



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:30 am BST

PDB ID : 3CR8  
Title : Hexameric APS kinase from *Thiobacillus denitrificans*  
Authors : Gay, S.C.; Segel, I.H.; Fisher, A.J.  
Deposited on : 2008-04-04  
Resolution : 2.95 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

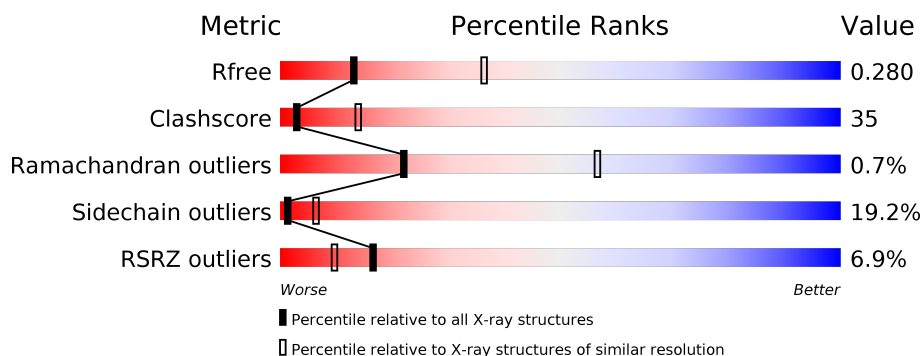
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	552	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>28%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	552	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>29%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	552	<div> <div>7%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>9%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11339 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 Sulfate adenylyltransferase, adenylylsulfate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3761	2390	676	679	16			
1	B	493	Total	C	N	O	S	0	0	0
			3744	2378	671	679	16			
1	C	493	Total	C	N	O	S	0	0	0
			3748	2380	670	682	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	LEU	-	EXPRESSION TAG	UNP Q3SM86
A	546	GLU	-	EXPRESSION TAG	UNP Q3SM86
A	547	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	548	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	549	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	550	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	551	HIS	-	EXPRESSION TAG	UNP Q3SM86
A	552	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	545	LEU	-	EXPRESSION TAG	UNP Q3SM86
B	546	GLU	-	EXPRESSION TAG	UNP Q3SM86
B	547	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	548	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	549	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	550	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	551	HIS	-	EXPRESSION TAG	UNP Q3SM86
B	552	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	545	LEU	-	EXPRESSION TAG	UNP Q3SM86
C	546	GLU	-	EXPRESSION TAG	UNP Q3SM86
C	547	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	548	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	549	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	550	HIS	-	EXPRESSION TAG	UNP Q3SM86
C	551	HIS	-	EXPRESSION TAG	UNP Q3SM86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	552	HIS	-	EXPRESSION TAG	UNP Q3SM86

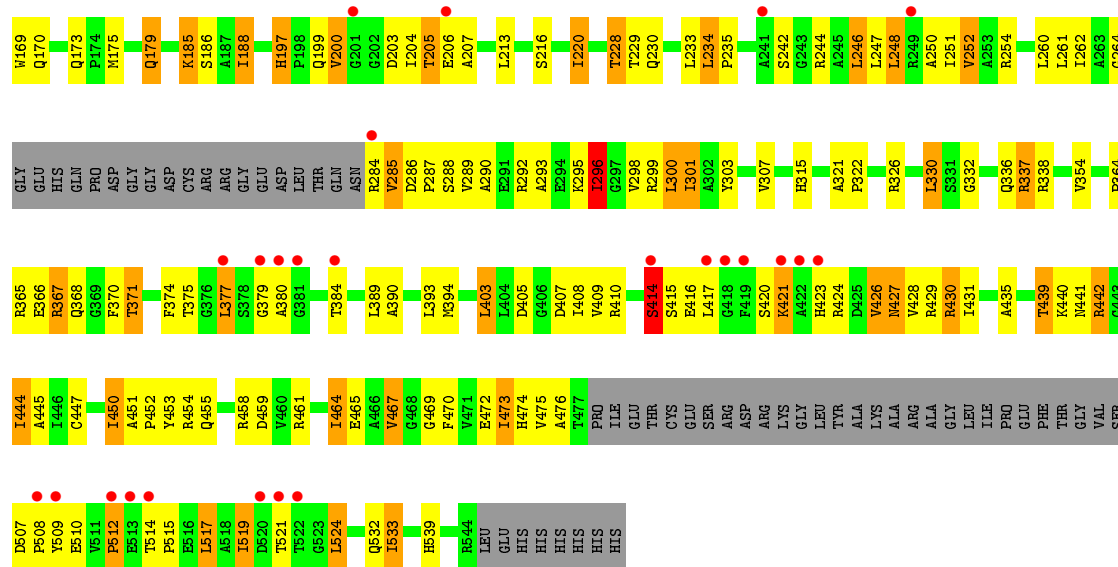
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	22	Total	O	0	0
			22	22		
2	C	33	Total	O	0	0
			33	33		

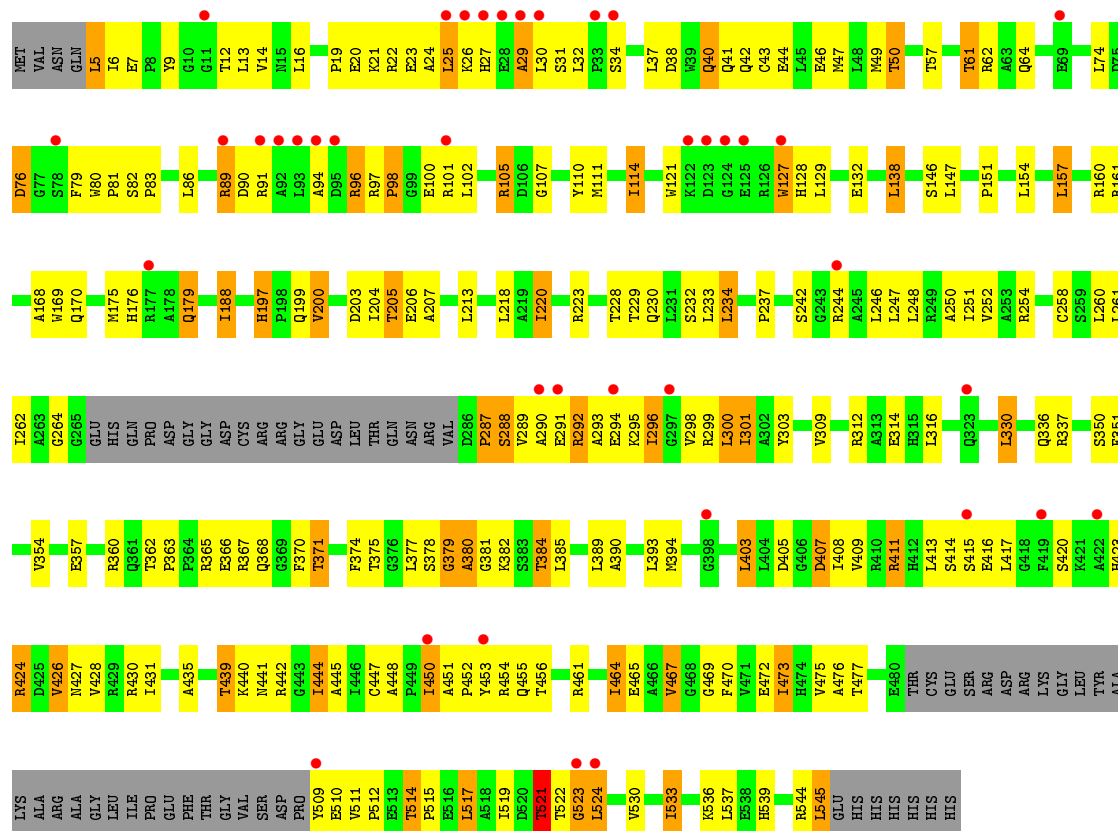
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Chain A:
- 
- Sequence logo for Chain A, showing amino acid conservation across 100 positions. The y-axis represents information content in bits, ranging from 0 to 5. The x-axis shows positions 1 to 100. A color scale at the top indicates the percentage of each amino acid at each position, with a maximum of 51% for Glycine (GLY) at position 1. Amino acids are listed on the left and right of the logo. Red dots above the logo indicate positions with high conservation (bits > 2).

- Chain B:
- 
- 6% 50% 29% 10% 11%
- | Label | Category |
|-------|----------|
| MET   | Grey     |
| VAL   | Grey     |
| ASN   | Grey     |
| Q4    | Red      |
| L5    | Red      |
| I6    | Orange   |
| E7    | Orange   |
| P8    | Orange   |
| Y9    | Orange   |
| G10   | Green    |
| G11   | Green    |
| T12   | Green    |
| L13   | Green    |
| V14   | Green    |
| H15   | Green    |
| L16   | Orange   |
| P19   | Red      |
| E20   | Red      |
| R21   | Green    |
| R22   | Green    |
| E23   | Green    |
| A24   | Green    |
| H27   | Green    |
| L30   | Yellow   |
| L35   | Yellow   |
| D36   | Green    |
| L37   | Green    |
| D38   | Green    |
| V39   | Green    |
| Q40   | Orange   |
| Q41   | Orange   |
| Q42   | Orange   |
| Q43   | Orange   |
| E44   | Orange   |
| L45   | Green    |
| L46   | Green    |
| E46   | Orange   |
| M47   | Orange   |
| T50   | Orange   |
| T57   | Yellow   |
| T61   | Orange   |
| A62   | Orange   |
| A63   | Orange   |
| Q64   | Orange   |
| R67   | Orange   |
| V68   | Orange   |
| E69   | Orange   |
| S70   | Orange   |
| A71   | Green    |
| L74   | Yellow   |
| D75   | Green    |
| D76   | Green    |
| F79   | Green    |
| W80   | Orange   |
| P81   | Orange   |
| L86   | Yellow   |
| R89   | Orange   |
| D90   | Orange   |
| R91   | Orange   |
| A92   | Green    |
| L93   | Green    |
| A94   | Orange   |
| D95   | Green    |
| R96   | Orange   |
| R97   | Orange   |
| E100  | Orange   |
| R101  | Orange   |
| R102  | Orange   |
| R105  | Orange   |
| D106  | Orange   |
| G107  | Red      |
| E108  | Orange   |
| M111  | Yellow   |
| L114  | Orange   |
| L115  | Green    |
| T116  | Yellow   |
| W121  | Yellow   |
| W127  | Orange   |
| H128  | Orange   |
| L129  | Orange   |
| G130  | Green    |
| A131  | Green    |
| E132  | Orange   |
| L138  | Orange   |
| P139  | Orange   |
| P140  | Yellow   |
| V145  | Orange   |
| S146  | Orange   |
| L147  | Orange   |
| P151  | Orange   |
| L154  | Orange   |
| L157  | Orange   |
| R160  | Orange   |
| R161  | Orange   |
| R164  | Yellow   |



• Molecule 1: Sulfate adenylyltransferase, adenylylsulfate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.07Å 227.21Å 106.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.03 – 2.95 35.03 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.1 (35.03-2.95) 92.1 (35.03-2.95)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.243 , 0.282 0.238 , 0.280	Depositor DCC
$R_{free}$ test set	1889 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

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	0.67	2/3843 (0.1%)	0.87	15/5227 (0.3%)
1	B	0.68	0/3825	0.83	8/5205 (0.2%)
1	C	0.65	0/3829	0.88	12/5209 (0.2%)
All	All	0.66	2/11497 (0.0%)	0.86	35/15641 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	CYS	CB-SG	-5.88	1.72	1.81
1	A	447	CYS	CB-SG	-5.42	1.73	1.81

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	SER	CB-CA-C	11.04	131.07	110.10
1	C	522	THR	N-CA-CB	-10.76	89.85	110.30
1	C	521	THR	CB-CA-C	-10.58	83.03	111.60
1	B	416	GLU	N-CA-CB	-9.50	93.50	110.60
1	C	29	ALA	CB-CA-C	-9.35	96.08	110.10
1	A	291	GLU	CB-CA-C	-7.80	94.79	110.40
1	A	410	ARG	CB-CA-C	-7.56	95.28	110.40
1	C	350	SER	CB-CA-C	-7.06	96.69	110.10
1	A	292	ARG	CB-CA-C	-6.81	96.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	522	THR	N-CA-C	6.67	128.99	111.00
1	A	511	VAL	CB-CA-C	-6.54	98.98	111.40
1	B	108	GLU	C-N-CA	-6.48	108.69	122.30
1	C	447	CYS	CB-CA-C	-6.45	97.49	110.40
1	B	380	ALA	N-CA-CB	-6.42	101.11	110.10
1	B	447	CYS	CB-CA-C	-6.39	97.61	110.40
1	A	291	GLU	N-CA-C	6.38	128.22	111.00
1	C	292	ARG	CB-CA-C	-6.17	98.06	110.40
1	B	205	THR	N-CA-C	6.12	127.52	111.00
1	C	205	THR	N-CA-C	6.11	127.49	111.00
1	B	414	SER	CB-CA-C	-5.97	98.75	110.10
1	A	454	ARG	C-N-CA	-5.94	106.85	121.70
1	A	89	ARG	N-CA-CB	5.89	121.21	110.60
1	A	88	SER	N-CA-C	-5.79	95.35	111.00
1	A	447	CYS	CB-CA-C	-5.75	98.90	110.40
1	A	89	ARG	N-CA-C	-5.67	95.69	111.00
1	A	410	ARG	N-CA-C	5.51	125.89	111.00
1	C	379	GLY	N-CA-C	-5.51	99.33	113.10
1	A	286	ASP	C-N-CD	-5.45	108.61	120.60
1	C	330	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	19	PRO	N-CA-C	5.43	126.23	112.10
1	A	330	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	448	ALA	N-CA-CB	-5.33	102.64	110.10
1	B	330	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	523	GLY	N-CA-C	-5.16	100.21	113.10
1	A	458	ARG	CG-CD-NE	-5.12	101.05	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ASP	Peptide
1	C	380	ALA	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	3761	0	3716	267	0
1	B	3744	0	3685	289	1
1	C	3748	0	3684	235	0
2	A	31	0	0	2	0
2	B	22	0	0	0	0
2	C	33	0	0	4	0
All	All	11339	0	11085	773	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (773) 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:414:SER:HB2	1:A:417:LEU:CD1	1.57	1.35
1:B:4:GLN:NE2	1:B:5:LEU:HB2	1.42	1.34
1:C:288:SER:O	1:C:291:GLU:HB2	1.32	1.28
1:A:244:ARG:N	1:A:244:ARG:HD2	1.40	1.22
1:C:287:PRO:O	1:C:291:GLU:HG2	1.32	1.22
1:C:21:LYS:O	1:C:24:ALA:HB3	1.35	1.22
1:A:286:ASP:CB	1:A:287:PRO:HA	1.69	1.21
1:B:414:SER:CB	1:B:417:LEU:HD12	1.68	1.21
1:B:61:THR:HG22	1:B:64:GLN:CG	1.73	1.18
1:A:545:LEU:HD23	1:A:546:GLU:N	1.59	1.16
1:A:244:ARG:H	1:A:244:ARG:CD	1.57	1.16
1:B:475:VAL:HG13	1:B:519:ILE:HD11	1.24	1.15
1:A:414:SER:CB	1:A:417:LEU:HD12	1.75	1.15
1:B:67:ARG:CG	1:B:67:ARG:HH11	1.59	1.13
1:B:61:THR:CG2	1:B:64:GLN:HG3	1.79	1.13
1:B:509:TYR:CE2	1:B:510:GLU:O	2.03	1.12
1:B:424:ARG:HE	1:B:450:ILE:HD11	1.01	1.11
1:B:424:ARG:NE	1:B:450:ILE:HD11	1.66	1.11
1:A:539:HIS:CE1	1:C:188:ILE:HA	1.86	1.10
1:B:521:THR:HG21	1:B:524:LEU:HG	1.26	1.10
1:A:96:ARG:HG3	1:A:96:ARG:HH11	0.95	1.10
1:B:89:ARG:CG	1:B:89:ARG:HH11	1.65	1.09
1:B:507:ASP:CB	1:B:508:PRO:CD	2.30	1.09
1:B:414:SER:CB	1:B:417:LEU:CD1	2.30	1.08
1:A:414:SER:HB2	1:A:417:LEU:HD12	1.10	1.08
1:A:507:ASP:CB	1:A:508:PRO:CD	2.30	1.08
1:A:89:ARG:CG	1:A:89:ARG:HH11	1.65	1.07
1:A:545:LEU:HD23	1:A:546:GLU:H	0.90	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ASP:CB	1:B:508:PRO:HD3	1.83	1.07
1:A:539:HIS:CD2	1:C:188:ILE:HG22	1.90	1.07
1:C:414:SER:HB2	1:C:417:LEU:HD12	1.09	1.07
1:B:367:ARG:CG	1:B:367:ARG:HH11	1.68	1.06
1:A:414:SER:CB	1:A:417:LEU:CD1	2.30	1.05
1:B:521:THR:CG2	1:B:524:LEU:HG	1.86	1.05
1:B:414:SER:HB2	1:B:417:LEU:HD12	1.30	1.04
1:B:442:ARG:HH11	1:B:442:ARG:HG2	1.22	1.04
1:C:61:THR:HG22	1:C:64:GLN:HG3	1.36	1.04
1:B:367:ARG:HG2	1:B:367:ARG:HH11	1.21	1.03
1:B:285:VAL:O	1:B:285:VAL:HG13	1.57	1.03
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.19	1.03
1:A:286:ASP:CB	1:A:287:PRO:CA	2.30	1.02
1:B:521:THR:HG21	1:B:524:LEU:CG	1.89	1.02
1:C:428:VAL:HG11	1:C:456:THR:CG2	1.90	1.02
1:B:4:GLN:NE2	1:B:5:LEU:H	1.57	1.01
1:B:509:TYR:O	1:B:510:GLU:HG3	1.61	1.00
1:B:424:ARG:HE	1:B:450:ILE:CD1	1.74	0.98
1:C:291:GLU:HA	1:C:291:GLU:OE1	1.63	0.98
1:B:67:ARG:NH1	1:B:67:ARG:HG3	1.63	0.98
1:A:96:ARG:NH1	1:A:96:ARG:HG3	1.67	0.97
1:B:67:ARG:HG3	1:B:67:ARG:HH11	0.83	0.97
1:A:61:THR:HG22	1:A:64:GLN:HG3	1.44	0.96
1:C:220:ILE:HG22	1:C:354:VAL:HG22	1.47	0.96
1:C:414:SER:CB	1:C:417:LEU:HD12	1.95	0.96
1:A:507:ASP:CB	1:A:508:PRO:HD3	1.91	0.96
1:A:220:ILE:HG22	1:A:354:VAL:HG22	1.47	0.96
1:B:296:ILE:O	1:B:296:ILE:CG1	2.08	0.96
1:B:61:THR:HG22	1:B:64:GLN:HG3	0.98	0.95
1:B:414:SER:HB3	1:B:417:LEU:CD1	1.97	0.95
1:B:220:ILE:HG22	1:B:354:VAL:HG22	1.44	0.94
1:C:289:VAL:HG23	1:C:290:ALA:N	1.81	0.94
1:A:246:LEU:O	1:A:246:LEU:HD22	1.67	0.94
1:B:296:ILE:O	1:B:296:ILE:HG12	1.65	0.94
1:B:509:TYR:CD2	1:B:510:GLU:N	2.34	0.94
1:A:122:LYS:NZ	1:A:127:TRP:CH2	2.35	0.94
1:B:4:GLN:NE2	1:B:5:LEU:CB	2.30	0.93
1:B:427:ASN:C	1:B:427:ASN:HD22	1.71	0.93
1:B:4:GLN:HE22	1:B:5:LEU:HB2	0.93	0.93
1:B:521:THR:CB	1:B:524:LEU:HG	1.99	0.93
1:B:161:ARG:HH21	1:B:230:GLN:HG2	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:H	1:B:89:ARG:HD3	1.35	0.92
1:A:545:LEU:CD2	1:A:546:GLU:H	1.83	0.92
1:B:96:ARG:HH11	1:B:96:ARG:HG3	1.32	0.91
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.36	0.90
1:A:89:ARG:HH11	1:A:89:ARG:HG2	1.37	0.90
1:C:415:SER:O	1:C:416:GLU:HG3	1.72	0.89
1:B:464:ILE:HD11	1:B:469:GLY:O	1.72	0.89
1:A:286:ASP:CB	1:A:287:PRO:HG3	2.02	0.89
1:A:414:SER:CA	1:A:417:LEU:HD12	2.01	0.89
1:C:428:VAL:HG11	1:C:456:THR:HG22	1.55	0.89
1:B:424:ARG:HD2	1:B:450:ILE:HD13	1.54	0.89
1:A:89:ARG:HH11	1:A:89:ARG:HG3	1.37	0.88
1:B:475:VAL:CG1	1:B:519:ILE:HD11	2.04	0.88
1:B:89:ARG:HG3	1:B:89:ARG:HH11	1.36	0.88
1:C:292:ARG:O	1:C:295:LYS:CB	2.22	0.88
1:C:161:ARG:HH21	1:C:230:GLN:HG2	1.39	0.87
1:A:290:ALA:HA	1:A:300:LEU:HD21	1.53	0.87
1:B:427:ASN:HD22	1:B:428:VAL:N	1.72	0.87
1:A:292:ARG:NH2	1:A:295:LYS:CB	2.38	0.87
1:C:475:VAL:HG13	1:C:519:ILE:HD11	1.55	0.87
1:B:89:ARG:HG2	1:B:89:ARG:HH11	1.38	0.86
1:C:157:LEU:HD23	1:C:160:ARG:HH21	1.40	0.86
1:A:161:ARG:HH21	1:A:230:GLN:HG2	1.41	0.86
1:A:62:ARG:HG3	1:A:121:TRP:CE2	2.11	0.85
1:B:427:ASN:C	1:B:427:ASN:ND2	2.29	0.85
1:A:414:SER:HB2	1:A:417:LEU:HD13	1.57	0.85
1:B:220:ILE:CG2	1:B:354:VAL:HG22	2.05	0.85
1:B:475:VAL:HG13	1:B:519:ILE:CD1	2.06	0.85
1:A:35:LEU:HD11	1:A:88:SER:OG	1.75	0.84
1:B:424:ARG:HD2	1:B:450:ILE:CD1	2.07	0.84
1:B:377:LEU:HD12	1:B:377:LEU:H	1.42	0.83
1:A:475:VAL:HG13	1:A:519:ILE:HD11	1.60	0.83
1:A:377:LEU:H	1:A:377:LEU:HD12	1.44	0.82
1:C:61:THR:CG2	1:C:64:GLN:HG3	2.09	0.82
1:A:157:LEU:HD23	1:A:160:ARG:HH21	1.42	0.82
1:B:414:SER:CA	1:B:417:LEU:CD1	2.58	0.82
1:C:426:VAL:HG12	1:C:427:ASN:N	1.92	0.82
1:B:393:LEU:HD13	1:B:444:ILE:CD1	2.09	0.81
1:A:289:VAL:HG23	1:A:290:ALA:N	1.94	0.81
1:B:414:SER:CA	1:B:417:LEU:HD12	2.10	0.81
1:A:97:ARG:O	1:A:100:GLU:HG3	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:VAL:CG2	1:C:290:ALA:N	2.44	0.80
1:B:424:ARG:NE	1:B:450:ILE:CD1	2.38	0.80
1:B:292:ARG:O	1:B:295:LYS:CB	2.30	0.80
1:C:544:ARG:HG2	1:C:545:LEU:N	1.95	0.80
1:C:19:PRO:O	1:C:22:ARG:CB	2.30	0.80
1:B:157:LEU:HD23	1:B:160:ARG:HH21	1.47	0.80
1:B:367:ARG:HG2	1:B:367:ARG:NH1	1.93	0.80
1:B:393:LEU:HD13	1:B:444:ILE:HD12	1.63	0.80
1:C:384:THR:HG22	2:C:555:HOH:O	1.81	0.80
1:B:4:GLN:NE2	1:B:5:LEU:N	2.30	0.79
1:A:377:LEU:O	1:A:379:GLY:HA3	1.83	0.79
1:C:428:VAL:CG1	1:C:456:THR:CG2	2.61	0.79
1:A:246:LEU:O	1:A:246:LEU:CD2	2.30	0.79
1:A:377:LEU:O	1:A:379:GLY:CA	2.31	0.79
1:B:46:GLU:O	1:B:50:THR:HB	1.83	0.78
1:C:521:THR:OG1	1:C:521:THR:O	1.93	0.78
1:B:4:GLN:CD	1:B:5:LEU:H	1.87	0.78
1:C:464:ILE:HD11	1:C:469:GLY:O	1.83	0.78
1:A:188:ILE:HG22	1:B:539:HIS:CD2	2.18	0.78
1:A:292:ARG:HH22	1:A:295:LYS:CB	1.97	0.78
1:B:19:PRO:O	1:B:22:ARG:CB	2.32	0.77
1:B:421:LYS:H	1:B:421:LYS:HD3	1.49	0.77
1:A:289:VAL:CG2	1:A:290:ALA:N	2.47	0.77
1:B:284:ARG:O	1:B:285:VAL:HG12	1.83	0.77
1:B:509:TYR:CG	1:B:510:GLU:N	2.48	0.77
1:A:220:ILE:CG2	1:A:354:VAL:HG22	2.14	0.76
1:A:4:GLN:HE21	1:A:5:LEU:H	1.33	0.76
1:A:517:LEU:CD1	1:A:533:ILE:HG22	2.15	0.76
1:B:424:ARG:CD	1:B:450:ILE:CD1	2.63	0.76
1:B:89:ARG:N	1:B:89:ARG:HD3	2.00	0.76
1:C:220:ILE:CG2	1:C:354:VAL:HG22	2.14	0.76
1:B:414:SER:HA	1:B:417:LEU:HD11	1.67	0.76
1:A:188:ILE:HA	1:B:539:HIS:CE1	2.20	0.76
1:B:509:TYR:O	1:B:510:GLU:CG	2.33	0.75
1:A:200:VAL:CG1	1:A:200:VAL:O	2.33	0.75
1:C:291:GLU:OE1	1:C:291:GLU:CA	2.30	0.75
1:B:89:ARG:NH1	1:B:89:ARG:CG	2.37	0.75
1:C:62:ARG:HG3	1:C:121:TRP:CE2	2.22	0.75
1:A:61:THR:CG2	1:A:64:GLN:HG3	2.17	0.74
1:A:96:ARG:HH11	1:A:96:ARG:CG	1.85	0.74
1:C:461:ARG:O	1:C:465:GLU:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:SER:CA	1:A:417:LEU:CD1	2.63	0.74
1:C:21:LYS:O	1:C:25:LEU:HG	1.87	0.74
1:B:285:VAL:O	1:B:285:VAL:CG1	2.30	0.74
1:A:46:GLU:O	1:A:50:THR:HB	1.88	0.74
1:A:517:LEU:HD13	1:A:533:ILE:HG22	1.70	0.74
1:B:97:ARG:O	1:B:100:GLU:HG3	1.88	0.73
1:C:21:LYS:C	1:C:24:ALA:HB3	2.08	0.73
1:A:286:ASP:CB	1:A:287:PRO:CG	2.66	0.73
1:A:203:ASP:O	1:A:208:PRO:HG3	1.88	0.73
1:B:19:PRO:O	1:B:22:ARG:HB3	1.87	0.73
1:A:200:VAL:HG13	1:A:200:VAL:O	1.87	0.73
1:B:138:LEU:H	1:B:138:LEU:HD12	1.53	0.73
1:B:519:ILE:HG13	1:B:519:ILE:O	1.88	0.73
1:B:67:ARG:NH1	1:B:67:ARG:CG	2.30	0.73
1:C:46:GLU:O	1:C:50:THR:HB	1.88	0.73
1:C:24:ALA:O	1:C:27:HIS:CB	2.37	0.73
1:A:204:ILE:C	1:A:208:PRO:HG3	2.09	0.72
1:C:414:SER:HB2	1:C:417:LEU:CD1	2.05	0.72
1:C:89:ARG:HG3	1:C:89:ARG:HH11	1.54	0.72
1:A:122:LYS:HD2	1:A:127:TRP:CZ2	2.25	0.72
1:C:38:ASP:OD1	1:C:41:GLN:HG2	1.90	0.72
1:C:517:LEU:CD1	1:C:533:ILE:HG22	2.20	0.72
1:B:517:LEU:CD1	1:B:533:ILE:HG22	2.21	0.71
1:A:458:ARG:HH11	1:A:461:ARG:HD2	1.55	0.71
1:B:424:ARG:CD	1:B:450:ILE:HD13	2.21	0.71
1:C:57:THR:HG23	1:C:132:GLU:OE1	1.90	0.71
1:A:207:ALA:N	1:A:208:PRO:HD3	2.04	0.71
1:B:96:ARG:NH1	1:B:96:ARG:HG3	2.00	0.71
1:A:442:ARG:CG	1:A:442:ARG:HH11	1.99	0.70
1:C:428:VAL:HG11	1:C:456:THR:HG21	1.71	0.70
1:A:169:TRP:CZ3	1:A:262:ILE:HG21	2.25	0.70
1:C:426:VAL:CG1	1:C:427:ASN:N	2.52	0.70
1:A:371:THR:HG23	1:A:464:ILE:HD13	1.74	0.70
1:A:461:ARG:O	1:A:465:GLU:HB2	1.92	0.70
1:A:454:ARG:O	1:A:455:GLN:C	2.27	0.70
1:B:442:ARG:HH11	1:B:442:ARG:CG	2.03	0.70
1:B:461:ARG:O	1:B:465:GLU:HB2	1.91	0.70
1:B:371:THR:HG23	1:B:464:ILE:HD13	1.73	0.69
1:A:35:LEU:HD21	1:A:88:SER:CB	2.22	0.69
1:C:199:GLN:HG3	1:C:234:LEU:HD13	1.74	0.69
1:B:169:TRP:CZ3	1:B:262:ILE:HG21	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:THR:CG2	1:A:439:THR:HG21	2.23	0.69
1:C:169:TRP:CZ3	1:C:262:ILE:HG21	2.27	0.69
1:C:138:LEU:H	1:C:138:LEU:HD12	1.57	0.69
1:A:393:LEU:HD13	1:A:444:ILE:CD1	2.22	0.69
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.37	0.69
1:A:96:ARG:NH1	1:A:96:ARG:CG	2.49	0.69
1:A:207:ALA:O	2:A:577:HOH:O	2.11	0.69
1:C:288:SER:OG	1:C:292:ARG:CZ	2.41	0.68
1:C:262:ILE:HG12	1:C:301:ILE:HD11	1.75	0.68
1:C:413:LEU:HG	1:C:430:ARG:HG2	1.76	0.68
1:A:57:THR:HG23	1:A:132:GLU:OE1	1.94	0.68
1:A:61:THR:HG21	2:A:572:HOH:O	1.93	0.68
1:B:106:ASP:C	1:B:106:ASP:OD1	2.29	0.68
1:C:371:THR:HG23	1:C:464:ILE:HD13	1.74	0.68
1:B:199:GLN:HG3	1:B:234:LEU:HD13	1.76	0.67
1:C:415:SER:O	1:C:416:GLU:CG	2.42	0.67
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.04	0.67
1:C:294:GLU:O	1:C:294:GLU:HG3	1.93	0.67
1:C:289:VAL:CG2	1:C:290:ALA:H	2.07	0.67
1:B:414:SER:CA	1:B:417:LEU:HD11	2.23	0.67
1:B:409:VAL:HG11	1:B:431:ILE:HD11	1.75	0.67
1:C:47:MET:HE2	1:C:47:MET:HA	1.74	0.67
1:A:376:GLY:CA	1:A:509:TYR:OH	2.43	0.67
1:B:296:ILE:O	1:B:296:ILE:HG13	1.95	0.67
1:C:287:PRO:O	1:C:291:GLU:CG	2.27	0.67
1:A:393:LEU:HD13	1:A:444:ILE:HD12	1.76	0.67
1:C:374:PHE:CE2	1:C:473:ILE:HD11	2.30	0.67
1:C:475:VAL:HA	1:C:519:ILE:HG12	1.77	0.67
1:A:246:LEU:CD2	1:A:246:LEU:C	2.64	0.67
1:B:68:VAL:C	1:B:70:SER:H	1.99	0.67
1:C:517:LEU:HD13	1:C:533:ILE:HG22	1.75	0.67
1:B:57:THR:HG23	1:B:132:GLU:OE1	1.94	0.66
1:C:288:SER:O	1:C:291:GLU:CB	2.27	0.66
1:C:454:ARG:HG3	1:C:510:GLU:OE1	1.95	0.66
1:A:371:THR:HG23	1:A:439:THR:HG21	1.77	0.66
1:B:517:LEU:HD13	1:B:533:ILE:HG22	1.76	0.66
1:B:47:MET:HE2	1:B:47:MET:HA	1.76	0.66
1:A:464:ILE:HD11	1:A:469:GLY:O	1.96	0.66
1:A:89:ARG:N	1:A:89:ARG:HD3	2.10	0.66
1:B:374:PHE:CE2	1:B:473:ILE:HD11	2.29	0.66
1:A:138:LEU:H	1:A:138:LEU:HD12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:CG	1:B:367:ARG:NH1	2.39	0.66
1:A:246:LEU:HD22	1:A:246:LEU:C	2.13	0.66
1:A:365:ARG:HA	1:A:368:GLN:HG2	1.76	0.66
1:B:106:ASP:OD1	1:B:108:GLU:N	2.28	0.66
1:B:7:GLU:CB	1:B:8:PRO:CD	2.74	0.66
1:A:4:GLN:NE2	1:A:5:LEU:H	1.94	0.65
1:A:545:LEU:CD2	1:A:546:GLU:N	2.50	0.65
1:A:122:LYS:HD2	1:A:127:TRP:CE2	2.31	0.65
1:A:507:ASP:CB	1:A:508:PRO:HD2	2.26	0.65
1:B:367:ARG:HG3	1:B:367:ARG:HH11	1.60	0.65
1:A:50:THR:HG23	1:A:151:PRO:HD2	1.77	0.65
1:A:288:SER:O	1:A:291:GLU:CB	2.45	0.65
1:B:89:ARG:HG2	1:B:89:ARG:NH1	2.09	0.65
1:C:289:VAL:HG23	1:C:290:ALA:H	1.62	0.65
1:B:286:ASP:O	1:B:289:VAL:HG22	1.97	0.64
1:B:185:LYS:O	1:B:186:SER:C	2.30	0.64
1:B:19:PRO:O	1:B:22:ARG:N	2.29	0.64
1:C:138:LEU:N	1:C:138:LEU:HD12	2.12	0.64
1:C:20:GLU:C	1:C:22:ARG:H	1.98	0.64
1:A:242:SER:OG	1:A:243:GLY:N	2.30	0.64
1:C:288:SER:OG	1:C:292:ARG:NH2	2.30	0.64
1:C:89:ARG:CG	1:C:89:ARG:HH11	2.10	0.64
1:B:509:TYR:C	1:B:510:GLU:HG3	2.18	0.64
1:C:378:SER:C	1:C:380:ALA:H	2.00	0.64
1:A:244:ARG:N	1:A:244:ARG:CD	2.29	0.64
1:C:97:ARG:O	1:C:100:GLU:HG3	1.99	0.63
1:A:376:GLY:N	1:A:509:TYR:OH	2.32	0.63
1:B:371:THR:CG2	1:B:439:THR:HG21	2.28	0.63
1:C:19:PRO:O	1:C:22:ARG:N	2.30	0.63
1:C:413:LEU:HG	1:C:430:ARG:CG	2.28	0.63
1:B:50:THR:HG23	1:B:151:PRO:HD2	1.81	0.63
1:B:38:ASP:OD1	1:B:41:GLN:HG2	1.98	0.63
1:B:368:GLN:HA	1:B:442:ARG:HD2	1.80	0.62
1:A:89:ARG:NH1	1:A:89:ARG:HG2	2.08	0.62
1:B:138:LEU:N	1:B:138:LEU:HD12	2.13	0.62
1:C:21:LYS:O	1:C:24:ALA:CB	2.30	0.62
1:A:374:PHE:CE2	1:A:473:ILE:HD11	2.35	0.62
1:B:62:ARG:HG2	1:B:121:TRP:CE2	2.34	0.62
1:B:169:TRP:HZ3	1:B:262:ILE:HG21	1.63	0.62
1:B:199:GLN:HG3	1:B:234:LEU:CD1	2.29	0.62
1:C:20:GLU:O	1:C:22:ARG:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLN:HG3	1:A:234:LEU:HD13	1.81	0.62
1:A:414:SER:HA	1:A:417:LEU:CD1	2.29	0.62
1:C:21:LYS:O	1:C:25:LEU:CD2	2.48	0.62
1:B:521:THR:HG21	1:B:524:LEU:CD1	2.29	0.62
1:A:442:ARG:HG2	1:A:442:ARG:NH1	1.98	0.61
1:C:169:TRP:HZ3	1:C:262:ILE:HG21	1.65	0.61
1:C:371:THR:CG2	1:C:439:THR:HG21	2.30	0.61
1:B:414:SER:HA	1:B:417:LEU:CD1	2.28	0.61
1:B:475:VAL:HA	1:B:519:ILE:HG12	1.82	0.61
1:A:89:ARG:NH1	1:A:89:ARG:HG3	2.08	0.61
1:B:509:TYR:CE2	1:B:510:GLU:C	2.74	0.61
1:C:378:SER:C	1:C:380:ALA:N	2.53	0.61
1:C:300:LEU:CD2	1:C:300:LEU:H	2.14	0.61
1:A:262:ILE:HG12	1:A:301:ILE:HD11	1.82	0.61
1:B:262:ILE:HG12	1:B:301:ILE:HD11	1.81	0.60
1:B:128:HIS:O	1:B:129:LEU:HD23	2.01	0.60
1:B:464:ILE:HG12	1:B:470:PHE:HD1	1.65	0.60
1:B:188:ILE:HG22	1:C:539:HIS:CD2	2.35	0.60
1:B:475:VAL:HA	1:B:519:ILE:CD1	2.31	0.60
1:B:61:THR:HG22	1:B:64:GLN:H	1.65	0.60
1:A:169:TRP:HZ3	1:A:262:ILE:HG21	1.64	0.60
1:A:47:MET:HE2	1:A:47:MET:HA	1.82	0.60
1:B:61:THR:CB	1:B:64:GLN:HG3	2.31	0.60
1:C:393:LEU:HD13	1:C:444:ILE:CD1	2.32	0.60
1:B:89:ARG:HG3	1:B:89:ARG:NH1	2.07	0.60
1:C:409:VAL:HG11	1:C:431:ILE:HD11	1.84	0.60
1:A:366:GLU:HG3	1:A:544:ARG:CB	2.32	0.59
1:A:89:ARG:H	1:A:89:ARG:HD3	1.67	0.59
1:B:421:LYS:CD	1:B:421:LYS:H	2.08	0.59
1:A:123:ASP:O	1:A:124:GLY:C	2.38	0.59
1:A:464:ILE:HG12	1:A:470:PHE:HD1	1.67	0.59
1:A:519:ILE:HG13	1:A:519:ILE:O	2.03	0.59
1:C:107:GLY:HA2	2:C:574:HOH:O	2.02	0.59
1:A:114:ILE:C	1:A:114:ILE:HD12	2.23	0.59
1:B:286:ASP:OD1	1:B:287:PRO:HD2	2.02	0.59
1:C:170:GLN:HA	1:C:197:HIS:O	2.02	0.59
1:C:20:GLU:C	1:C:22:ARG:N	2.51	0.59
1:C:105:ARG:HB3	1:C:110:TYR:O	2.02	0.59
1:C:61:THR:HG22	1:C:64:GLN:CG	2.22	0.59
1:C:50:THR:HG23	1:C:151:PRO:HD2	1.85	0.59
1:C:393:LEU:HD13	1:C:444:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLN:HA	1:B:197:HIS:O	2.02	0.59
1:A:114:ILE:O	1:A:114:ILE:HD12	2.03	0.59
1:B:377:LEU:HD12	1:B:377:LEU:N	2.16	0.59
1:C:94:ALA:HB2	1:C:127:TRP:CZ2	2.37	0.59
1:A:138:LEU:N	1:A:138:LEU:HD12	2.18	0.58
1:C:427:ASN:O	1:C:430:ARG:N	2.36	0.58
1:A:203:ASP:HB3	1:A:206:GLU:CB	2.33	0.58
1:B:371:THR:HG23	1:B:439:THR:HG21	1.84	0.58
1:C:365:ARG:HA	1:C:368:GLN:HG2	1.85	0.58
1:C:79:PHE:CE2	1:C:81:PRO:HD3	2.39	0.58
1:A:300:LEU:H	1:A:300:LEU:CD2	2.16	0.58
1:C:94:ALA:HB2	1:C:127:TRP:CH2	2.39	0.58
1:A:38:ASP:OD1	1:A:41:GLN:HG2	2.04	0.58
1:B:300:LEU:CD2	1:B:300:LEU:H	2.17	0.58
1:B:424:ARG:CD	1:B:450:ILE:HD11	2.28	0.58
1:A:188:ILE:HA	1:B:539:HIS:CD2	2.38	0.58
1:A:539:HIS:ND1	1:C:188:ILE:HA	2.18	0.58
1:C:89:ARG:N	1:C:89:ARG:HD3	2.19	0.58
1:B:475:VAL:HA	1:B:519:ILE:HD11	1.84	0.57
1:A:300:LEU:HD23	1:A:300:LEU:H	1.69	0.57
1:C:199:GLN:HG3	1:C:234:LEU:CD1	2.34	0.57
1:A:61:THR:HG22	1:A:64:GLN:H	1.69	0.57
1:B:441:ASN:O	1:B:442:ARG:HB2	2.05	0.57
1:A:375:THR:HG21	1:A:472:GLU:OE2	2.03	0.57
1:C:61:THR:HG22	1:C:64:GLN:H	1.68	0.57
1:A:35:LEU:HD13	1:A:93:LEU:HD21	1.87	0.57
1:B:521:THR:OG1	1:B:524:LEU:HG	2.04	0.57
1:A:461:ARG:HB2	1:A:470:PHE:CE2	2.39	0.57
1:B:453:TYR:O	1:B:454:ARG:C	2.43	0.56
1:A:403:LEU:HD22	1:A:405:ASP:HB2	1.87	0.56
1:C:114:ILE:HD12	1:C:114:ILE:C	2.25	0.56
1:C:544:ARG:CG	1:C:545:LEU:N	2.66	0.56
1:A:204:ILE:O	1:A:208:PRO:HG2	2.05	0.56
1:B:429:ARG:NH2	1:B:459:ASP:OD1	2.38	0.56
1:B:475:VAL:HA	1:B:519:ILE:CG1	2.36	0.56
1:A:4:GLN:HE21	1:A:5:LEU:N	1.99	0.56
1:B:365:ARG:C	1:B:367:ARG:H	2.08	0.56
1:B:97:ARG:HH11	1:B:97:ARG:HG2	1.71	0.56
1:C:264:GLY:HA3	1:C:303:TYR:HB3	1.88	0.56
1:B:68:VAL:C	1:B:70:SER:N	2.59	0.56
1:A:414:SER:HA	1:A:417:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:OE1	1:B:44:GLU:HA	2.04	0.56
1:A:204:ILE:C	1:A:208:PRO:CG	2.74	0.56
1:B:300:LEU:HD23	1:B:300:LEU:H	1.70	0.56
1:B:507:ASP:CB	1:B:508:PRO:HD2	2.29	0.56
1:C:464:ILE:HG12	1:C:470:PHE:HD1	1.69	0.56
1:A:62:ARG:HG3	1:A:121:TRP:NE1	2.21	0.55
1:B:293:ALA:C	1:B:295:LYS:N	2.58	0.55
1:B:61:THR:CG2	1:B:64:GLN:CG	2.59	0.55
1:C:14:VAL:CG1	1:C:16:LEU:HD13	2.36	0.55
1:C:21:LYS:O	1:C:25:LEU:CG	2.53	0.55
1:A:410:ARG:O	1:A:415:SER:N	2.38	0.55
1:B:89:ARG:N	1:B:89:ARG:CD	2.68	0.55
1:A:188:ILE:HA	1:B:539:HIS:CG	2.42	0.55
1:A:475:VAL:HA	1:A:519:ILE:HG12	1.88	0.55
1:A:6:ILE:HD13	1:A:254:ARG:HG3	1.88	0.55
1:B:114:ILE:C	1:B:114:ILE:HD12	2.27	0.55
1:C:371:THR:HG23	1:C:439:THR:HG21	1.88	0.55
1:C:521:THR:OG1	1:C:524:LEU:HG	2.07	0.55
1:B:5:LEU:O	1:B:6:ILE:C	2.46	0.55
1:B:250:ALA:HB1	1:B:298:VAL:HG11	1.88	0.55
1:B:62:ARG:HG2	1:B:121:TRP:CZ2	2.41	0.54
1:A:440:LYS:HB2	1:A:467:VAL:HG21	1.88	0.54
1:B:121:TRP:CH2	1:B:128:HIS:HB3	2.43	0.54
1:A:161:ARG:NH2	1:A:229:THR:O	2.41	0.54
1:A:87:THR:O	1:A:88:SER:HB2	2.07	0.54
1:B:375:THR:HG21	1:B:472:GLU:OE2	2.07	0.54
1:B:86:LEU:HD12	1:B:129:LEU:HD12	1.89	0.54
1:C:453:TYR:O	1:C:454:ARG:C	2.46	0.54
1:C:519:ILE:O	1:C:519:ILE:HG13	2.08	0.54
1:C:6:ILE:HD13	1:C:254:ARG:HG3	1.89	0.54
1:C:86:LEU:HD12	1:C:129:LEU:HD12	1.89	0.54
1:A:170:GLN:HA	1:A:197:HIS:O	2.07	0.54
1:A:204:ILE:O	1:A:208:PRO:CG	2.56	0.54
1:B:264:GLY:HA3	1:B:303:TYR:HB3	1.91	0.54
1:A:86:LEU:HD12	1:A:129:LEU:HD12	1.90	0.53
1:B:403:LEU:HD22	1:B:405:ASP:HB2	1.91	0.53
1:A:377:LEU:N	1:A:377:LEU:HD12	2.18	0.53
1:B:262:ILE:HG12	1:B:301:ILE:CD1	2.38	0.53
1:B:35:LEU:HD13	1:B:93:LEU:HD21	1.90	0.53
1:C:262:ILE:HG12	1:C:301:ILE:CD1	2.38	0.53
1:B:220:ILE:HG13	1:B:220:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:CD1	1:B:444:ILE:CD1	2.85	0.53
1:C:428:VAL:CG1	1:C:456:THR:HG21	2.35	0.53
1:A:188:ILE:HA	1:B:539:HIS:NE2	2.23	0.53
1:A:91:ARG:C	1:A:93:LEU:H	2.13	0.53
1:B:439:THR:HG21	1:B:464:ILE:HD13	1.91	0.53
1:C:476:ALA:O	1:C:477:THR:C	2.47	0.53
1:B:101:ARG:CZ	1:B:114:ILE:HD11	2.39	0.52
1:B:67:ARG:O	1:B:67:ARG:HG2	2.09	0.52
1:B:453:TYR:N	1:B:453:TYR:HD1	2.07	0.52
1:C:439:THR:HG21	1:C:464:ILE:HD13	1.90	0.52
1:C:375:THR:HG21	1:C:472:GLU:OE2	2.09	0.52
1:A:44:GLU:HA	1:A:44:GLU:OE1	2.09	0.52
1:B:440:LYS:HB2	1:B:467:VAL:HG21	1.91	0.52
1:B:374:PHE:CE2	1:B:473:ILE:CD1	2.92	0.52
1:B:5:LEU:C	1:B:6:ILE:O	2.47	0.52
1:B:68:VAL:O	1:B:70:SER:N	2.43	0.52
1:B:188:ILE:HA	1:C:539:HIS:CE1	2.44	0.52
1:A:104:LEU:HD11	1:A:115:LEU:HB2	1.90	0.52
1:A:262:ILE:HG12	1:A:301:ILE:CD1	2.40	0.52
1:C:453:TYR:N	1:C:453:TYR:HD1	2.08	0.52
1:A:408:ILE:O	1:A:412:HIS:HD2	1.93	0.51
1:B:452:PRO:C	1:B:453:TYR:HD1	2.14	0.51
1:B:453:TYR:N	1:B:453:TYR:CD1	2.77	0.51
1:B:62:ARG:CG	1:B:121:TRP:CE2	2.93	0.51
1:C:25:LEU:HD23	1:C:25:LEU:N	2.25	0.51
1:C:475:VAL:HG22	1:C:519:ILE:HD11	1.92	0.51
1:B:121:TRP:CE2	1:B:128:HIS:HB2	2.46	0.51
1:C:6:ILE:CD1	1:C:254:ARG:HG3	2.39	0.51
1:A:289:VAL:CG2	1:A:290:ALA:H	2.23	0.51
1:B:220:ILE:CG2	1:B:354:VAL:CG2	2.84	0.51
1:C:455:GLN:HA	1:C:455:GLN:NE2	2.25	0.51
1:C:374:PHE:CE2	1:C:473:ILE:CD1	2.93	0.51
1:A:199:GLN:HG3	1:A:234:LEU:CD1	2.40	0.51
1:B:79:PHE:CE2	1:B:81:PRO:HD3	2.46	0.51
1:A:441:ASN:O	1:A:442:ARG:HB2	2.11	0.51
1:C:128:HIS:O	1:C:129:LEU:HD23	2.10	0.51
1:A:512:PRO:HB2	1:A:515:PRO:HG3	1.92	0.51
1:C:220:ILE:HG13	1:C:220:ILE:O	2.12	0.51
1:C:44:GLU:HA	1:C:44:GLU:OE1	2.11	0.51
1:C:523:GLY:O	1:C:524:LEU:HD23	2.10	0.51
1:B:7:GLU:HB2	1:B:8:PRO:CD	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:N	1:C:453:TYR:CD1	2.78	0.50
1:C:90:ASP:OD1	1:C:91:ARG:N	2.44	0.50
1:B:365:ARG:O	1:B:367:ARG:N	2.45	0.50
1:C:175:MET:HG3	1:C:179:GLN:CG	2.41	0.50
1:A:220:ILE:O	1:A:220:ILE:HG13	2.11	0.50
1:B:442:ARG:NH1	1:B:442:ARG:HG2	2.01	0.50
1:C:300:LEU:HD23	1:C:300:LEU:H	1.75	0.50
1:C:377:LEU:C	1:C:379:GLY:H	2.15	0.50
1:A:242:SER:OG	1:A:244:ARG:HD3	2.12	0.50
1:A:439:THR:HG21	1:A:464:ILE:HD13	1.93	0.50
1:C:357:GLU:OE1	1:C:360:ARG:NH1	2.43	0.50
1:A:62:ARG:HG3	1:A:121:TRP:CD2	2.47	0.50
1:B:47:MET:CE	1:B:47:MET:HA	2.42	0.50
1:A:251:ILE:HG12	1:A:296:ILE:HD12	1.94	0.49
1:A:311:ASP:C	1:B:338:ARG:HH21	2.15	0.49
1:B:390:ALA:O	1:B:394:MET:HG3	2.13	0.49
1:C:260:LEU:HA	1:C:299:ARG:O	2.12	0.49
1:C:440:LYS:HB2	1:C:467:VAL:HG21	1.94	0.49
1:B:414:SER:HB3	1:B:417:LEU:HD11	1.90	0.49
1:B:61:THR:HG23	1:B:63:ALA:H	1.77	0.49
1:C:461:ARG:HB2	1:C:470:PHE:CE2	2.47	0.49
1:A:453:TYR:HD1	1:A:453:TYR:N	2.10	0.49
1:B:5:LEU:O	1:B:6:ILE:O	2.30	0.49
1:A:458:ARG:HH11	1:A:461:ARG:CD	2.23	0.49
1:B:440:LYS:HB2	1:B:467:VAL:CG2	2.42	0.49
1:C:250:ALA:HB1	1:C:298:VAL:HG11	1.94	0.49
1:A:539:HIS:NE2	1:C:188:ILE:HA	2.21	0.49
1:C:475:VAL:HG22	1:C:519:ILE:CD1	2.42	0.49
1:A:157:LEU:HD23	1:A:160:ARG:NH2	2.21	0.49
1:B:455:GLN:O	1:B:458:ARG:CB	2.61	0.49
1:A:371:THR:HA	1:A:445:ALA:O	2.13	0.49
1:B:393:LEU:CD1	1:B:444:ILE:HD11	2.43	0.49
1:C:157:LEU:HD23	1:C:160:ARG:NH2	2.19	0.49
1:A:39:TRP:CD1	1:A:206:GLU:CB	2.96	0.49
1:A:414:SER:O	1:A:417:LEU:HD12	2.13	0.49
1:A:440:LYS:HB2	1:A:467:VAL:CG2	2.43	0.49
1:B:509:TYR:CD2	1:B:510:GLU:C	2.86	0.49
1:C:114:ILE:HD12	1:C:114:ILE:O	2.12	0.49
1:C:19:PRO:O	1:C:20:GLU:C	2.50	0.49
1:C:312:ARG:O	1:C:314:GLU:HG2	2.13	0.49
1:A:97:ARG:O	1:A:98:PRO:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASP:O	1:C:42:GLN:HG3	2.13	0.48
1:A:453:TYR:CD1	1:A:453:TYR:N	2.80	0.48
1:B:220:ILE:HG22	1:B:354:VAL:CG2	2.29	0.48
1:B:509:TYR:CD2	1:B:510:GLU:O	2.62	0.48
1:B:4:GLN:HE21	1:B:5:LEU:N	2.07	0.48
1:B:121:TRP:CZ2	1:B:128:HIS:CB	2.96	0.48
1:C:380:ALA:C	1:C:382:LYS:N	2.67	0.48
1:C:475:VAL:CG1	1:C:519:ILE:HD11	2.37	0.48
1:A:514:THR:O	1:A:514:THR:HG23	2.14	0.48
1:B:61:THR:O	1:B:64:GLN:N	2.47	0.48
1:A:452:PRO:C	1:A:453:TYR:HD1	2.17	0.48
1:A:97:ARG:O	1:A:98:PRO:C	2.50	0.48
1:B:114:ILE:O	1:B:114:ILE:HD12	2.14	0.48
1:C:476:ALA:C	1:C:477:THR:O	2.48	0.48
1:B:289:VAL:HG23	1:B:290:ALA:N	2.28	0.48
1:A:164:ARG:HH21	1:B:532:GLN:HB2	1.78	0.48
1:A:169:TRP:CE3	1:A:262:ILE:HG21	2.48	0.48
1:A:205:THR:HG23	1:A:206:GLU:N	2.28	0.48
1:A:427:ASN:O	1:A:430:ARG:HB3	2.14	0.48
1:A:309:VAL:HG21	1:A:316:LEU:HD12	1.96	0.47
1:B:97:ARG:HG2	1:B:97:ARG:NH1	2.28	0.47
1:C:247:LEU:HD11	1:C:292:ARG:HD2	1.94	0.47
1:A:442:ARG:HD3	1:A:442:ARG:HA	1.62	0.47
1:C:25:LEU:O	1:C:26:LYS:C	2.52	0.47
1:C:29:ALA:C	1:C:31:SER:H	2.17	0.47
1:C:514:THR:N	1:C:515:PRO:HD3	2.29	0.47
1:A:300:LEU:N	1:A:300:LEU:CD2	2.76	0.47
1:A:409:VAL:HG11	1:A:431:ILE:HD11	1.96	0.47
1:B:377:LEU:H	1:B:377:LEU:CD1	2.21	0.47
1:A:128:HIS:O	1:A:129:LEU:HD23	2.14	0.47
1:A:453:TYR:O	1:A:454:ARG:C	2.47	0.47
1:C:251:ILE:HG12	1:C:296:ILE:HD12	1.96	0.47
1:A:247:LEU:O	1:A:251:ILE:HG13	2.14	0.47
1:B:414:SER:CB	1:B:417:LEU:HD11	2.33	0.47
1:B:461:ARG:HB2	1:B:470:PHE:CE2	2.50	0.47
1:A:250:ALA:HB1	1:A:298:VAL:HG11	1.96	0.47
1:B:365:ARG:C	1:B:367:ARG:N	2.68	0.47
1:B:157:LEU:HD23	1:B:160:ARG:NH2	2.24	0.47
1:B:300:LEU:CD2	1:B:300:LEU:N	2.77	0.47
1:A:35:LEU:HD21	1:A:88:SER:HB3	1.95	0.47
1:B:370:PHE:HA	1:B:469:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:HH11	1:B:424:ARG:HG2	1.79	0.47
1:C:403:LEU:HD22	1:C:405:ASP:HB2	1.97	0.47
1:C:452:PRO:C	1:C:453:TYR:HD1	2.18	0.47
1:A:539:HIS:CD2	1:C:188:ILE:CG2	2.81	0.46
1:A:205:THR:C	1:A:208:PRO:HD3	2.36	0.46
1:B:14:VAL:CG1	1:B:16:LEU:HD13	2.45	0.46
1:C:530:VAL:O	1:C:533:ILE:HG12	2.15	0.46
1:B:185:LYS:HG3	1:B:186:SER:N	2.30	0.46
1:C:415:SER:OG	1:C:416:GLU:N	2.49	0.46
1:A:14:VAL:CG1	1:A:16:LEU:HD13	2.45	0.46
1:A:414:SER:C	1:A:417:LEU:HD12	2.36	0.46
1:B:409:VAL:O	1:B:410:ARG:C	2.54	0.46
1:B:414:SER:O	1:B:417:LEU:HD12	2.15	0.46
1:C:23:GLU:OE2	1:C:23:GLU:HA	2.15	0.46
1:C:427:ASN:O	1:C:430:ARG:HB3	2.14	0.46
1:B:138:LEU:CD1	1:B:138:LEU:H	2.27	0.46
1:C:293:ALA:C	1:C:295:LYS:N	2.69	0.46
1:A:371:THR:CG2	1:A:439:THR:CG2	2.92	0.46
1:A:9:TYR:C	1:A:11:GLY:H	2.19	0.46
1:B:514:THR:O	1:B:514:THR:HG23	2.16	0.46
1:C:451:ALA:HA	1:C:452:PRO:HD3	1.72	0.46
1:A:74:LEU:HD13	1:A:80:TRP:CB	2.46	0.46
1:B:451:ALA:HA	1:B:452:PRO:HD3	1.69	0.46
1:A:455:GLN:NE2	1:A:455:GLN:HA	2.31	0.46
1:A:79:PHE:CE2	1:A:81:PRO:HD3	2.50	0.46
1:B:161:ARG:NH2	1:B:229:THR:O	2.47	0.46
1:B:61:THR:HG22	1:B:64:GLN:HG2	1.84	0.46
1:A:357:GLU:OE1	1:A:360:ARG:NH1	2.47	0.46
1:A:379:GLY:HA3	1:A:382:LYS:HE2	1.98	0.46
1:C:16:LEU:HD11	1:C:57:THR:OG1	2.16	0.46
1:C:220:ILE:CG2	1:C:354:VAL:CG2	2.92	0.46
1:A:216:SER:O	1:A:220:ILE:HG23	2.16	0.45
1:A:242:SER:OG	1:A:244:ARG:CD	2.64	0.45
1:B:364:PRO:O	1:B:365:ARG:C	2.53	0.45
1:B:475:VAL:CA	1:B:519:ILE:HD11	2.46	0.45
1:C:509:TYR:CG	1:C:510:GLU:N	2.84	0.45
1:A:292:ARG:HD2	1:A:292:ARG:HA	1.66	0.45
1:B:116:THR:O	1:B:131:GLY:HA3	2.16	0.45
1:C:441:ASN:O	1:C:442:ARG:HB2	2.16	0.45
1:A:289:VAL:C	1:A:291:GLU:N	2.65	0.45
1:A:530:VAL:O	1:A:533:ILE:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:O	1:B:251:ILE:HG13	2.15	0.45
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.41	0.45
1:B:514:THR:N	1:B:515:PRO:HD3	2.31	0.45
1:A:292:ARG:O	1:A:295:LYS:CB	2.65	0.45
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.79	0.45
1:A:374:PHE:CE2	1:A:473:ILE:CD1	3.00	0.45
1:A:6:ILE:HG23	1:A:6:ILE:O	2.16	0.45
1:A:33:PRO:O	1:A:102:LEU:HD23	2.16	0.45
1:A:76:ASP:OD1	1:A:76:ASP:N	2.48	0.45
1:B:377:LEU:C	1:B:379:GLY:H	2.19	0.45
1:C:97:ARG:O	1:C:98:PRO:O	2.35	0.45
1:A:370:PHE:HA	1:A:469:GLY:O	2.16	0.45
1:B:260:LEU:HA	1:B:299:ARG:O	2.17	0.45
1:B:371:THR:CG2	1:B:439:THR:CG2	2.95	0.45
1:B:96:ARG:CG	1:B:96:ARG:NH1	2.73	0.45
1:A:450:ILE:O	1:A:450:ILE:HD12	2.16	0.45
1:C:454:ARG:NH1	1:C:511:VAL:O	2.49	0.45
1:A:168:ALA:HB2	1:A:258:CYS:SG	2.57	0.45
1:A:50:THR:HG23	1:A:151:PRO:CD	2.45	0.45
1:C:175:MET:HG3	1:C:179:GLN:HG3	1.99	0.45
1:C:374:PHE:CD2	1:C:473:ILE:HD11	2.52	0.45
1:C:411:ARG:HA	1:C:411:ARG:HD3	1.53	0.45
1:C:440:LYS:HB2	1:C:467:VAL:CG2	2.46	0.45
1:A:188:ILE:HA	1:B:539:HIS:ND1	2.30	0.45
1:A:474:HIS:CE1	1:A:476:ALA:HB2	2.52	0.45
1:A:101:ARG:CZ	1:A:114:ILE:HD11	2.46	0.45
1:A:6:ILE:CD1	1:A:254:ARG:HG3	2.47	0.45
1:A:90:ASP:HB3	1:A:93:LEU:HG	1.98	0.45
1:B:365:ARG:HA	1:B:368:GLN:HG2	1.97	0.45
1:B:76:ASP:OD1	1:B:76:ASP:N	2.49	0.45
1:B:96:ARG:CG	1:B:96:ARG:HH11	2.14	0.45
1:B:286:ASP:OD1	1:B:287:PRO:CD	2.64	0.44
1:B:40:GLN:O	1:B:43:CYS:HB2	2.17	0.44
1:B:474:HIS:CE1	1:B:476:ALA:HB2	2.52	0.44
1:A:254:ARG:NH1	1:A:296:ILE:O	2.49	0.44
1:A:514:THR:N	1:A:515:PRO:HD3	2.31	0.44
1:A:519:ILE:CG1	1:A:519:ILE:O	2.64	0.44
1:C:34:SER:HB2	1:C:105:ARG:HD2	1.99	0.44
1:C:5:LEU:HA	1:C:5:LEU:HD23	1.64	0.44
1:A:314:GLU:OE2	1:B:337:ARG:NH2	2.49	0.44
1:B:450:ILE:O	1:B:450:ILE:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:TYR:C	1:B:455:GLN:N	2.71	0.44
1:C:200:VAL:HG21	1:C:233:LEU:HD22	2.00	0.44
1:C:377:LEU:C	1:C:379:GLY:N	2.70	0.44
1:A:122:LYS:NZ	1:A:127:TRP:CZ3	2.78	0.44
1:A:260:LEU:HA	1:A:299:ARG:O	2.17	0.44
1:B:442:ARG:HD3	1:B:442:ARG:HA	1.65	0.44
1:C:20:GLU:O	1:C:21:LYS:C	2.54	0.44
1:C:300:LEU:N	1:C:300:LEU:CD2	2.76	0.44
1:C:370:PHE:HA	1:C:469:GLY:O	2.17	0.44
1:B:435:ALA:O	1:B:439:THR:CG2	2.65	0.44
1:B:435:ALA:O	1:B:439:THR:HG22	2.17	0.44
1:C:82:SER:HA	1:C:83:PRO:HD3	1.86	0.44
1:A:220:ILE:CG2	1:A:354:VAL:CG2	2.92	0.44
1:A:451:ALA:HA	1:A:452:PRO:HD3	1.69	0.44
1:B:27:HIS:O	1:B:30:LEU:HB2	2.17	0.44
1:B:509:TYR:OH	1:B:512:PRO:HD3	2.18	0.44
1:A:371:THR:HG21	1:A:435:ALA:HB1	1.99	0.44
1:C:203:ASP:H	1:C:207:ALA:HB3	1.82	0.44
1:C:379:GLY:O	1:C:381:GLY:N	2.47	0.44
1:C:544:ARG:HG2	1:C:545:LEU:H	1.78	0.44
1:C:76:ASP:OD1	1:C:76:ASP:N	2.50	0.44
1:A:414:SER:CB	1:A:417:LEU:HD11	2.39	0.44
1:B:19:PRO:HA	1:B:22:ARG:HB2	1.99	0.44
1:C:427:ASN:O	1:C:428:VAL:C	2.56	0.44
1:C:464:ILE:O	1:C:464:ILE:HD12	2.18	0.44
1:C:30:LEU:HA	1:C:30:LEU:HD23	1.80	0.43
1:A:424:ARG:HA	1:A:424:ARG:HD3	1.67	0.43
1:B:509:TYR:CZ	1:B:510:GLU:O	2.66	0.43
1:B:9:TYR:C	1:B:11:GLY:H	2.21	0.43
1:B:38:ASP:O	1:B:42:GLN:HG3	2.18	0.43
1:C:101:ARG:CZ	1:C:114:ILE:HD11	2.49	0.43
1:C:390:ALA:O	1:C:394:MET:HG3	2.18	0.43
1:A:9:TYR:HD1	1:A:254:ARG:NH1	2.16	0.43
1:B:4:GLN:NE2	1:B:5:LEU:CA	2.81	0.43
1:C:220:ILE:HG22	1:C:354:VAL:CG2	2.33	0.43
1:C:385:LEU:HA	1:C:385:LEU:HD23	1.76	0.43
1:C:417:LEU:HD21	1:C:426:VAL:HG11	1.98	0.43
1:C:371:THR:HA	1:C:445:ALA:O	2.19	0.43
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.72	0.43
1:B:216:SER:O	1:B:220:ILE:HG23	2.17	0.43
1:B:4:GLN:HA	1:B:164:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:TRP:NE1	1:C:82:SER:O	2.48	0.43
1:A:435:ALA:O	1:A:439:THR:CG2	2.67	0.43
1:B:185:LYS:HA	1:B:188:ILE:CD1	2.48	0.43
1:B:203:ASP:H	1:B:207:ALA:HB3	1.82	0.43
1:B:246:LEU:HD22	1:B:246:LEU:O	2.19	0.43
1:C:169:TRP:CE3	1:C:262:ILE:HG21	2.54	0.43
1:C:96:ARG:HG3	1:C:100:GLU:OE2	2.18	0.43
1:A:200:VAL:HG21	1:A:233:LEU:HD22	2.00	0.43
1:C:47:MET:HA	1:C:47:MET:CE	2.46	0.43
1:A:414:SER:CA	1:A:417:LEU:HD11	2.44	0.43
1:C:40:GLN:O	1:C:43:CYS:HB2	2.19	0.43
1:B:228:THR:CG2	1:B:228:THR:O	2.64	0.43
1:B:9:TYR:HD1	1:B:254:ARG:NH1	2.16	0.43
1:C:413:LEU:HG	1:C:430:ARG:HG3	2.01	0.43
1:C:477:THR:CB	1:C:521:THR:O	2.67	0.43
1:A:175:MET:HG3	1:A:179:GLN:CG	2.49	0.42
1:A:207:ALA:N	1:A:208:PRO:CD	2.81	0.42
1:A:223:ARG:HD2	1:A:351:PHE:CE2	2.54	0.42
1:B:175:MET:HG3	1:B:179:GLN:CG	2.49	0.42
1:B:234:LEU:HA	1:B:235:PRO:HD3	1.91	0.42
1:B:250:ALA:HB1	1:B:298:VAL:CG1	2.49	0.42
1:B:426:VAL:CG1	1:B:427:ASN:N	2.80	0.42
1:C:21:LYS:C	1:C:24:ALA:CB	2.83	0.42
1:C:512:PRO:HB2	1:C:515:PRO:HG3	2.01	0.42
1:C:536:LYS:O	1:C:537:LEU:C	2.55	0.42
1:C:89:ARG:CG	1:C:89:ARG:NH1	2.72	0.42
1:A:289:VAL:HG22	1:A:290:ALA:H	1.84	0.42
1:B:147:LEU:HB3	1:B:233:LEU:HG	2.00	0.42
1:B:409:VAL:CG1	1:B:431:ILE:HD11	2.48	0.42
1:B:90:ASP:OD1	1:B:91:ARG:N	2.52	0.42
1:C:223:ARG:HD2	1:C:351:PHE:CE2	2.54	0.42
1:A:169:TRP:CZ3	1:A:262:ILE:CG2	2.99	0.42
1:A:368:GLN:HA	1:A:442:ARG:HD2	2.01	0.42
1:A:413:LEU:O	1:A:430:ARG:NH2	2.48	0.42
1:B:228:THR:HG23	1:B:228:THR:O	2.19	0.42
1:C:379:GLY:C	1:C:381:GLY:H	2.20	0.42
1:C:426:VAL:O	1:C:427:ASN:C	2.56	0.42
1:A:414:SER:O	1:A:416:GLU:N	2.52	0.42
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.62	0.42
1:A:82:SER:HA	1:A:83:PRO:HD3	1.93	0.42
1:C:147:LEU:HD11	1:C:218:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:HA	1:B:539:HIS:CE1	2.53	0.42
1:A:346:PRO:HB3	1:A:348:TRP:CE2	2.54	0.42
1:A:387:ARG:HG3	1:A:403:LEU:HD11	2.01	0.42
1:B:453:TYR:O	1:B:455:GLN:N	2.53	0.42
1:A:3:ASN:O	1:A:164:ARG:HD2	2.19	0.42
1:A:425:ASP:OD2	1:A:425:ASP:O	2.36	0.42
1:A:517:LEU:HG	1:A:536:LYS:HG2	2.01	0.42
1:B:414:SER:C	1:B:417:LEU:HD12	2.39	0.42
1:A:314:GLU:CD	1:B:337:ARG:HH22	2.22	0.42
1:B:23:GLU:O	1:B:24:ALA:C	2.58	0.42
1:C:29:ALA:O	1:C:31:SER:N	2.52	0.42
1:A:167:ILE:HA	1:A:260:LEU:HB2	2.02	0.42
1:B:321:ALA:HA	1:B:322:PRO:HD3	1.95	0.42
1:C:21:LYS:O	1:C:25:LEU:HD21	2.20	0.42
1:A:205:THR:HA	1:A:208:PRO:HG2	2.02	0.42
1:A:444:ILE:HD13	1:A:444:ILE:HG21	1.76	0.42
1:A:47:MET:CE	1:A:47:MET:HA	2.47	0.42
1:B:96:ARG:HG3	1:B:100:GLU:OE2	2.19	0.42
1:C:309:VAL:HG21	1:C:316:LEU:HD12	2.01	0.42
1:C:450:ILE:O	1:C:450:ILE:HD12	2.20	0.42
1:C:138:LEU:CD1	1:C:138:LEU:N	2.83	0.41
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.71	0.41
1:A:74:LEU:HD13	1:A:80:TRP:HB3	2.01	0.41
1:B:200:VAL:HG13	1:B:200:VAL:O	2.19	0.41
1:C:94:ALA:CB	1:C:127:TRP:CZ2	3.01	0.41
1:C:435:ALA:O	1:C:439:THR:CG2	2.68	0.41
1:B:332:GLY:O	1:B:336:GLN:HB2	2.21	0.41
1:C:19:PRO:O	1:C:22:ARG:CA	2.69	0.41
1:C:371:THR:HG21	1:C:435:ALA:HB1	2.01	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.55	0.41
1:B:94:ALA:HB2	1:B:127:TRP:CZ2	2.55	0.41
1:B:139:PRO:HA	1:B:140:PRO:HD3	1.95	0.41
1:B:19:PRO:C	1:B:22:ARG:H	2.23	0.41
1:C:168:ALA:HB2	1:C:258:CYS:SG	2.60	0.41
1:C:424:ARG:HD2	1:C:424:ARG:HA	1.25	0.41
1:A:393:LEU:CD1	1:A:444:ILE:HD11	2.50	0.41
1:A:91:ARG:C	1:A:93:LEU:N	2.73	0.41
1:B:307:VAL:O	1:B:315:HIS:HA	2.21	0.41
1:C:176:HIS:H	1:C:179:GLN:HE21	1.68	0.41
1:C:521:THR:HG23	1:C:521:THR:H	1.59	0.41
1:A:414:SER:C	1:A:416:GLU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:THR:HG22	1:A:439:THR:CG2	2.50	0.41
1:B:200:VAL:O	1:B:200:VAL:CG1	2.69	0.41
1:B:521:THR:HG21	1:B:524:LEU:HD11	2.02	0.41
1:C:107:GLY:CA	2:C:574:HOH:O	2.63	0.41
1:C:97:ARG:O	1:C:98:PRO:C	2.58	0.41
1:A:35:LEU:HD21	1:A:88:SER:HB2	2.00	0.41
1:B:371:THR:HA	1:B:445:ALA:O	2.19	0.41
1:C:200:VAL:HG13	1:C:200:VAL:O	2.19	0.41
1:C:407:ASP:O	1:C:411:ARG:HG2	2.21	0.41
1:A:408:ILE:HG22	1:A:409:VAL:N	2.36	0.41
1:A:5:LEU:HD23	1:A:164:ARG:O	2.21	0.41
1:A:89:ARG:O	1:A:89:ARG:HG2	2.21	0.41
1:B:410:ARG:O	1:B:415:SER:HB3	2.20	0.41
1:B:421:LYS:N	1:B:421:LYS:HD3	2.27	0.41
1:C:247:LEU:O	1:C:251:ILE:HG13	2.20	0.41
1:C:362:THR:HA	1:C:363:PRO:HD3	1.82	0.41
1:C:9:TYR:HD1	1:C:254:ARG:NH1	2.18	0.41
1:A:97:ARG:CB	1:A:98:PRO:CD	2.99	0.41
1:C:384:THR:CG2	2:C:555:HOH:O	2.52	0.41
1:C:408:ILE:HG22	1:C:409:VAL:N	2.35	0.41
1:B:286:ASP:OD2	1:B:288:SER:HB3	2.21	0.41
1:C:450:ILE:HD12	1:C:450:ILE:H	1.86	0.41
1:C:61:THR:CB	1:C:64:GLN:HG3	2.50	0.41
1:A:292:ARG:HH21	1:A:292:ARG:CA	2.33	0.41
1:C:29:ALA:C	1:C:31:SER:N	2.74	0.41
1:C:371:THR:CG2	1:C:439:THR:CG2	2.96	0.41
1:A:286:ASP:CB	1:A:287:PRO:CB	2.95	0.40
1:A:301:ILE:O	1:A:301:ILE:HG12	2.20	0.40
1:A:321:ALA:HA	1:A:322:PRO:HD3	1.94	0.40
1:A:61:THR:HG23	1:A:63:ALA:H	1.85	0.40
1:B:169:TRP:CZ3	1:B:262:ILE:CG2	3.01	0.40
1:B:9:TYR:CE2	1:B:251:ILE:HD13	2.56	0.40
1:B:169:TRP:CE3	1:B:262:ILE:HG21	2.56	0.40
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.76	0.40
1:C:105:ARG:CB	1:C:110:TYR:O	2.69	0.40
1:C:161:ARG:NH2	1:C:229:THR:O	2.54	0.40
1:A:40:GLN:O	1:A:43:CYS:HB2	2.21	0.40
1:C:32:LEU:HD23	1:C:32:LEU:HA	1.84	0.40
1:A:374:PHE:CE2	1:A:385:LEU:HB3	2.56	0.40
1:B:4:GLN:CG	1:B:5:LEU:H	2.31	0.40
1:C:29:ALA:O	1:C:30:LEU:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:THR:HG22	1:C:439:THR:CG2	2.51	0.40
1:A:288:SER:C	1:A:291:GLU:CB	2.89	0.40
1:A:303:TYR:HA	1:A:304:PRO:HD3	1.80	0.40
1:B:248:LEU:O	1:B:252:VAL:HG13	2.21	0.40
1:B:423:HIS:O	1:B:426:VAL:HG12	2.21	0.40
1:B:408:ILE:HG22	1:B:409:VAL:N	2.36	0.40
1:B:519:ILE:CG1	1:B:519:ILE:O	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:NH2	1:B:430:ARG:NH2[3_455]	1.87	0.33

## 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	487/552 (88%)	441 (91%)	44 (9%)	2 (0%)	34 69
1	B	487/552 (88%)	440 (90%)	42 (9%)	5 (1%)	15 48
1	C	487/552 (88%)	438 (90%)	46 (9%)	3 (1%)	25 60
All	All	1461/1656 (88%)	1319 (90%)	132 (9%)	10 (1%)	22 56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	GLU
1	C	366	GLU
1	A	98	PRO
1	B	69	GLU
1	B	366	GLU

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Mol	Chain	Res	Type
1	B	6	ILE
1	B	296	ILE
1	C	514	THR
1	C	98	PRO
1	B	519	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	376/449 (84%)	311 (83%)	65 (17%)	2	8
1	B	373/449 (83%)	295 (79%)	78 (21%)	1	4
1	C	373/449 (83%)	301 (81%)	72 (19%)	1	6
All	All	1122/1347 (83%)	907 (81%)	215 (19%)	1	6

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	LEU
1	A	12	THR
1	A	13	LEU
1	A	23	GLU
1	A	37	LEU
1	A	40	GLN
1	A	44	GLU
1	A	50	THR
1	A	61	THR
1	A	74	LEU
1	A	76	ASP
1	A	89	ARG
1	A	96	ARG
1	A	97	ARG
1	A	102	LEU
1	A	111	MET

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Mol	Chain	Res	Type
1	A	114	ILE
1	A	123	ASP
1	A	127	TRP
1	A	138	LEU
1	A	154	LEU
1	A	157	LEU
1	A	173	GLN
1	A	179	GLN
1	A	188	ILE
1	A	197	HIS
1	A	200	VAL
1	A	213	LEU
1	A	220	ILE
1	A	228	THR
1	A	234	LEU
1	A	244	ARG
1	A	246	LEU
1	A	248	LEU
1	A	261	LEU
1	A	287	PRO
1	A	292	ARG
1	A	300	LEU
1	A	301	ILE
1	A	330	LEU
1	A	337	ARG
1	A	346	PRO
1	A	367	ARG
1	A	377	LEU
1	A	384	THR
1	A	389	LEU
1	A	403	LEU
1	A	407	ASP
1	A	413	LEU
1	A	415	SER
1	A	424	ARG
1	A	426	VAL
1	A	430	ARG
1	A	439	THR
1	A	442	ARG
1	A	444	ILE
1	A	450	ILE
1	A	464	ILE

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Mol	Chain	Res	Type
1	A	467	VAL
1	A	473	ILE
1	A	517	LEU
1	A	533	ILE
1	A	536	LYS
1	A	545	LEU
1	B	4	GLN
1	B	7	GLU
1	B	12	THR
1	B	13	LEU
1	B	16	LEU
1	B	19	PRO
1	B	37	LEU
1	B	40	GLN
1	B	44	GLU
1	B	50	THR
1	B	61	THR
1	B	62	ARG
1	B	67	ARG
1	B	74	LEU
1	B	76	ASP
1	B	89	ARG
1	B	96	ARG
1	B	97	ARG
1	B	102	LEU
1	B	105	ARG
1	B	111	MET
1	B	114	ILE
1	B	127	TRP
1	B	138	LEU
1	B	145	VAL
1	B	146	SER
1	B	154	LEU
1	B	157	LEU
1	B	173	GLN
1	B	179	GLN
1	B	185	LYS
1	B	188	ILE
1	B	197	HIS
1	B	200	VAL
1	B	204	ILE
1	B	205	THR

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Mol	Chain	Res	Type
1	B	206	GLU
1	B	213	LEU
1	B	220	ILE
1	B	228	THR
1	B	234	LEU
1	B	242	SER
1	B	244	ARG
1	B	246	LEU
1	B	248	LEU
1	B	252	VAL
1	B	261	LEU
1	B	285	VAL
1	B	296	ILE
1	B	300	LEU
1	B	301	ILE
1	B	326	ARG
1	B	330	LEU
1	B	337	ARG
1	B	367	ARG
1	B	371	THR
1	B	377	LEU
1	B	384	THR
1	B	389	LEU
1	B	403	LEU
1	B	407	ASP
1	B	414	SER
1	B	420	SER
1	B	421	LYS
1	B	426	VAL
1	B	427	ASN
1	B	430	ARG
1	B	439	THR
1	B	442	ARG
1	B	444	ILE
1	B	450	ILE
1	B	464	ILE
1	B	467	VAL
1	B	473	ILE
1	B	512	PRO
1	B	517	LEU
1	B	524	LEU
1	B	533	ILE

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Mol	Chain	Res	Type
1	C	5	LEU
1	C	7	GLU
1	C	12	THR
1	C	13	LEU
1	C	25	LEU
1	C	37	LEU
1	C	40	GLN
1	C	49	MET
1	C	50	THR
1	C	61	THR
1	C	74	LEU
1	C	76	ASP
1	C	89	ARG
1	C	96	ARG
1	C	102	LEU
1	C	105	ARG
1	C	111	MET
1	C	114	ILE
1	C	127	TRP
1	C	138	LEU
1	C	146	SER
1	C	154	LEU
1	C	157	LEU
1	C	179	GLN
1	C	188	ILE
1	C	197	HIS
1	C	200	VAL
1	C	204	ILE
1	C	205	THR
1	C	206	GLU
1	C	213	LEU
1	C	220	ILE
1	C	228	THR
1	C	232	SER
1	C	234	LEU
1	C	237	PRO
1	C	242	SER
1	C	244	ARG
1	C	246	LEU
1	C	248	LEU
1	C	252	VAL
1	C	261	LEU

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Mol	Chain	Res	Type
1	C	287	PRO
1	C	288	SER
1	C	296	ILE
1	C	300	LEU
1	C	301	ILE
1	C	330	LEU
1	C	336	GLN
1	C	337	ARG
1	C	367	ARG
1	C	371	THR
1	C	384	THR
1	C	389	LEU
1	C	403	LEU
1	C	407	ASP
1	C	411	ARG
1	C	420	SER
1	C	423	HIS
1	C	424	ARG
1	C	426	VAL
1	C	439	THR
1	C	444	ILE
1	C	450	ILE
1	C	464	ILE
1	C	467	VAL
1	C	473	ILE
1	C	517	LEU
1	C	521	THR
1	C	524	LEU
1	C	533	ILE
1	C	545	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	173	GLN
1	A	230	GLN
1	A	368	GLN
1	A	412	HIS
1	A	455	GLN
1	A	474	HIS
1	A	539	HIS

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Mol	Chain	Res	Type
1	B	4	GLN
1	B	27	HIS
1	B	173	GLN
1	B	230	GLN
1	B	368	GLN
1	B	427	ASN
1	B	474	HIS
1	B	539	HIS
1	C	230	GLN
1	C	368	GLN
1	C	455	GLN
1	C	539	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	493/552 (89%)	0.26	30 (6%)	21 12	30, 55, 94, 118	11 (2%)
1	B	493/552 (89%)	0.24	33 (6%)	17 10	26, 57, 93, 129	6 (1%)
1	C	493/552 (89%)	0.24	39 (7%)	12 7	26, 57, 94, 114	7 (1%)
All	All	1479/1656 (89%)	0.24	102 (6%)	16 10	26, 56, 94, 129	24 (1%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	GLY	5.7
1	B	422	ALA	5.6
1	B	379	GLY	5.6
1	B	380	ALA	5.4
1	B	418	GLY	5.3
1	A	476	ALA	4.9
1	C	30	LEU	4.8
1	B	423	HIS	4.5
1	C	127	TRP	4.4
1	B	508	PRO	4.3
1	C	450	ILE	4.2
1	C	95	ASP	4.2
1	A	520	ASP	4.0
1	B	206	GLU	3.8
1	B	522	THR	3.8
1	B	421	LYS	3.8
1	C	290	ALA	3.6
1	A	322	PRO	3.6
1	B	71	ALA	3.6
1	B	4	GLN	3.6
1	A	241	ALA	3.5
1	C	509	TYR	3.5
1	C	93	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	96	ARG	3.4
1	A	521	THR	3.4
1	A	240	GLU	3.3
1	B	520	ASP	3.3
1	A	89	ARG	3.3
1	A	326	ARG	3.3
1	C	92	ALA	3.2
1	C	123	ASP	3.2
1	B	509	TYR	3.1
1	C	294	GLU	3.1
1	C	125	GLU	2.9
1	C	323	GLN	2.9
1	C	297	GLY	2.9
1	C	94	ALA	2.9
1	B	414	SER	2.9
1	B	521	THR	2.8
1	A	77	GLY	2.8
1	C	29	ALA	2.8
1	A	24	ALA	2.8
1	B	384	THR	2.8
1	B	19	PRO	2.8
1	A	453	TYR	2.7
1	B	241	ALA	2.7
1	C	33	PRO	2.7
1	B	417	LEU	2.7
1	C	27	HIS	2.7
1	B	201	GLY	2.7
1	C	419	PHE	2.7
1	A	125	GLU	2.7
1	C	398	GLY	2.7
1	C	453	TYR	2.7
1	A	75	ASP	2.7
1	C	524	LEU	2.7
1	C	415	SER	2.7
1	A	378	SER	2.6
1	C	26	LYS	2.6
1	C	122	LYS	2.6
1	C	177	ARG	2.6
1	A	249	ARG	2.6
1	C	25	LEU	2.6
1	A	351	PHE	2.6
1	C	11	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	522	THR	2.5
1	B	107	GLY	2.5
1	B	419	PHE	2.5
1	B	21	LYS	2.4
1	A	62	ARG	2.4
1	C	101	ARG	2.4
1	B	381	GLY	2.3
1	C	91	ARG	2.3
1	B	514	THR	2.3
1	B	22	ARG	2.3
1	C	34	SER	2.3
1	A	69	GLU	2.3
1	A	122	LYS	2.3
1	B	30	LEU	2.3
1	C	89	ARG	2.2
1	B	512	PRO	2.2
1	A	124	GLY	2.2
1	C	244	ARG	2.2
1	C	523	GLY	2.2
1	B	5	LEU	2.1
1	A	426	VAL	2.1
1	C	28	GLU	2.1
1	A	161	ARG	2.1
1	C	291	GLU	2.1
1	B	284	ARG	2.1
1	A	3	ASN	2.1
1	A	21	LYS	2.1
1	B	377	LEU	2.1
1	A	507	ASP	2.1
1	A	207	ALA	2.0
1	C	69	GLU	2.0
1	B	249	ARG	2.0
1	B	513	GLU	2.0
1	C	422	ALA	2.0
1	A	127	TRP	2.0
1	C	78	SER	2.0
1	A	22	ARG	2.0

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

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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.