL:CG1	2.42	0.49
1:A:168:TYR:O	1:A:299:THR:HG21	2.13	0.49
1:A:147:ALA:CB	1:A:343:THR:HG22	2.37	0.49
1:A:588:GLU:HG2	1:A:589:ILE:H	1.78	0.49
1:A:61:VAL:HG21	1:A:88:TRP:CZ3	2.47	0.49
1:B:144:PRO:HA	1:B:149:TYR:CG	2.47	0.49
1:B:499:THR:CG2	1:B:500:ALA:N	2.76	0.49
1:B:506:ARG:HB2	1:B:568:VAL:HB	1.94	0.49
1:C:59:PHE:HE2	1:C:119:LEU:HG	1.77	0.49
1:C:470:GLU:OE2	1:C:473:MET:N	2.46	0.49
1:C:63:THR:HG22	1:C:73:THR:O	2.13	0.49
1:A:513:THR:HG22	1:A:561:ILE:HG12	1.94	0.49
1:A:77:PHE:HE1	1:A:90:ALA:HB2	1.78	0.49
1:B:77:PHE:CE1	1:B:90:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:CD2	1:C:227:MET:HB3	2.42	0.49
1:C:5:LEU:HD13	1:C:6:VAL:N	2.28	0.49
1:B:237:LEU:HD21	1:B:260:ILE:HG21	1.94	0.49
1:B:305:HIS:HD2	1:B:332:TRP:CZ2	2.31	0.49
1:C:237:LEU:HD21	1:C:260:ILE:HG21	1.93	0.49
1:C:375:PRO:O	1:C:378:ALA:HB3	2.12	0.49
1:A:59:PHE:HE2	1:A:119:LEU:HG	1.78	0.48
1:B:186:GLU:OE1	1:B:627:ALA:HB2	2.13	0.48
1:B:307:GLN:HG3	1:B:313:ILE:HD11	1.94	0.48
1:C:377:ARG:O	1:C:381:GLU:HG2	2.13	0.48
1:A:321:GLY:O	1:A:564:ARG:HD2	2.12	0.48
1:B:168:TYR:O	1:B:299:THR:HG21	2.13	0.48
1:C:163:GLN:CG	1:C:184:GLN:NE2	2.70	0.48
1:C:499:THR:CG2	1:C:500:ALA:N	2.75	0.48
1:A:201:PRO:O	1:A:203:PHE:N	2.46	0.48
1:A:308:ASN:O	1:A:309:SER:HB3	2.13	0.48
1:B:10:CYS:CB	1:B:44:HIS:HB2	2.41	0.48
1:B:537:PHE:HB3	1:C:540:LYS:HZ2	1.78	0.48
1:B:7:LEU:H	1:B:7:LEU:HD12	1.78	0.48
1:C:326:ASP:O	1:C:328:SER:N	2.47	0.48
1:A:4:GLU:CG	1:A:5:LEU:H	2.25	0.48
1:A:5:LEU:HD13	1:A:6:VAL:N	2.29	0.48
1:B:624:VAL:HG13	1:B:664:LEU:HD11	1.95	0.48
1:C:12:LEU:CD2	1:C:14:LEU:H	2.27	0.48
1:C:638:ILE:HG13	1:C:648:VAL:HG11	1.96	0.48
1:A:240:ARG:HB2	1:A:274:TYR:CD1	2.48	0.48
1:A:591:ILE:HG12	1:A:607:VAL:HG12	1.96	0.48
1:A:77:PHE:CE1	1:A:90:ALA:HB2	2.49	0.48
1:B:467:GLU:HB3	1:B:469:GLU:OE1	2.14	0.48
1:B:321:GLY:O	1:B:564:ARG:HD2	2.13	0.48
1:C:608:SER:HA	1:C:648:VAL:O	2.14	0.48
1:B:19:ARG:CB	1:B:19:ARG:NH1	2.77	0.48
1:B:470:GLU:OE2	1:B:473:MET:N	2.46	0.48
1:C:591:ILE:HG12	1:C:607:VAL:HG12	1.96	0.48
1:C:63:THR:CG2	1:C:64:GLY:H	2.25	0.48
1:A:470:GLU:OE2	1:A:473:MET:N	2.47	0.48
1:A:80:ARG:O	1:A:91:THR:HA	2.12	0.48
1:B:28:ARG:NH2	1:B:187:ASP:HA	2.26	0.48
1:B:642:VAL:HG21	1:B:648:VAL:CG2	2.42	0.48
1:C:38:PRO:HA	1:C:104:LEU:O	2.14	0.48
1:C:317:ARG:HA	1:C:324:GLN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ARG:HB2	1:C:568:VAL:HB	1.96	0.48
1:A:144:PRO:HA	1:A:149:TYR:CG	2.49	0.48
1:A:160:VAL:CG2	1:A:294:PRO:HG3	2.44	0.48
1:A:326:ASP:O	1:A:328:SER:N	2.47	0.48
1:B:636:VAL:HG23	1:B:652:MET:CE	2.44	0.48
1:A:638:ILE:HG13	1:A:648:VAL:HG11	1.96	0.48
1:C:308:ASN:O	1:C:309:SER:HB3	2.14	0.48
1:A:511:ALA:C	1:A:512:ARG:HG3	2.35	0.47
1:A:661:LEU:HD13	1:A:683:ILE:HD13	1.96	0.47
1:A:514:VAL:CG1	1:A:515:SER:N	2.76	0.47
1:B:21:HIS:O	1:B:23:THR:HG23	2.14	0.47
1:B:479:VAL:HG21	2:B:701:ATP:C8	2.48	0.47
1:B:4:GLU:OE2	1:B:4:GLU:HA	2.14	0.47
1:B:636:VAL:HG23	1:B:652:MET:HE3	1.94	0.47
1:C:307:GLN:HG3	1:C:313:ILE:HD11	1.95	0.47
1:C:7:LEU:H	1:C:7:LEU:HD12	1.79	0.47
1:C:43:LEU:O	1:C:99:THR:HA	2.14	0.47
1:A:88:TRP:CH2	1:A:106:THR:HG22	2.49	0.47
1:B:63:THR:CG2	1:B:64:GLY:N	2.76	0.47
1:C:344:ARG:HD2	1:C:355:GLN:CD	2.35	0.47
2:C:702:ATP:O1G	2:C:702:ATP:O1B	2.31	0.47
1:A:62:VAL:HG12	1:A:74:LYS:CG	2.42	0.47
1:B:61:VAL:HG21	1:B:88:TRP:CZ3	2.49	0.47
1:C:57:LEU:O	1:C:57:LEU:HD23	2.14	0.47
1:A:661:LEU:HD13	1:A:683:ILE:CD1	2.44	0.47
1:A:613:LEU:CD1	1:A:672:LYS:HB3	2.44	0.47
1:B:163:GLN:CA	1:B:184:GLN:HE22	2.26	0.47
1:B:43:LEU:O	1:B:99:THR:HA	2.14	0.47
1:C:29:GLU:O	1:C:30:LYS:CB	2.60	0.47
1:C:7:LEU:HD13	1:C:46:GLU:O	2.14	0.47
1:A:163:GLN:HG2	1:A:184:GLN:HE21	1.72	0.47
1:B:390:ALA:HB3	1:B:391:PRO:HD3	1.97	0.47
1:C:555:LEU:HD21	1:C:559:ASN:HA	1.96	0.47
1:B:59:PHE:HE2	1:B:119:LEU:HG	1.80	0.47
1:C:144:PRO:HA	1:C:149:TYR:CG	2.50	0.47
1:C:237:LEU:HD23	1:C:272:VAL:HB	1.96	0.47
1:C:147:ALA:CB	1:C:343:THR:HG22	2.40	0.47
1:A:407:GLN:C	1:A:409:ASP:H	2.18	0.47
1:A:12:LEU:CD2	1:A:14:LEU:H	2.27	0.47
1:B:511:ALA:C	1:B:512:ARG:HG3	2.35	0.47
1:C:186:GLU:OE1	1:C:627:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LEU:HD21	1:C:260:ILE:CG2	2.45	0.47
1:C:407:GLN:C	1:C:409:ASP:H	2.18	0.47
1:B:213:ARG:C	1:B:215:SER:H	2.19	0.47
1:C:321:GLY:O	1:C:564:ARG:HD2	2.14	0.47
1:C:79:LEU:O	1:C:79:LEU:HD13	2.14	0.47
1:B:344:ARG:CD	1:B:347:LEU:HD12	2.42	0.47
1:B:57:LEU:O	1:B:57:LEU:HD23	2.14	0.47
1:B:638:ILE:HG13	1:B:648:VAL:HG11	1.97	0.47
1:A:273:LYS:HD2	1:A:274:TYR:CE2	2.51	0.46
1:A:355:GLN:HB3	1:A:373:PRO:HB2	1.97	0.46
1:A:309:SER:HB2	1:A:392:PHE:CD1	2.50	0.46
2:B:701:ATP:O2G	2:B:701:ATP:O1B	2.34	0.46
1:C:416:ILE:HB	1:C:576:LEU:CD1	2.42	0.46
1:A:42:THR:HG22	1:A:101:SER:CB	2.46	0.46
1:A:236:VAL:HA	1:A:264:TRP:CD1	2.49	0.46
1:A:499:THR:CG2	1:A:500:ALA:N	2.78	0.46
1:A:94:ASP:OD2	1:A:95:GLN:N	2.44	0.46
1:B:7:LEU:HD13	1:B:46:GLU:O	2.14	0.46
1:A:262:ARG:O	1:A:266:ASN:HB2	2.15	0.46
1:A:81:ASP:HB2	1:B:600:LYS:HZ1	1.80	0.46
1:B:407:GLN:C	1:B:409:ASP:H	2.19	0.46
1:C:390:ALA:HB3	1:C:391:PRO:HD3	1.98	0.46
1:A:420:LEU:C	1:A:420:LEU:HD23	2.35	0.46
1:B:237:LEU:HD23	1:B:272:VAL:HB	1.98	0.46
1:B:29:GLU:O	1:B:30:LYS:CB	2.62	0.46
1:B:514:VAL:CG1	1:B:515:SER:N	2.78	0.46
1:C:168:TYR:O	1:C:299:THR:HG21	2.15	0.46
1:C:202:LYS:HG2	1:C:219:TYR:OH	2.15	0.46
1:C:222:ARG:CG	1:C:373:PRO:HD2	2.46	0.46
1:C:549:GLU:OE1	1:C:549:GLU:HA	2.15	0.46
1:A:317:ARG:NH2	1:A:323:ILE:HD11	2.29	0.46
1:B:317:ARG:HA	1:B:324:GLN:H	1.80	0.46
1:B:350:GLY:N	1:B:352:GLU:OE2	2.46	0.46
1:C:309:SER:HB2	1:C:392:PHE:CE1	2.51	0.46
1:A:19:ARG:CB	1:A:19:ARG:NH1	2.78	0.46
1:A:551:TYR:CD1	1:A:551:TYR:C	2.88	0.46
1:B:309:SER:HB2	1:B:392:PHE:CD1	2.51	0.46
1:C:279:VAL:O	1:C:283:VAL:HG13	2.15	0.46
1:C:57:LEU:HD22	1:C:57:LEU:H	1.81	0.46
1:A:28:ARG:NH2	1:A:187:ASP:HA	2.29	0.46
1:A:323:ILE:HD12	1:A:323:ILE:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:OD2	1:B:243:ASN:N	2.49	0.46
1:B:467:GLU:C	1:B:469:GLU:H	2.20	0.46
1:C:323:ILE:N	1:C:323:ILE:HD12	2.29	0.46
1:C:44:HIS:CD2	1:C:99:THR:HG22	2.50	0.46
1:A:277:CYS:SG	1:A:516:TYR:OH	2.67	0.46
1:A:344:ARG:HD2	1:A:355:GLN:CD	2.36	0.46
1:B:549:GLU:HA	1:B:549:GLU:OE1	2.15	0.46
1:A:279:VAL:O	1:A:283:VAL:HG13	2.15	0.46
1:C:236:VAL:HA	1:C:264:TRP:CD1	2.51	0.46
1:A:216:SER:O	1:A:220:VAL:HG23	2.16	0.46
1:A:309:SER:HB2	1:A:392:PHE:CE1	2.51	0.46
1:A:608:SER:HA	1:A:648:VAL:O	2.16	0.46
1:B:323:ILE:HD12	1:B:323:ILE:N	2.30	0.46
1:B:420:LEU:HD23	1:B:420:LEU:C	2.36	0.46
1:B:532:LEU:HD21	1:B:540:LYS:HG2	1.97	0.46
1:C:19:ARG:CB	1:C:19:ARG:NH1	2.79	0.46
1:B:87:ASP:OD1	1:B:107:PRO:HA	2.16	0.45
1:C:213:ARG:C	1:C:215:SER:H	2.19	0.45
1:C:514:VAL:CG1	1:C:515:SER:N	2.79	0.45
1:C:613:LEU:CD1	1:C:672:LYS:HB3	2.46	0.45
1:A:44:HIS:CD2	1:A:99:THR:HG22	2.52	0.45
1:C:305:HIS:HD2	1:C:332:TRP:CZ2	2.35	0.45
1:C:60:SER:OG	1:C:118:SER:HB2	2.16	0.45
1:A:237:LEU:HD21	1:A:260:ILE:CG2	2.47	0.45
1:B:237:LEU:HD21	1:B:260:ILE:CG2	2.47	0.45
1:C:231:ASN:C	1:C:233:ASP:H	2.18	0.45
1:C:420:LEU:C	1:C:420:LEU:HD23	2.36	0.45
1:B:238:LEU:O	1:B:274:TYR:HA	2.16	0.45
1:B:79:LEU:C	1:B:79:LEU:HD13	2.37	0.45
1:C:467:GLU:C	1:C:469:GLU:H	2.19	0.45
1:A:312:LEU:HD23	1:A:312:LEU:C	2.36	0.45
1:A:467:GLU:C	1:A:469:GLU:H	2.19	0.45
1:C:4:GLU:OE2	1:C:4:GLU:HA	2.17	0.45
1:C:505:CYS:HB3	1:C:568:VAL:O	2.17	0.45
1:A:197:LEU:O	1:A:200:ASN:ND2	2.49	0.45
1:A:317:ARG:HA	1:A:324:GLN:H	1.82	0.45
1:B:312:LEU:HD23	1:B:312:LEU:C	2.36	0.45
1:B:309:SER:HB2	1:B:392:PHE:CE1	2.51	0.45
1:B:591:ILE:HG12	1:B:607:VAL:HG12	1.99	0.45
1:B:62:VAL:HG12	1:B:74:LYS:CG	2.42	0.45
1:C:238:LEU:O	1:C:274:TYR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ILE:CG2	1:C:603:LEU:HD11	2.47	0.45
1:A:29:GLU:O	1:A:30:LYS:CB	2.62	0.45
1:B:206:ASN:OD1	1:B:209:ARG:HB2	2.16	0.45
1:B:551:TYR:C	1:B:551:TYR:CD1	2.89	0.45
1:C:532:LEU:HD21	1:C:540:LYS:HG2	1.98	0.45
1:A:237:LEU:HD23	1:A:272:VAL:HB	1.99	0.45
1:A:238:LEU:O	1:A:274:TYR:HA	2.17	0.45
1:A:43:LEU:O	1:A:99:THR:HA	2.16	0.45
1:B:593:ILE:CG2	1:B:603:LEU:HD11	2.46	0.45
1:C:197:LEU:O	1:C:200:ASN:ND2	2.49	0.45
1:C:41:LEU:HD23	1:C:41:LEU:C	2.38	0.45
1:B:636:VAL:HG11	1:B:650:VAL:CG2	2.34	0.45
1:C:309:SER:HB2	1:C:392:PHE:CD1	2.52	0.45
2:C:702:ATP:H2'	2:C:702:ATP:O5'	2.16	0.45
1:B:236:VAL:HA	1:B:264:TRP:CD1	2.52	0.45
1:B:492:PHE:CD1	1:B:492:PHE:N	2.85	0.45
1:B:94:ASP:OD2	1:B:95:GLN:N	2.45	0.45
1:C:620:CYS:HB2	1:C:638:ILE:HB	1.99	0.45
1:B:231:ASN:C	1:B:233:ASP:H	2.19	0.44
1:B:222:ARG:CG	1:B:373:PRO:HD2	2.48	0.44
1:C:33:VAL:HG23	1:C:137:LEU:CD1	2.45	0.44
1:A:390:ALA:N	1:A:391:PRO:CD	2.79	0.44
1:A:532:LEU:HD21	1:A:540:LYS:HG2	1.98	0.44
1:A:549:GLU:HA	1:A:549:GLU:OE1	2.17	0.44
1:B:242:ASP:O	1:B:243:ASN:CB	2.65	0.44
1:B:348:GLN:CD	1:B:348:GLN:H	2.21	0.44
1:B:4:GLU:CG	1:B:5:LEU:H	2.27	0.44
1:C:21:HIS:O	1:C:23:THR:HG23	2.17	0.44
1:A:344:ARG:CD	1:A:347:LEU:HD12	2.43	0.44
1:A:596:GLU:HA	1:A:597:PRO:HD3	1.82	0.44
1:A:478:ARG:NE	2:A:700:ATP:O3G	2.42	0.44
1:B:147:ALA:HB1	1:B:343:THR:CG2	2.42	0.44
1:B:344:ARG:NH1	1:B:347:LEU:HD11	2.32	0.44
1:B:390:ALA:N	1:B:391:PRO:CD	2.80	0.44
1:B:416:ILE:HB	1:B:576:LEU:CD1	2.44	0.44
1:C:130:PHE:CD2	1:C:130:PHE:N	2.85	0.44
1:C:206:ASN:OD1	1:C:209:ARG:HB2	2.17	0.44
1:C:242:ASP:OD2	1:C:243:ASN:N	2.50	0.44
1:C:42:THR:HG22	1:C:101:SER:CB	2.47	0.44
1:A:60:SER:OG	1:A:118:SER:HB2	2.17	0.44
1:B:355:GLN:HB3	1:B:373:PRO:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:LEU:HG	1:B:509:LEU:CD1	2.46	0.44
1:B:502:GLU:HB3	1:B:536:PRO:HD3	2.00	0.44
1:A:298:VAL:HG12	1:A:299:THR:N	2.32	0.44
1:A:222:ARG:CG	1:A:373:PRO:HD2	2.47	0.44
1:A:451:GLU:HA	1:A:454:GLU:HG2	1.98	0.44
1:C:355:GLN:HB3	1:C:373:PRO:HB2	1.99	0.44
1:C:502:GLU:HB3	1:C:536:PRO:HD3	1.99	0.44
1:C:636:VAL:CG1	1:C:650:VAL:HG21	2.32	0.44
1:B:687:ALA:O	1:B:688:LEU:CB	2.66	0.44
1:C:7:LEU:HD23	1:C:9:ARG:HH21	1.83	0.44
1:A:687:ALA:O	1:A:688:LEU:CB	2.66	0.44
1:C:368:THR:O	1:C:368:THR:HG22	2.18	0.44
1:C:659:MET:HA	1:C:684:ILE:HB	2.00	0.44
1:C:206:ASN:C	1:C:206:ASN:ND2	2.71	0.44
1:C:551:TYR:C	1:C:551:TYR:CD1	2.91	0.44
1:C:642:VAL:CG2	1:C:648:VAL:HG22	2.45	0.44
1:C:687:ALA:O	1:C:688:LEU:CB	2.65	0.44
1:A:176:LYS:HG3	1:A:583:TYR:CE2	2.53	0.43
1:A:186:GLU:OE1	1:A:627:ALA:HB2	2.18	0.43
1:A:206:ASN:OD1	1:A:209:ARG:HB2	2.18	0.43
1:A:79:LEU:O	1:A:79:LEU:HD13	2.18	0.43
1:B:348:GLN:OE1	1:B:348:GLN:N	2.44	0.43
1:B:527:LYS:O	1:B:528:TYR:CD2	2.71	0.43
1:B:571:VAL:C	1:B:573:ASN:H	2.21	0.43
1:B:588:GLU:HG2	1:B:589:ILE:H	1.82	0.43
1:C:28:ARG:NH2	1:C:187:ASP:HA	2.28	0.43
1:C:636:VAL:HG23	1:C:652:MET:HE3	2.00	0.43
1:A:130:PHE:N	1:A:130:PHE:CD2	2.85	0.43
1:A:163:GLN:CA	1:A:184:GLN:HE22	2.30	0.43
1:C:451:GLU:HA	1:C:454:GLU:HG2	1.98	0.43
1:B:539:GLU:O	1:C:539:GLU:N	2.51	0.43
1:B:12:LEU:CD2	1:B:14:LEU:H	2.29	0.43
1:C:344:ARG:CD	1:C:347:LEU:HD12	2.44	0.43
1:C:348:GLN:OE1	1:C:348:GLN:N	2.46	0.43
1:A:348:GLN:H	1:A:348:GLN:CD	2.22	0.43
1:A:63:THR:HG22	1:A:73:THR:O	2.18	0.43
1:B:41:LEU:HD23	1:B:41:LEU:C	2.38	0.43
1:B:659:MET:HA	1:B:684:ILE:HB	2.01	0.43
1:A:593:ILE:CG2	1:A:603:LEU:HD11	2.49	0.43
1:B:44:HIS:CD2	1:B:99:THR:HG22	2.54	0.43
1:C:218:VAL:HG21	1:C:344:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:GLY:N	1:C:452:GLU:OE2	2.51	0.43
1:C:311:LEU:HB3	1:C:461:HIS:ND1	2.33	0.43
1:B:199:VAL:HG22	1:B:199:VAL:O	2.18	0.43
1:B:57:LEU:CD2	1:B:57:LEU:N	2.77	0.43
1:B:63:THR:HG22	1:B:73:THR:O	2.18	0.43
1:C:390:ALA:N	1:C:391:PRO:CD	2.81	0.43
1:C:492:PHE:N	1:C:492:PHE:CD1	2.86	0.43
1:A:87:ASP:OD1	1:A:107:PRO:HA	2.19	0.43
1:B:451:GLU:HA	1:B:454:GLU:HG2	2.01	0.43
1:B:527:LYS:O	1:B:528:TYR:HD2	2.02	0.43
1:C:344:ARG:NH1	1:C:347:LEU:HD11	2.33	0.43
1:C:514:VAL:HG22	1:C:520:LEU:CD2	2.48	0.43
1:C:588:GLU:HG2	1:C:589:ILE:H	1.83	0.43
1:C:63:THR:CG2	1:C:64:GLY:N	2.78	0.43
1:C:87:ASP:OD1	1:C:107:PRO:HA	2.19	0.43
1:A:10:CYS:CB	1:A:44:HIS:HB2	2.45	0.43
1:A:7:LEU:HD13	1:A:46:GLU:O	2.19	0.43
1:A:527:LYS:O	1:A:528:TYR:CD2	2.72	0.43
1:B:197:LEU:O	1:B:200:ASN:ND2	2.50	0.43
1:B:19:ARG:NH1	1:B:19:ARG:HB2	2.34	0.43
1:B:229:ASN:O	1:B:230:CYS:C	2.57	0.43
1:B:33:VAL:HG23	1:B:137:LEU:CD1	2.47	0.43
1:B:535:GLU:HB3	1:C:535:GLU:HG3	2.01	0.43
1:B:634:LYS:C	1:B:652:MET:HE1	2.39	0.43
1:A:492:PHE:CD1	1:A:492:PHE:N	2.86	0.43
1:B:273:LYS:HA	1:B:273:LYS:HD3	1.81	0.43
1:B:469:GLU:C	1:B:470:GLU:HG3	2.39	0.43
1:B:81:ASP:OD2	1:B:81:ASP:N	2.51	0.43
1:A:344:ARG:NH1	1:A:347:LEU:HD11	2.34	0.43
1:B:232:ASP:C	1:B:234:GLN:N	2.72	0.43
1:A:199:VAL:HG22	1:A:199:VAL:O	2.19	0.42
1:A:555:LEU:HD21	1:A:559:ASN:HA	2.01	0.42
1:A:508:LEU:O	1:A:565:ALA:HA	2.19	0.42
1:C:310:ASN:C	1:C:312:LEU:H	2.22	0.42
1:C:312:LEU:HD23	1:C:312:LEU:C	2.40	0.42
1:C:617:LEU:O	1:C:641:PRO:HA	2.19	0.42
1:A:229:ASN:O	1:A:230:CYS:C	2.57	0.42
1:A:305:HIS:HD2	1:A:332:TRP:CZ2	2.38	0.42
1:A:348:GLN:N	1:A:348:GLN:OE1	2.47	0.42
1:A:41:LEU:C	1:A:41:LEU:HD23	2.40	0.42
1:B:130:PHE:N	1:B:130:PHE:CD2	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASN:ND2	1:B:206:ASN:C	2.70	0.42
1:B:7:LEU:HD23	1:B:9:ARG:HH21	1.84	0.42
1:A:571:VAL:C	1:A:573:ASN:H	2.22	0.42
1:B:199:VAL:HG22	1:B:234:GLN:HG2	2.00	0.42
1:B:508:LEU:O	1:B:565:ALA:HA	2.18	0.42
1:B:176:LYS:HG3	1:B:583:TYR:CE2	2.55	0.42
1:B:601:ARG:O	1:B:655:LEU:HD12	2.19	0.42
1:C:176:LYS:HG3	1:C:583:TYR:CE2	2.55	0.42
1:A:196:LEU:HD21	1:A:227:MET:HB3	2.00	0.42
1:A:542:VAL:HA	1:A:543:PRO:HD3	1.72	0.42
1:B:163:GLN:CG	1:B:184:GLN:NE2	2.72	0.42
1:B:344:ARG:HD2	1:B:355:GLN:CD	2.39	0.42
1:B:368:THR:HG22	1:B:368:THR:O	2.20	0.42
1:A:19:ARG:HB2	1:A:19:ARG:NH1	2.34	0.42
1:A:7:LEU:HD23	1:A:9:ARG:HH21	1.83	0.42
1:C:146:ASP:OD1	1:C:147:ALA:N	2.52	0.42
1:C:364:LYS:C	1:C:366:GLU:H	2.23	0.42
1:A:202:LYS:HG2	1:A:219:TYR:OH	2.19	0.42
1:A:216:SER:OG	1:A:218:VAL:HG13	2.19	0.42
1:B:317:ARG:NH2	1:B:323:ILE:HD11	2.34	0.42
1:B:431:VAL:O	1:B:431:VAL:HG22	2.19	0.42
1:B:608:SER:HA	1:B:648:VAL:O	2.20	0.42
1:C:273:LYS:HD2	1:C:274:TYR:CE2	2.55	0.42
1:A:323:ILE:CD1	1:A:323:ILE:H	2.31	0.42
1:B:115:TYR:HB2	1:B:135:PHE:CE1	2.55	0.42
1:B:202:LYS:HG2	1:B:219:TYR:OH	2.19	0.42
1:B:160:VAL:CG2	1:B:294:PRO:HG3	2.50	0.42
1:A:213:ARG:C	1:A:215:SER:H	2.23	0.42
1:A:624:VAL:HG13	1:A:664:LEU:HD11	2.01	0.42
1:B:512:ARG:HG2	1:B:523:GLU:CA	2.47	0.42
1:B:80:ARG:O	1:B:91:THR:HA	2.19	0.42
1:C:202:LYS:NZ	1:C:213:ARG:HH22	2.18	0.42
1:C:317:ARG:HD3	1:C:321:GLY:C	2.40	0.42
1:C:424:LEU:HD12	1:C:424:LEU:HA	1.88	0.42
1:C:507:LEU:HG	1:C:509:LEU:CD1	2.49	0.42
1:C:571:VAL:C	1:C:573:ASN:H	2.21	0.42
1:A:177:ASN:CG	1:A:177:ASN:O	2.58	0.42
1:A:300:ASN:O	1:A:334:PHE:HA	2.19	0.42
1:A:527:LYS:O	1:A:528:TYR:HD2	2.03	0.42
1:B:143:CYS:HA	1:B:144:PRO:HD3	1.88	0.42
1:B:317:ARG:HD3	1:B:321:GLY:C	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ASN:HD21	1:B:420:LEU:HB2	1.84	0.42
1:C:229:ASN:ND2	1:C:361:PRO:HG2	2.35	0.42
1:C:599:GLN:O	1:C:600:LYS:C	2.58	0.42
1:A:311:LEU:HB3	1:A:461:HIS:ND1	2.35	0.42
1:A:502:GLU:HB3	1:A:536:PRO:HD3	2.02	0.42
1:A:4:GLU:CG	1:A:5:LEU:N	2.83	0.42
1:B:262:ARG:O	1:B:266:ASN:HB2	2.20	0.42
1:B:276:GLN:O	1:B:279:VAL:N	2.52	0.42
1:C:199:VAL:HG22	1:C:199:VAL:O	2.20	0.42
1:A:232:ASP:C	1:A:234:GLN:N	2.72	0.41
1:A:81:ASP:N	1:A:81:ASP:OD2	2.52	0.41
1:B:6:VAL:HG21	1:B:121:ALA:HB1	2.02	0.41
1:B:240:ARG:NH1	1:B:274:TYR:CZ	2.88	0.41
1:B:42:THR:HG22	1:B:101:SER:CB	2.47	0.41
1:A:273:LYS:HA	1:A:273:LYS:HD3	1.85	0.41
1:A:33:VAL:HG23	1:A:137:LEU:CD1	2.48	0.41
1:A:599:GLN:O	1:A:600:LYS:C	2.58	0.41
1:A:659:MET:HA	1:A:684:ILE:HB	2.02	0.41
1:A:479:VAL:HG21	2:A:700:ATP:C8	2.55	0.41
1:B:146:ASP:OD1	1:B:147:ALA:N	2.52	0.41
1:B:650:VAL:HG22	1:B:651:ARG:N	2.35	0.41
1:C:175:ILE:HG23	1:C:301:TYR:OH	2.20	0.41
1:C:320:PHE:HE2	1:C:528:TYR:CE1	2.38	0.41
1:A:231:ASN:C	1:A:233:ASP:H	2.21	0.41
1:A:350:GLY:N	1:A:352:GLU:OE2	2.49	0.41
1:A:617:LEU:O	1:A:641:PRO:HA	2.21	0.41
1:B:279:VAL:O	1:B:283:VAL:HG13	2.20	0.41
1:C:19:ARG:HB2	1:C:19:ARG:NH1	2.35	0.41
1:C:199:VAL:HG22	1:C:234:GLN:HG2	2.02	0.41
1:C:469:GLU:C	1:C:470:GLU:HG3	2.40	0.41
1:C:89:THR:HG23	1:C:105:THR:HB	2.02	0.41
1:A:62:VAL:HB	1:A:67:PRO:HG3	2.02	0.41
1:B:273:LYS:HD2	1:B:274:TYR:CE2	2.55	0.41
1:B:305:HIS:CG	1:B:306:ASP:N	2.88	0.41
1:B:46:GLU:O	1:B:48:ARG:N	2.52	0.41
1:C:160:VAL:CG2	1:C:294:PRO:HG3	2.50	0.41
1:C:242:ASP:O	1:C:243:ASN:CB	2.68	0.41
1:C:305:HIS:CG	1:C:306:ASP:N	2.88	0.41
1:C:673:LEU:HD22	1:C:676:VAL:HG11	2.02	0.41
1:A:153:GLU:OE2	1:A:153:GLU:HA	2.21	0.41
1:A:231:ASN:OD1	1:A:233:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:C	1:A:312:LEU:H	2.22	0.41
1:A:318:ASN:C	1:A:320:PHE:H	2.24	0.41
1:A:448:GLY:N	1:A:452:GLU:OE2	2.52	0.41
1:A:457:THR:C	1:A:459:ALA:H	2.24	0.41
1:A:507:LEU:HG	1:A:509:LEU:CD1	2.48	0.41
1:B:242:ASP:O	1:B:243:ASN:HB3	2.21	0.41
2:B:701:ATP:H5'1	2:B:701:ATP:O1B	2.20	0.41
1:C:6:VAL:HG21	1:C:121:ALA:HB1	2.02	0.41
1:C:262:ARG:O	1:C:266:ASN:HB2	2.20	0.41
1:C:348:GLN:CD	1:C:348:GLN:H	2.21	0.41
1:C:381:GLU:O	1:C:455:ALA:HA	2.21	0.41
1:B:538:SER:CB	1:C:538:SER:HB3	2.42	0.41
1:A:364:LYS:C	1:A:366:GLU:H	2.24	0.41
1:A:464:LYS:O	1:A:464:LYS:HG3	2.21	0.41
1:B:307:GLN:C	1:B:309:SER:H	2.23	0.41
1:C:62:VAL:HG12	1:C:74:LYS:CG	2.41	0.41
1:A:317:ARG:CZ	1:A:323:ILE:CD1	2.94	0.41
1:A:469:GLU:C	1:A:470:GLU:HG3	2.40	0.41
1:A:640:ASP:HB3	1:A:641:PRO:HD2	2.02	0.41
1:B:196:LEU:HD21	1:B:227:MET:HB3	2.02	0.41
1:B:310:ASN:C	1:B:312:LEU:H	2.24	0.41
1:C:431:VAL:HG22	1:C:431:VAL:O	2.21	0.41
1:C:4:GLU:CG	1:C:5:LEU:H	2.28	0.41
1:C:79:LEU:C	1:C:79:LEU:HD13	2.40	0.41
1:A:242:ASP:OD2	1:A:243:ASN:N	2.53	0.41
1:A:317:ARG:HD3	1:A:321:GLY:C	2.41	0.41
1:A:57:LEU:CD2	1:A:57:LEU:N	2.78	0.41
1:A:642:VAL:CG2	1:A:648:VAL:HG22	2.48	0.41
1:C:232:ASP:C	1:C:234:GLN:N	2.73	0.41
1:C:231:ASN:OD1	1:C:233:ASP:HB2	2.19	0.41
1:A:242:ASP:O	1:A:243:ASN:CB	2.68	0.41
1:A:502:GLU:HB3	1:A:536:PRO:HG3	2.03	0.41
1:B:317:ARG:HG2	1:B:323:ILE:HA	2.03	0.41
1:B:323:ILE:H	1:B:323:ILE:CD1	2.32	0.41
1:B:535:GLU:HB3	1:C:535:GLU:CB	2.51	0.41
1:B:505:CYS:HB3	1:B:568:VAL:O	2.20	0.41
1:C:187:ASP:OD2	1:C:188:GLY:N	2.54	0.41
1:B:535:GLU:HG3	1:C:535:GLU:HB3	2.03	0.41
1:C:508:LEU:O	1:C:565:ALA:HA	2.20	0.41
1:A:326:ASP:O	1:A:327:LYS:HB2	2.21	0.41
1:B:34:ARG:HB3	1:B:140:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASN:ND2	1:B:361:PRO:HG2	2.36	0.41
1:B:448:GLY:N	1:B:452:GLU:OE2	2.53	0.41
1:B:502:GLU:HB3	1:B:536:PRO:HG3	2.03	0.41
1:B:53:SER:HB2	1:B:54:VAL:H	1.66	0.41
1:B:583:TYR:H	2:B:701:ATP:N6	1.97	0.41
1:B:600:LYS:CD	1:B:600:LYS:O	2.69	0.41
1:B:60:SER:OG	1:B:118:SER:HB2	2.20	0.41
1:C:229:ASN:O	1:C:230:CYS:C	2.58	0.41
1:A:6:VAL:HG21	1:A:121:ALA:HB1	2.03	0.40
1:A:216:SER:OG	1:A:218:VAL:CG1	2.69	0.40
1:A:636:VAL:HG23	1:A:652:MET:HE3	2.03	0.40
1:C:10:CYS:CB	1:C:44:HIS:HB2	2.45	0.40
1:C:502:GLU:HB3	1:C:536:PRO:HG3	2.03	0.40
1:C:638:ILE:HA	1:C:639:PRO:HD2	1.89	0.40
1:A:63:THR:CG2	1:A:64:GLY:N	2.80	0.40
1:B:379:ILE:HD12	1:B:393:VAL:HB	2.04	0.40
1:B:311:LEU:HB3	1:B:461:HIS:ND1	2.37	0.40
1:B:596:GLU:HA	1:B:597:PRO:HD3	1.83	0.40
1:C:308:ASN:O	1:C:309:SER:HB2	2.21	0.40
1:A:147:ALA:HB1	1:A:343:THR:CG2	2.39	0.40
1:A:508:LEU:HD22	1:A:508:LEU:N	2.36	0.40
1:A:600:LYS:O	1:A:600:LYS:CD	2.68	0.40
1:B:136:ILE:HD12	1:B:190:LEU:HD13	2.03	0.40
1:B:343:THR:O	1:B:345:PRO:HD3	2.22	0.40
1:B:593:ILE:HG22	1:B:603:LEU:HD11	2.03	0.40
1:C:307:GLN:C	1:C:309:SER:H	2.25	0.40
1:C:57:LEU:CD2	1:C:57:LEU:N	2.82	0.40
1:C:655:LEU:HA	1:C:655:LEU:HD12	1.86	0.40
1:A:201:PRO:O	1:A:202:LYS:C	2.59	0.40
1:A:416:ILE:HB	1:A:576:LEU:CD1	2.46	0.40
1:A:63:THR:CG2	1:A:64:GLY:H	2.29	0.40
1:B:240:ARG:NH1	1:B:274:TYR:OH	2.55	0.40
1:B:300:ASN:O	1:B:334:PHE:HA	2.22	0.40
1:B:335:HIS:NE2	1:B:358:ASP:OD2	2.46	0.40
1:B:9:ARG:NE	1:B:46:GLU:HB2	2.36	0.40
1:C:242:ASP:O	1:C:243:ASN:HB3	2.22	0.40
1:C:318:ASN:C	1:C:320:PHE:H	2.24	0.40
1:C:81:ASP:N	1:C:81:ASP:OD2	2.53	0.40
1:A:601:ARG:O	1:A:655:LEU:HD12	2.22	0.40
1:A:673:LEU:HD22	1:A:676:VAL:HG11	2.04	0.40
1:A:93:VAL:HG12	1:A:101:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HG13	1:B:625:GLU:OE1	2.22	0.40
1:C:350:GLY:N	1:C:352:GLU:OE2	2.48	0.40
1:C:62:VAL:HB	1:C:67:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	679/697 (97%)	561 (83%)	81 (12%)	37 (5%)	2	10
1	B	679/697 (97%)	564 (83%)	77 (11%)	38 (6%)	2	10
1	C	679/697 (97%)	563 (83%)	78 (12%)	38 (6%)	2	10
All	All	2037/2091 (97%)	1688 (83%)	236 (12%)	113 (6%)	2	10

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	30	LYS
1	A	67	PRO
1	A	87	ASP
1	A	309	SER
1	A	323	ILE
1	A	325	GLY
1	A	326	ASP
1	A	349	PRO
1	A	425	LYS
1	A	449	SER
1	A	466	ALA
1	A	470	GLU
1	A	571	VAL

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Mol	Chain	Res	Type
1	A	646	GLU
1	B	14	LEU
1	B	30	LYS
1	B	67	PRO
1	B	87	ASP
1	B	309	SER
1	B	323	ILE
1	B	325	GLY
1	B	326	ASP
1	B	349	PRO
1	B	449	SER
1	B	466	ALA
1	B	470	GLU
1	B	571	VAL
1	B	646	GLU
1	C	14	LEU
1	C	30	LYS
1	C	67	PRO
1	C	87	ASP
1	C	309	SER
1	C	323	ILE
1	C	325	GLY
1	C	326	ASP
1	C	349	PRO
1	C	425	LYS
1	C	449	SER
1	C	466	ALA
1	C	470	GLU
1	C	571	VAL
1	C	646	GLU
1	A	53	SER
1	A	202	LYS
1	A	388	TYR
1	A	409	ASP
1	B	53	SER
1	B	388	TYR
1	B	409	ASP
1	B	425	LYS
1	C	53	SER
1	C	388	TYR
1	C	409	ASP
1	A	10	CYS

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Mol	Chain	Res	Type
1	A	11	ASP
1	A	47	GLY
1	A	183	GLY
1	A	206	ASN
1	A	243	ASN
1	A	365	SER
1	B	10	CYS
1	B	11	ASP
1	B	47	GLY
1	B	202	LYS
1	B	206	ASN
1	B	243	ASN
1	B	365	SER
1	C	10	CYS
1	C	11	ASP
1	C	47	GLY
1	C	202	LYS
1	C	206	ASN
1	C	243	ASN
1	C	365	SER
1	A	95	GLN
1	A	97	ASP
1	A	234	GLN
1	A	273	LYS
1	A	274	TYR
1	A	468	LYS
1	B	95	GLN
1	B	97	ASP
1	B	234	GLN
1	B	274	TYR
1	B	468	LYS
1	C	95	GLN
1	C	97	ASP
1	C	234	GLN
1	C	274	TYR
1	C	468	LYS
1	A	68	SER
1	A	214	ARG
1	A	230	CYS
1	B	68	SER
1	B	214	ARG
1	B	230	CYS

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Mol	Chain	Res	Type
1	B	273	LYS
1	C	123	THR
1	C	214	ARG
1	C	230	CYS
1	C	273	LYS
1	A	123	THR
1	B	123	THR
1	C	68	SER
1	A	201	PRO
1	C	183	GLY
1	B	183	GLY
1	B	201	PRO
1	B	246	GLY
1	C	201	PRO
1	C	426	ILE

### 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	593/606 (98%)	534 (90%)	59 (10%)	8	27
1	B	593/606 (98%)	531 (90%)	62 (10%)	7	24
1	C	593/606 (98%)	533 (90%)	60 (10%)	7	26
All	All	1779/1818 (98%)	1598 (90%)	181 (10%)	7	25

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	VAL
1	A	10	CYS
1	A	12	LEU
1	A	15	GLU
1	A	51	GLU
1	A	57	LEU

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Mol	Chain	Res	Type
1	A	58	THR
1	A	79	LEU
1	A	80	ARG
1	A	89	THR
1	A	96	GLN
1	A	102	LEU
1	A	106	THR
1	A	114	LEU
1	A	119	LEU
1	A	125	TYR
1	A	126	GLN
1	A	128	SER
1	A	130	PHE
1	A	151	ASP
1	A	157	GLN
1	A	176	LYS
1	A	190	LEU
1	A	196	LEU
1	A	206	ASN
1	A	230	CYS
1	A	257	SER
1	A	271	ARG
1	A	291	LEU
1	A	297	VAL
1	A	306	ASP
1	A	346	ASP
1	A	349	PRO
1	A	363	GLU
1	A	377	ARG
1	A	424	LEU
1	A	427	SER
1	A	431	VAL
1	A	435	GLU
1	A	458	ARG
1	A	468	LYS
1	A	469	GLU
1	A	470	GLU
1	A	481	GLN
1	A	485	MET
1	A	504	VAL
1	A	516	TYR
1	A	532	LEU

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Mol	Chain	Res	Type
1	A	557	GLU
1	A	569	GLU
1	A	577	LEU
1	A	582	LEU
1	A	609	LEU
1	A	617	LEU
1	A	629	LEU
1	A	630	THR
1	A	666	VAL
1	A	673	LEU
1	B	5	LEU
1	B	6	VAL
1	B	10	CYS
1	B	12	LEU
1	B	15	GLU
1	B	26	LEU
1	B	51	GLU
1	B	53	SER
1	B	57	LEU
1	B	58	THR
1	B	79	LEU
1	B	80	ARG
1	B	89	THR
1	B	96	GLN
1	B	102	LEU
1	B	106	THR
1	B	114	LEU
1	B	119	LEU
1	B	125	TYR
1	B	126	GLN
1	B	128	SER
1	B	130	PHE
1	B	151	ASP
1	B	157	GLN
1	B	176	LYS
1	B	190	LEU
1	B	196	LEU
1	B	206	ASN
1	B	230	CYS
1	B	244	ASN
1	B	257	SER
1	B	271	ARG

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Mol	Chain	Res	Type
1	B	291	LEU
1	B	297	VAL
1	B	306	ASP
1	B	346	ASP
1	B	349	PRO
1	B	363	GLU
1	B	377	ARG
1	B	424	LEU
1	B	427	SER
1	B	431	VAL
1	B	435	GLU
1	B	458	ARG
1	B	468	LYS
1	B	469	GLU
1	B	470	GLU
1	B	481	GLN
1	B	485	MET
1	B	504	VAL
1	B	516	TYR
1	B	532	LEU
1	B	557	GLU
1	B	569	GLU
1	B	577	LEU
1	B	582	LEU
1	B	609	LEU
1	B	617	LEU
1	B	629	LEU
1	B	630	THR
1	B	666	VAL
1	B	673	LEU
1	C	5	LEU
1	C	6	VAL
1	C	10	CYS
1	C	12	LEU
1	C	15	GLU
1	C	26	LEU
1	C	51	GLU
1	C	53	SER
1	C	57	LEU
1	C	58	THR
1	C	79	LEU
1	C	80	ARG

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Mol	Chain	Res	Type
1	C	89	THR
1	C	96	GLN
1	C	102	LEU
1	C	106	THR
1	C	114	LEU
1	C	125	TYR
1	C	126	GLN
1	C	128	SER
1	C	130	PHE
1	C	151	ASP
1	C	157	GLN
1	C	176	LYS
1	C	190	LEU
1	C	196	LEU
1	C	206	ASN
1	C	230	CYS
1	C	257	SER
1	C	271	ARG
1	C	291	LEU
1	C	297	VAL
1	C	306	ASP
1	C	346	ASP
1	C	349	PRO
1	C	363	GLU
1	C	377	ARG
1	C	424	LEU
1	C	427	SER
1	C	431	VAL
1	C	435	GLU
1	C	458	ARG
1	C	468	LYS
1	C	469	GLU
1	C	470	GLU
1	C	481	GLN
1	C	485	MET
1	C	504	VAL
1	C	516	TYR
1	C	532	LEU
1	C	557	GLU
1	C	569	GLU
1	C	577	LEU
1	C	582	LEU

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Mol	Chain	Res	Type
1	C	609	LEU
1	C	617	LEU
1	C	629	LEU
1	C	630	THR
1	C	666	VAL
1	C	673	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	95	GLN
1	A	103	GLN
1	A	157	GLN
1	A	164	GLN
1	A	169	GLN
1	A	184	GLN
1	A	206	ASN
1	A	229	ASN
1	A	243	ASN
1	A	276	GLN
1	A	302	ASN
1	A	307	GLN
1	A	362	GLN
1	A	413	HIS
1	A	417	ASN
1	A	573	ASN
1	B	17	ASN
1	B	95	GLN
1	B	103	GLN
1	B	157	GLN
1	B	164	GLN
1	B	169	GLN
1	B	184	GLN
1	B	206	ASN
1	B	229	ASN
1	B	243	ASN
1	B	276	GLN
1	B	302	ASN
1	B	307	GLN
1	B	362	GLN
1	B	413	HIS

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Mol	Chain	Res	Type
1	B	417	ASN
1	B	573	ASN
1	C	17	ASN
1	C	95	GLN
1	C	103	GLN
1	C	157	GLN
1	C	164	GLN
1	C	169	GLN
1	C	184	GLN
1	C	206	ASN
1	C	229	ASN
1	C	243	ASN
1	C	276	GLN
1	C	302	ASN
1	C	307	GLN
1	C	362	GLN
1	C	413	HIS
1	C	417	ASN
1	C	573	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ATP	B	701	-	26,33,33	1.29	3 (11%)	31,52,52	1.57	5 (16%)
2	ATP	C	702	-	26,33,33	1.30	3 (11%)	31,52,52	1.53	5 (16%)
2	ATP	A	700	-	26,33,33	1.31	3 (11%)	31,52,52	1.67	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	701	-	-	1/18/38/38	0/3/3/3
2	ATP	C	702	-	-	4/18/38/38	0/3/3/3
2	ATP	A	700	-	-	3/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	702	ATP	PG-O1G	3.45	1.61	1.50
2	B	701	ATP	PG-O1G	3.41	1.61	1.50
2	A	700	ATP	PG-O1G	3.36	1.61	1.50
2	A	700	ATP	PB-O1B	3.02	1.61	1.50
2	B	701	ATP	PB-O1B	2.98	1.61	1.50
2	C	702	ATP	PB-O1B	2.95	1.61	1.50
2	C	702	ATP	O4'-C1'	2.34	1.44	1.41
2	A	700	ATP	O4'-C1'	2.28	1.44	1.41
2	B	701	ATP	O4'-C1'	2.23	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ATP	N3-C2-N1	-4.61	121.47	128.68
2	A	700	ATP	PB-O3B-PG	-4.61	117.00	132.83
2	C	702	ATP	N3-C2-N1	-4.59	121.50	128.68
2	B	701	ATP	N3-C2-N1	-4.45	121.73	128.68
2	B	701	ATP	PB-O3B-PG	-4.06	118.88	132.83
2	C	702	ATP	PB-O3B-PG	-3.36	121.29	132.83
2	A	700	ATP	PA-O3A-PB	-2.91	122.83	132.83
2	C	702	ATP	PA-O3A-PB	-2.84	123.08	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ATP	PA-O3A-PB	-2.75	123.39	132.83
2	A	700	ATP	O2G-PG-O3B	2.52	113.10	104.64
2	B	701	ATP	O2G-PG-O3B	2.39	112.65	104.64
2	A	700	ATP	C3'-C2'-C1'	-2.35	97.44	100.98
2	A	700	ATP	O4'-C1'-C2'	-2.26	103.63	106.93
2	C	702	ATP	C3'-C2'-C1'	-2.21	97.66	100.98
2	C	702	ATP	O2G-PG-O3B	2.13	111.77	104.64
2	B	701	ATP	C3'-C2'-C1'	-2.05	97.89	100.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	702	ATP	PB-O3B-PG-O3G
2	C	702	ATP	PB-O3A-PA-O1A
2	A	700	ATP	PB-O3A-PA-O1A
2	A	700	ATP	PB-O3A-PA-O2A
2	B	701	ATP	PA-O3A-PB-O2B
2	C	702	ATP	PA-O3A-PB-O2B
2	C	702	ATP	PB-O3A-PA-O2A
2	A	700	ATP	PG-O3B-PB-O2B

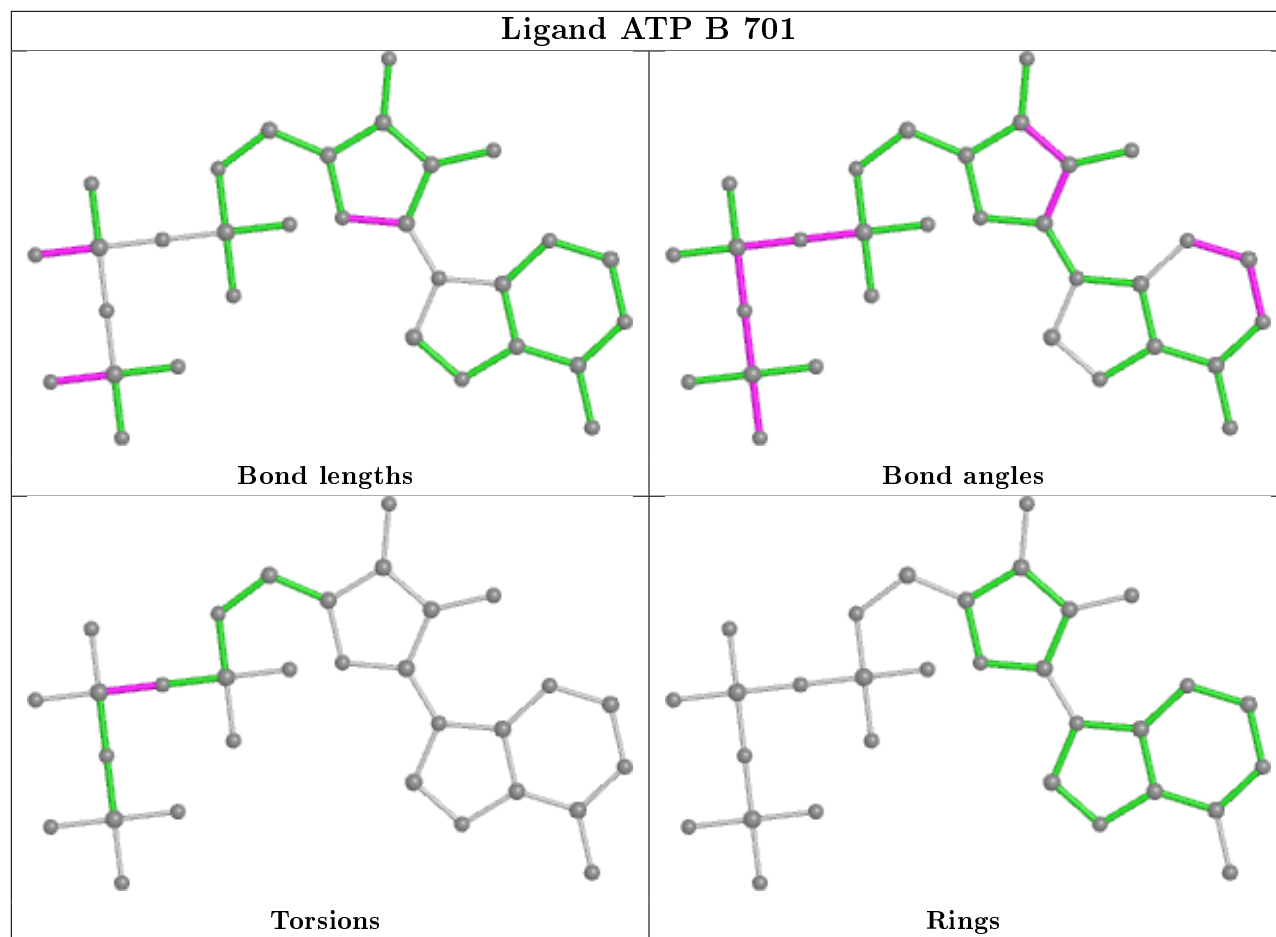
There are no ring outliers.

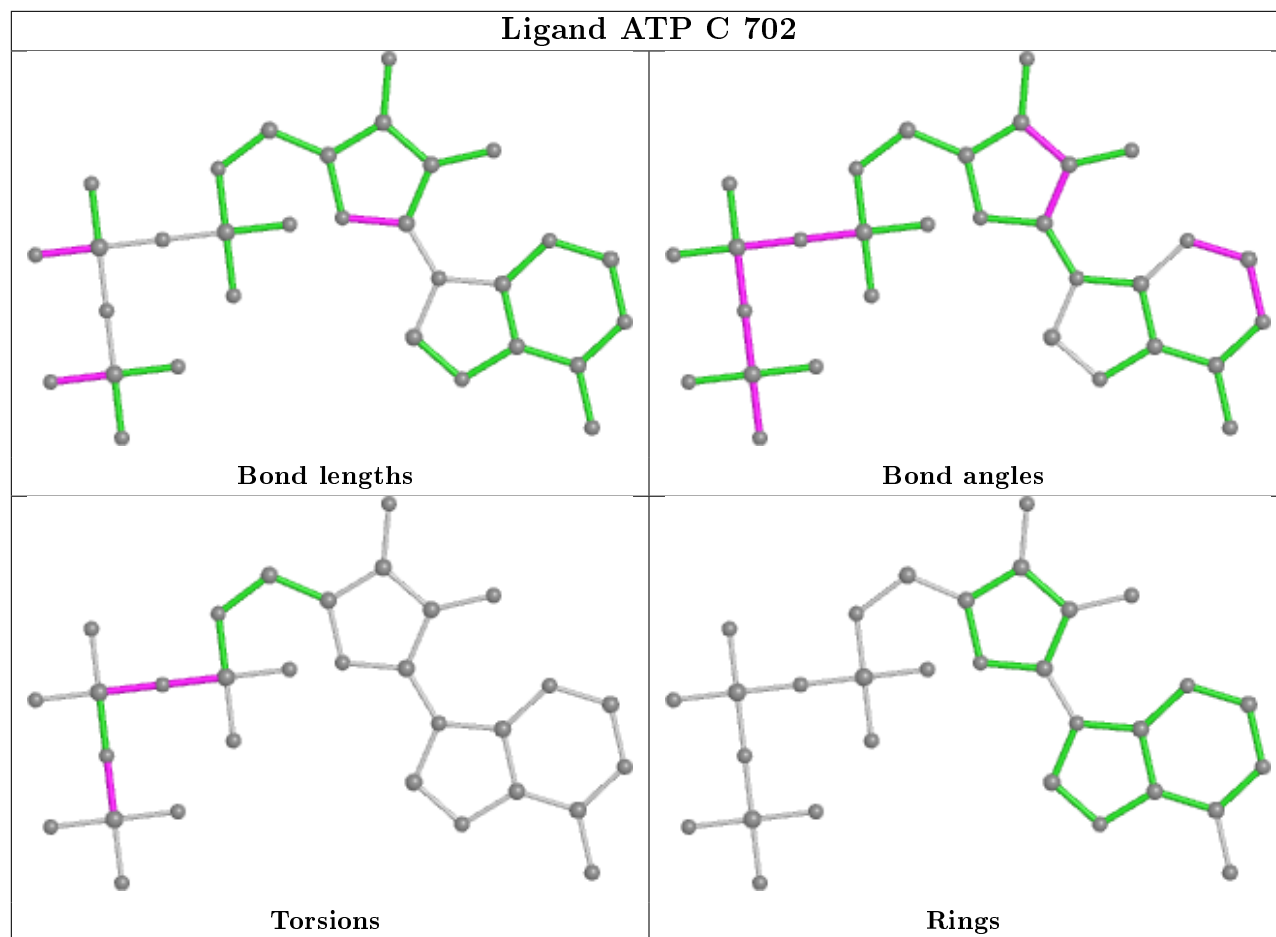
3 monomers are involved in 17 short contacts:

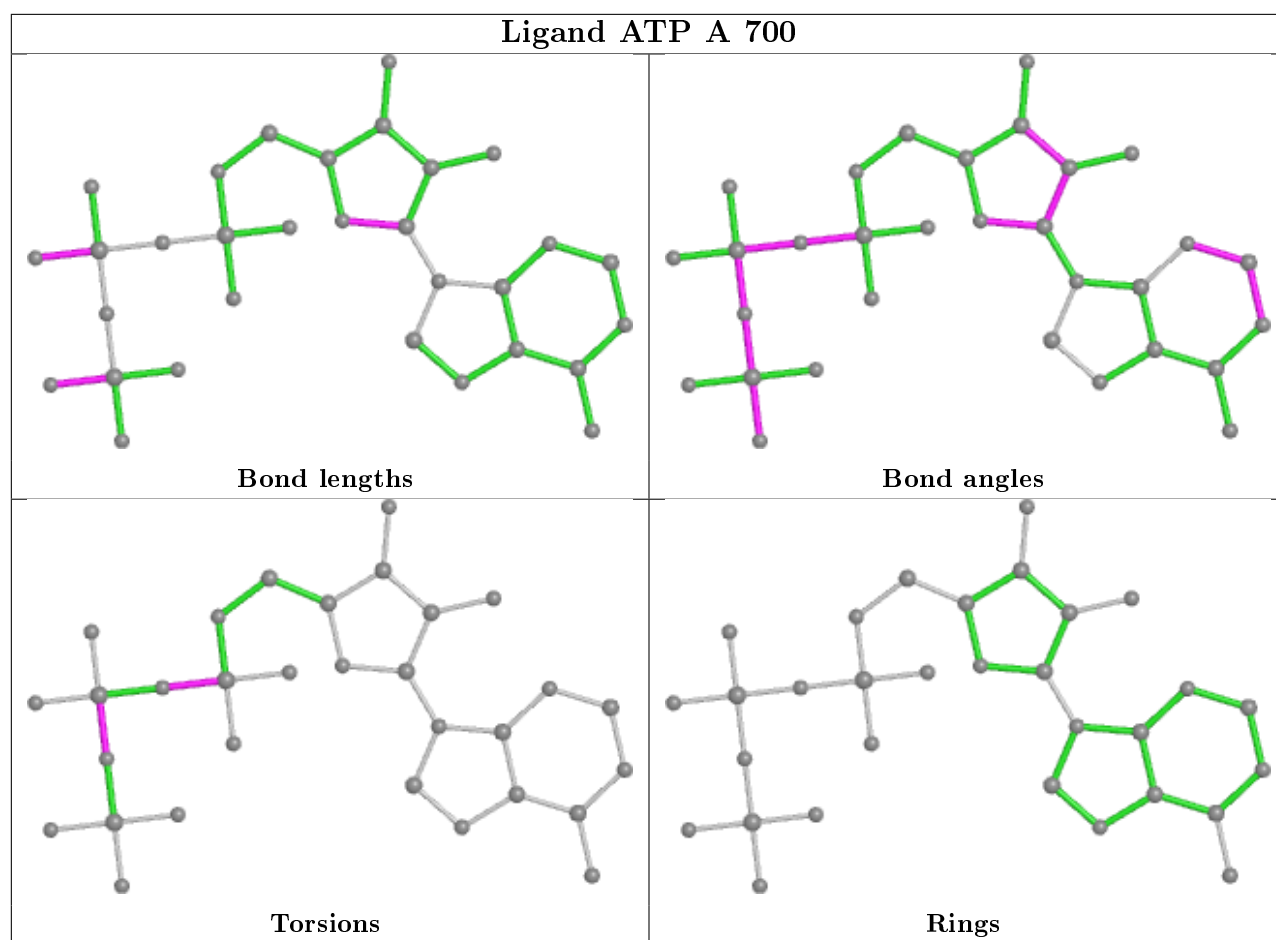
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ATP	7	0
2	C	702	ATP	6	0
2	A	700	ATP	4	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	683/697 (97%)	0.09	18 (2%) 56 35	32, 65, 109, 145	0
1	B	683/697 (97%)	0.26	28 (4%) 37 19	35, 75, 129, 174	0
1	C	683/697 (97%)	0.32	46 (6%) 17 7	40, 76, 137, 183	0
All	All	2049/2091 (97%)	0.22	92 (4%) 33 16	32, 72, 126, 183	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	SER	5.3
1	C	121	ALA	5.3
1	A	471	THR	5.2
1	C	130	PHE	5.0
1	C	46	GLU	5.0
1	B	9	ARG	4.9
1	C	47	GLY	4.9
1	B	468	LYS	4.7
1	C	4	GLU	4.4
1	B	4	GLU	4.3
1	B	8	GLU	4.2
1	B	128	SER	4.1
1	A	7	LEU	4.1
1	C	119	LEU	4.1
1	C	127	GLY	3.9
1	C	133	GLY	3.8
1	C	365	SER	3.7
1	A	8	GLU	3.7
1	B	87	ASP	3.7
1	C	6	VAL	3.6
1	C	48	ARG	3.5
1	B	123	THR	3.5
1	B	125	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLN	3.4
1	B	45	PHE	3.4
1	A	95	GLN	3.4
1	B	688	LEU	3.4
1	B	47	GLY	3.4
1	B	52	ALA	3.3
1	A	128	SER	3.3
1	C	5	LEU	3.2
1	A	119	LEU	3.1
1	C	125	TYR	3.1
1	C	69	GLN	3.1
1	A	47	GLY	3.0
1	B	572	ILE	2.9
1	A	41	LEU	2.9
1	C	100	LEU	2.9
1	C	8	GLU	2.9
1	C	102	LEU	2.9
1	B	97	ASP	2.9
1	C	56	SER	2.9
1	B	129	SER	2.8
1	A	11	ASP	2.7
1	C	10	CYS	2.7
1	C	57	LEU	2.7
1	C	117	LEU	2.6
1	B	469	GLU	2.6
1	C	135	PHE	2.6
1	B	46	GLU	2.5
1	B	100	LEU	2.5
1	C	147	ALA	2.5
1	C	132	LEU	2.4
1	C	646	GLU	2.4
1	C	54	VAL	2.4
1	A	129	SER	2.4
1	B	132	LEU	2.4
1	C	87	ASP	2.4
1	B	130	PHE	2.4
1	C	95	GLN	2.4
1	C	126	GLN	2.4
1	C	368	THR	2.3
1	C	128	SER	2.3
1	C	528	TYR	2.3
1	B	83	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	319	GLU	2.3
1	B	43	LEU	2.2
1	C	9	ARG	2.2
1	C	79	LEU	2.2
1	C	55	ASP	2.2
1	B	10	CYS	2.1
1	C	129	SER	2.1
1	C	131	VAL	2.1
1	C	468	LYS	2.1
1	A	98	CYS	2.1
1	C	7	LEU	2.1
1	A	9	ARG	2.1
1	A	46	GLU	2.1
1	C	76	ARG	2.1
1	C	74	LYS	2.1
1	A	45	PHE	2.1
1	C	77	PHE	2.1
1	A	466	ALA	2.1
1	B	81	ASP	2.1
1	B	274	TYR	2.0
1	B	408	ASP	2.0
1	A	468	LYS	2.0
1	A	42	THR	2.0
1	A	123	THR	2.0
1	B	11	ASP	2.0
1	C	41	LEU	2.0
1	C	63	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

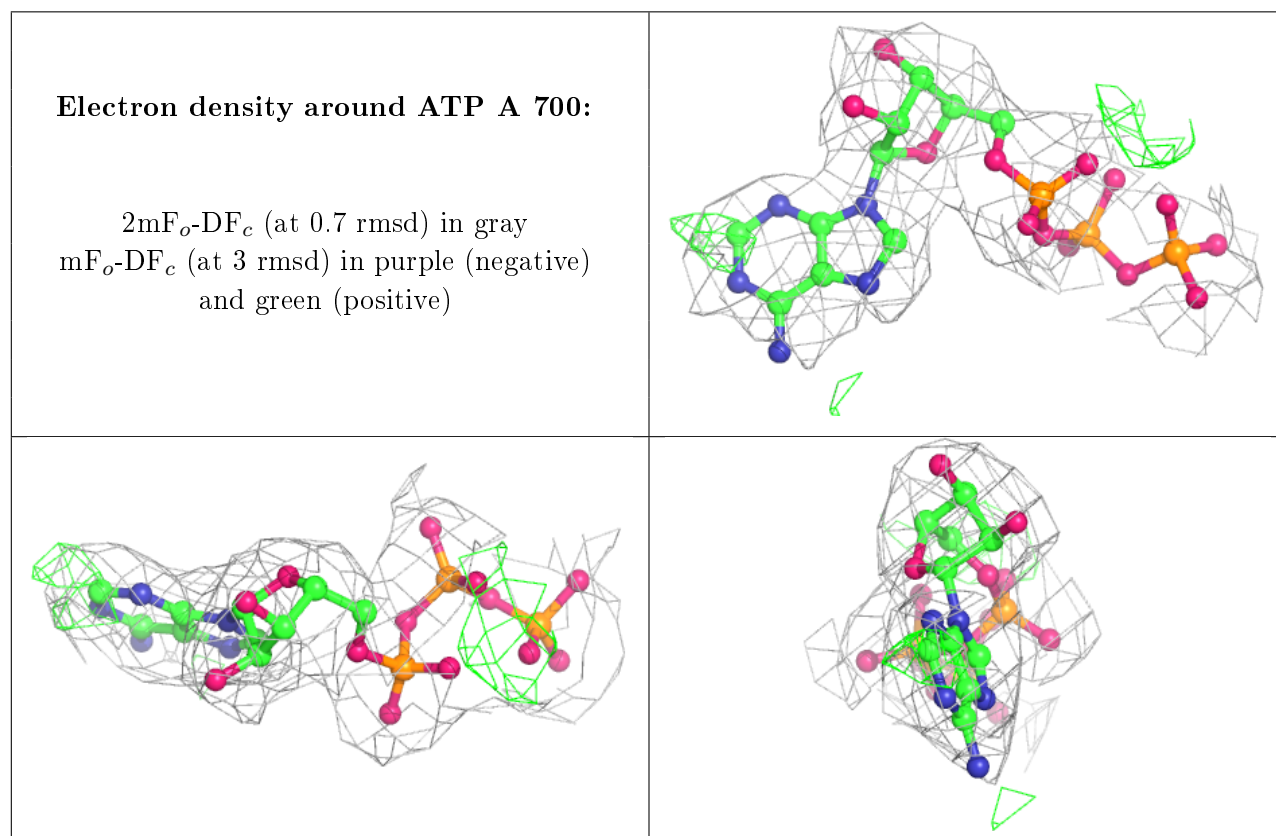
## 6.4 Ligands [i](#)

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.

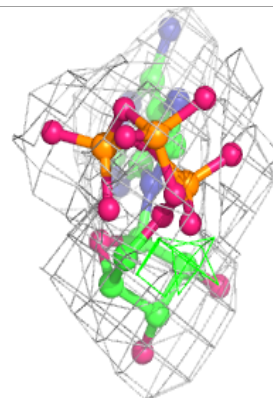
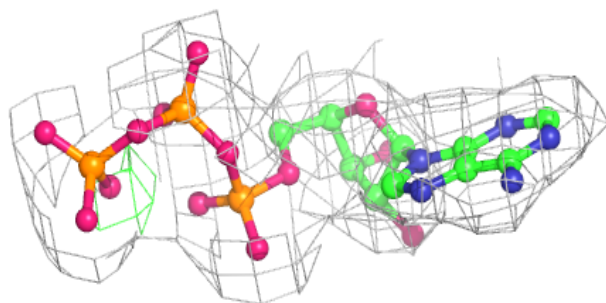
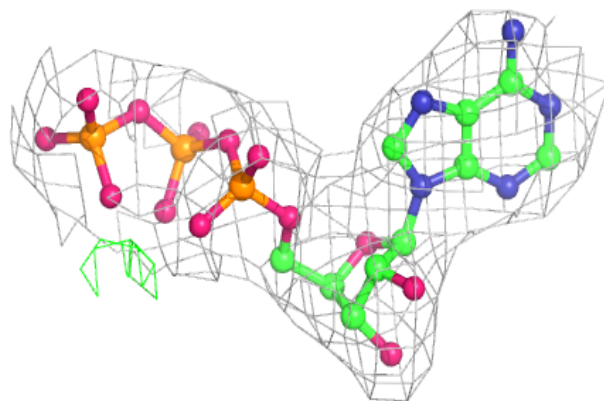
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ATP	A	700	31/31	0.93	0.19	72,72,72,72	0
2	ATP	C	702	31/31	0.94	0.17	72,72,72,72	0
2	ATP	B	701	31/31	0.94	0.17	72,72,72,72	0

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.

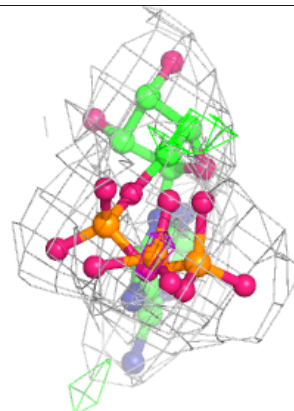
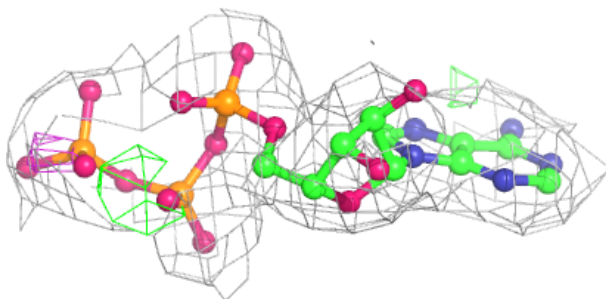
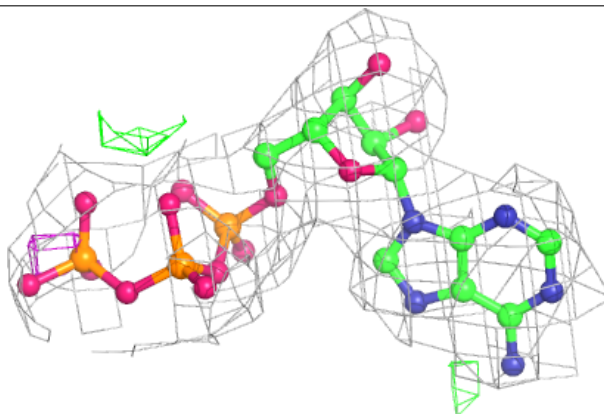


**Electron density around ATP C 702:**

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

**Electron density around ATP B 701:**

$2mF_o-DF_c$  (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.