



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:10 pm BST

PDB ID : 3DYU  
Title : Crystal structure of Snx9PX-BAR (230-595), H32  
Authors : Wang, Q.; Kaan, H.Y.K.; Sondermann, H.  
Deposited on : 2008-07-28  
Resolution : 4.10 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

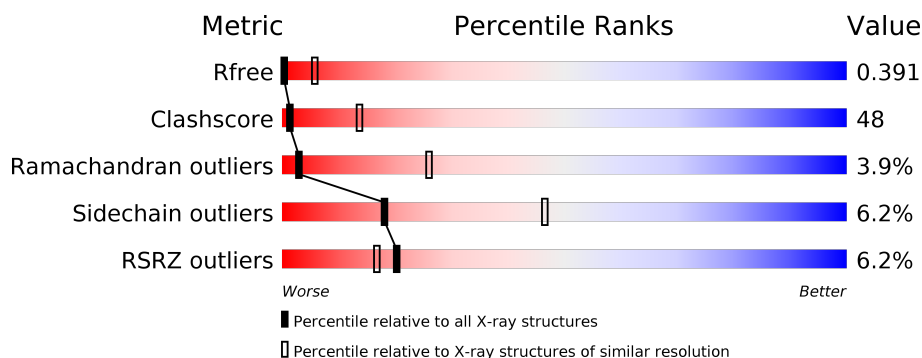
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	366	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>• •</div> </div> </div>
1	B	366	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	366	<div> <div>11%</div> <div> <div></div> <div>49%</div> <div>42%</div> <div>5%</div> <div>•</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8931 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.

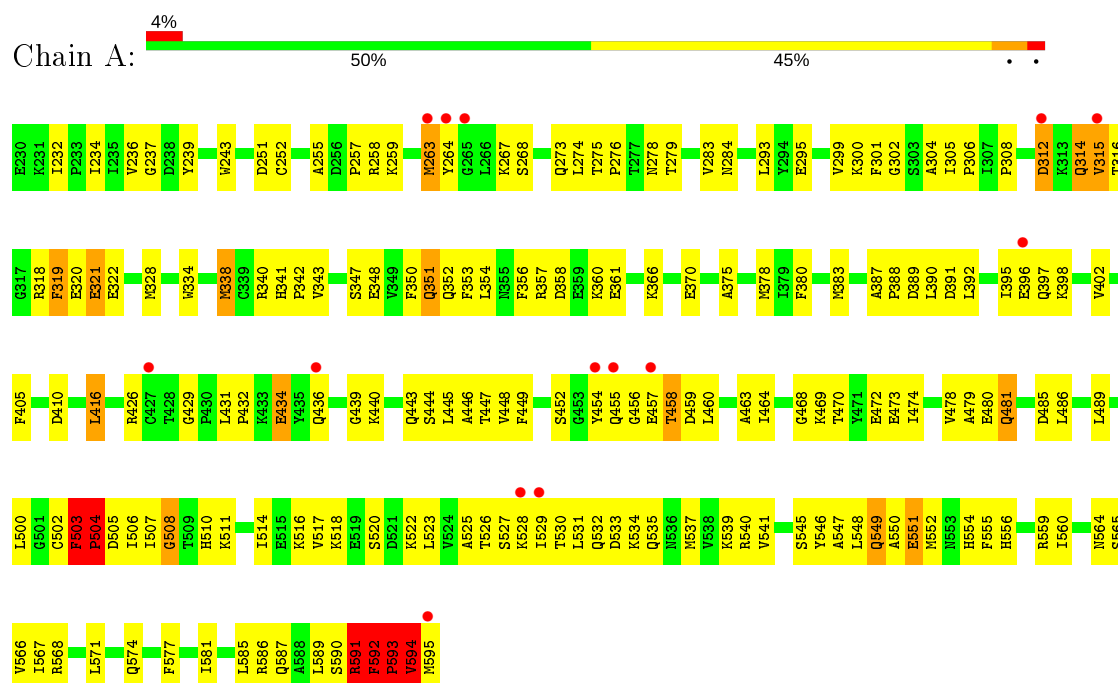
- Molecule 1 is a protein called Sorting nexin-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			
1	B	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			
1	C	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			

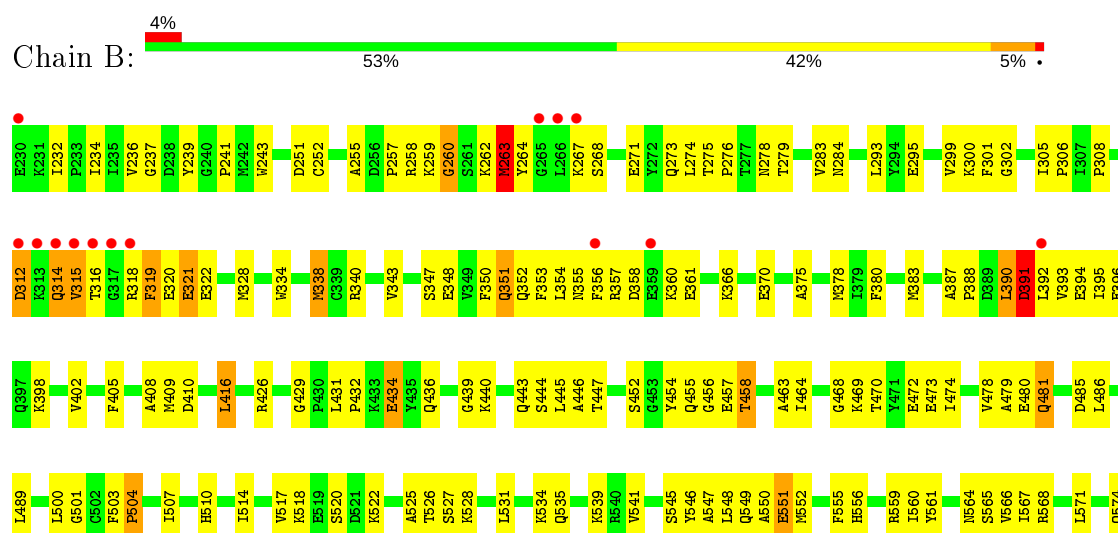
### 3 Residue-property plots

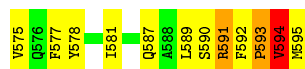
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Sorting nexin-9

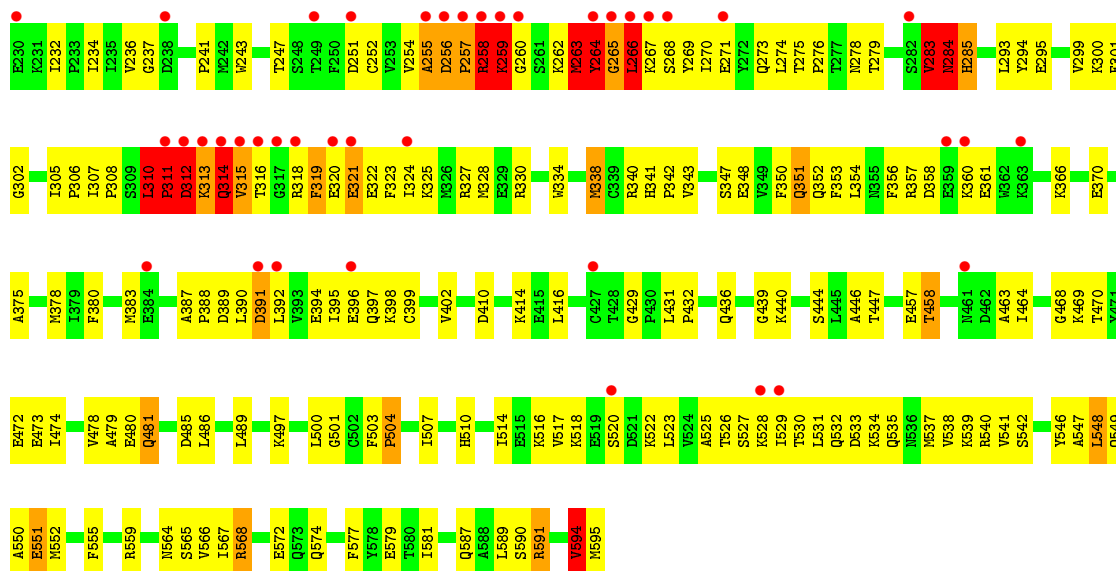


#### • Molecule 1: Sorting nexin-9





• Molecule 1: Sorting nexin-9



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.76 Å   131.76 Å   569.07 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	32.94 – 4.10 47.42 – 4.10	Depositor EDS
% Data completeness (in resolution range)	89.2 (32.94-4.10) 89.0 (47.42-4.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.24 (at 4.14 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.388   ,   0.403 0.391   ,   0.391	Depositor DCC
$R_{free}$ test set	764 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	8931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.42	0/3044	0.71	6/4100 (0.1%)
1	B	0.43	0/3044	0.65	2/4100 (0.0%)
1	C	0.44	1/3044 (0.0%)	0.67	3/4100 (0.1%)
All	All	0.43	1/9132 (0.0%)	0.68	11/12300 (0.1%)

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	3	6
1	B	0	3
1	C	5	16
All	All	8	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	548	LEU	C-N	5.73	1.47	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	LEU	O-C-N	-12.41	102.84	122.70
1	C	548	LEU	O-C-N	10.65	139.75	122.70
1	A	390	LEU	C-N-CA	8.87	143.88	121.70
1	A	390	LEU	CA-C-N	8.63	136.18	117.20
1	C	548	LEU	CA-C-N	-7.93	99.75	117.20
1	B	314	GLN	N-CA-C	7.63	131.59	111.00
1	A	314	GLN	N-CA-C	7.59	131.50	111.00
1	B	319	PHE	N-CA-C	7.12	130.23	111.00
1	C	319	PHE	N-CA-C	7.09	130.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	319	PHE	N-CA-C	7.09	130.13	111.00
1	A	263	MET	N-CA-C	6.32	128.07	111.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	503	PHE	CA
1	A	592	PHE	CA
1	A	594	VAL	CA
1	C	266	LEU	CA
1	C	284	ASN	CA
1	C	310	LEU	CA
1	C	312	ASP	CA
1	C	314	GLN	CA

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	PHE	Peptide
1	A	504	PRO	Peptide
1	A	508	GLY	Peptide
1	A	591	ARG	Peptide
1	A	592	PHE	Peptide
1	A	593	PRO	Peptide
1	B	260	GLY	Peptide
1	B	593	PRO	Peptide
1	B	594	VAL	Peptide
1	C	255	ALA	Peptide
1	C	258	ARG	Peptide
1	C	259	LYS	Peptide
1	C	260	GLY	Peptide
1	C	264	TYR	Peptide
1	C	265	GLY	Peptide
1	C	266	LEU	Peptide
1	C	283	VAL	Peptide
1	C	284	ASN	Peptide
1	C	310	LEU	Peptide
1	C	311	PRO	Peptide
1	C	312	ASP	Peptide
1	C	314	GLN	Peptide
1	C	389	ASP	Peptide
1	C	391	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	C	594	VAL	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	2977	0	2958	358	0
1	B	2977	0	2958	279	0
1	C	2977	0	2958	369	2
All	All	8931	0	8874	855	2

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 48.

All (855) 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:523:LEU:CD2	1:A:529:ILE:HG12	1.50	1.41
1:A:523:LEU:HD22	1:A:529:ILE:CG1	1.53	1.37
1:C:312:ASP:HB2	1:C:313:LYS:CG	1.56	1.33
1:C:255:ALA:CB	1:C:273:GLN:HE21	1.40	1.32
1:C:283:VAL:HG22	1:C:284:ASN:CG	1.51	1.29
1:C:523:LEU:HD23	1:C:529:ILE:CD1	1.66	1.26
1:C:391:ASP:HB3	1:C:538:VAL:CG1	1.63	1.26
1:A:568:ARG:NH1	1:B:589:LEU:HD11	1.48	1.26
1:C:254:VAL:HG22	1:C:274:LEU:CD2	1.65	1.25
1:B:395:ILE:CD1	1:B:541:VAL:HG13	1.67	1.24
1:C:391:ASP:CB	1:C:538:VAL:HG13	1.68	1.23
1:C:284:ASN:HB2	1:C:285:HIS:CG	1.74	1.22
1:C:283:VAL:HG22	1:C:284:ASN:CB	1.70	1.21
1:C:523:LEU:HD11	1:C:528:LYS:CB	1.70	1.20
1:C:312:ASP:CA	1:C:313:LYS:HG3	1.71	1.20
1:A:452:SER:HA	1:B:405:PHE:CD1	1.77	1.19
1:C:255:ALA:CB	1:C:256:ASP:HB2	1.71	1.18
1:C:523:LEU:CD1	1:C:528:LYS:CB	2.22	1.18
1:C:395:ILE:CD1	1:C:541:VAL:HG13	1.74	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LEU:N	1:C:311:PRO:HD3	1.42	1.16
1:B:594:VAL:O	1:B:595:MET:HG3	1.47	1.15
1:A:523:LEU:CD1	1:C:529:ILE:HG23	1.77	1.14
1:C:312:ASP:CB	1:C:313:LYS:CG	2.25	1.13
1:C:523:LEU:HD23	1:C:529:ILE:HD13	1.17	1.12
1:C:255:ALA:HB3	1:C:256:ASP:HB2	1.26	1.12
1:C:254:VAL:HG22	1:C:274:LEU:HD23	1.12	1.11
1:A:454:TYR:CE1	1:B:556:HIS:HB2	1.85	1.11
1:A:452:SER:HB3	1:B:405:PHE:CE1	1.85	1.11
1:C:392:LEU:HD13	1:C:517:VAL:HB	1.32	1.11
1:A:264:TYR:HD2	1:A:267:LYS:CB	1.63	1.11
1:A:452:SER:CB	1:B:405:PHE:CE1	2.34	1.11
1:C:324:ILE:HG22	1:C:328:MET:HE2	1.34	1.10
1:C:312:ASP:CB	1:C:313:LYS:HG2	1.78	1.09
1:C:523:LEU:HD12	1:C:528:LYS:HB2	1.29	1.09
1:B:395:ILE:HD13	1:B:541:VAL:HG13	1.22	1.09
1:C:264:TYR:O	1:C:267:LYS:HB2	1.52	1.09
1:A:568:ARG:HH11	1:B:589:LEU:CD1	1.66	1.09
1:C:594:VAL:HG13	1:C:595:MET:HG2	1.35	1.09
1:A:239:TYR:CE2	1:B:456:GLY:HA3	1.87	1.09
1:A:591:ARG:HB2	1:A:591:ARG:HH11	1.17	1.09
1:C:313:LYS:HB2	1:C:327:ARG:HH21	1.05	1.08
1:C:313:LYS:HB2	1:C:327:ARG:NH2	1.67	1.08
1:A:454:TYR:CD2	1:B:556:HIS:HB3	1.89	1.07
1:C:312:ASP:HA	1:C:313:LYS:HG3	1.34	1.07
1:A:452:SER:HA	1:B:405:PHE:HD1	1.02	1.07
1:C:312:ASP:HB3	1:C:313:LYS:HA	1.36	1.06
1:A:523:LEU:HD11	1:C:523:LEU:HD21	1.09	1.06
1:A:568:ARG:NH1	1:B:589:LEU:CD1	2.19	1.06
1:A:537:MET:HG2	1:C:533:ASP:OD1	1.55	1.05
1:B:591:ARG:HH11	1:B:591:ARG:HB2	1.17	1.04
1:C:523:LEU:CD1	1:C:528:LYS:HB2	1.83	1.04
1:C:313:LYS:CB	1:C:327:ARG:HH21	1.69	1.04
1:A:264:TYR:CE2	1:A:267:LYS:HD2	1.92	1.04
1:A:589:LEU:HD13	1:B:571:LEU:HB2	1.39	1.04
1:C:324:ILE:HG22	1:C:328:MET:CE	1.86	1.04
1:A:454:TYR:CD1	1:B:556:HIS:CD2	2.45	1.04
1:B:396:GLU:HA	1:B:514:ILE:HD13	1.37	1.04
1:C:591:ARG:HB2	1:C:591:ARG:HH11	1.17	1.03
1:C:523:LEU:HD11	1:C:528:LYS:HB3	1.07	1.03
1:C:391:ASP:CB	1:C:538:VAL:CG1	2.31	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD11	1:C:523:LEU:CD2	1.89	1.02
1:A:264:TYR:CD2	1:A:267:LYS:CD	2.41	1.02
1:A:454:TYR:CE2	1:B:556:HIS:HB3	1.94	1.02
1:B:392:LEU:HD13	1:B:517:VAL:CG1	1.90	1.01
1:A:457:GLU:HB3	1:B:560:ILE:HD11	1.38	1.01
1:C:255:ALA:HB1	1:C:256:ASP:CB	1.89	1.01
1:C:283:VAL:HG13	1:C:284:ASN:OD1	1.60	1.01
1:C:255:ALA:CB	1:C:273:GLN:NE2	2.23	1.00
1:C:283:VAL:HG22	1:C:284:ASN:OD1	1.60	1.00
1:C:284:ASN:ND2	1:C:285:HIS:CD2	2.30	1.00
1:C:255:ALA:HB1	1:C:256:ASP:CG	1.81	0.99
1:A:564:ASN:ND2	1:B:595:MET:HA	1.77	0.99
1:C:284:ASN:HB2	1:C:285:HIS:CD2	1.98	0.99
1:A:452:SER:HB3	1:B:405:PHE:HE1	1.20	0.98
1:C:258:ARG:O	1:C:270:ILE:HA	1.63	0.98
1:C:255:ALA:HB2	1:C:273:GLN:HE21	1.26	0.98
1:B:594:VAL:C	1:B:595:MET:HG3	1.82	0.98
1:C:310:LEU:H	1:C:311:PRO:HD3	0.88	0.97
1:A:264:TYR:HD2	1:A:267:LYS:HB2	1.28	0.97
1:A:503:PHE:HD2	1:A:507:ILE:HD11	1.28	0.97
1:A:545:SER:HB3	1:A:549:GLN:HE21	1.28	0.97
1:C:255:ALA:CB	1:C:256:ASP:CB	2.42	0.97
1:C:391:ASP:HB2	1:C:538:VAL:HG13	1.42	0.97
1:C:523:LEU:HG	1:C:529:ILE:HG12	1.46	0.96
1:C:395:ILE:HD13	1:C:541:VAL:HG13	1.48	0.96
1:A:445:LEU:HD22	1:B:416:LEU:HD12	1.48	0.95
1:C:283:VAL:CG2	1:C:284:ASN:CG	2.35	0.95
1:A:593:PRO:C	1:A:595:MET:H	1.70	0.95
1:C:310:LEU:N	1:C:311:PRO:CD	2.30	0.95
1:C:414:LYS:HE2	1:C:497:LYS:HE3	1.47	0.94
1:A:264:TYR:CD2	1:A:267:LYS:CB	2.51	0.94
1:C:258:ARG:O	1:C:271:GLU:N	2.01	0.94
1:C:310:LEU:H	1:C:311:PRO:CD	1.80	0.94
1:C:294:TYR:CG	1:C:310:LEU:HD22	2.03	0.94
1:A:523:LEU:CD1	1:C:529:ILE:CG2	2.45	0.94
1:A:452:SER:CA	1:B:405:PHE:CD1	2.51	0.93
1:A:533:ASP:OD1	1:C:537:MET:HG2	1.69	0.93
1:B:594:VAL:C	1:B:595:MET:CG	2.34	0.93
1:C:523:LEU:CD2	1:C:529:ILE:HD13	1.98	0.93
1:C:319:PHE:O	1:C:319:PHE:CG	2.17	0.92
1:A:568:ARG:HH11	1:B:589:LEU:HD11	0.76	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:LEU:CD1	1:C:528:LYS:HB3	1.90	0.92
1:A:264:TYR:CD2	1:A:267:LYS:HD2	2.05	0.92
1:A:503:PHE:CD2	1:A:507:ILE:HD11	2.05	0.91
1:C:284:ASN:HD22	1:C:285:HIS:CD2	1.85	0.91
1:C:319:PHE:O	1:C:319:PHE:CD2	2.24	0.91
1:C:395:ILE:HG22	1:C:514:ILE:HD11	1.52	0.91
1:C:312:ASP:HB3	1:C:313:LYS:CA	1.98	0.90
1:A:456:GLY:HA3	1:B:239:TYR:CE2	2.07	0.90
1:C:306:PRO:HD3	1:C:551:GLU:HG3	1.53	0.90
1:A:454:TYR:CZ	1:B:556:HIS:HB2	2.06	0.90
1:C:294:TYR:CB	1:C:310:LEU:HD22	2.01	0.90
1:C:392:LEU:HD13	1:C:517:VAL:CB	2.02	0.89
1:C:391:ASP:HB3	1:C:538:VAL:HG11	1.54	0.89
1:B:395:ILE:CD1	1:B:541:VAL:CG1	2.50	0.89
1:C:395:ILE:HD11	1:C:541:VAL:HG13	1.54	0.89
1:B:564:ASN:O	1:B:568:ARG:HG3	1.71	0.89
1:A:516:LYS:HG2	1:C:530:THR:HG22	1.54	0.88
1:A:459:ASP:OD2	1:A:593:PRO:HG3	1.70	0.88
1:A:523:LEU:CD1	1:C:523:LEU:HD21	2.01	0.88
1:A:239:TYR:HA	1:B:455:GLN:HG3	1.56	0.88
1:C:283:VAL:CG2	1:C:284:ASN:CB	2.52	0.88
1:C:254:VAL:CG2	1:C:274:LEU:CD2	2.52	0.88
1:A:460:LEU:HD21	1:A:464:ILE:HD11	1.56	0.87
1:A:529:ILE:HG23	1:C:523:LEU:HD22	1.55	0.87
1:C:395:ILE:CD1	1:C:541:VAL:CG1	2.51	0.87
1:A:523:LEU:HD11	1:C:529:ILE:HG23	1.56	0.87
1:B:392:LEU:HD13	1:B:517:VAL:HG11	1.54	0.86
1:C:392:LEU:CD1	1:C:517:VAL:HB	2.04	0.86
1:C:266:LEU:HG	1:C:266:LEU:O	1.75	0.86
1:A:454:TYR:CE1	1:B:556:HIS:CB	2.59	0.86
1:C:258:ARG:O	1:C:270:ILE:CA	2.23	0.85
1:A:264:TYR:CD2	1:A:267:LYS:HD3	2.11	0.85
1:A:264:TYR:CD2	1:A:267:LYS:HB2	2.09	0.85
1:C:523:LEU:HD21	1:C:529:ILE:CG2	2.06	0.85
1:C:305:ILE:HA	1:C:551:GLU:HG2	1.58	0.85
1:A:454:TYR:CD1	1:B:556:HIS:CG	2.64	0.85
1:A:389:ASP:OD1	1:A:539:LYS:HB3	1.77	0.85
1:A:457:GLU:HB3	1:B:560:ILE:CD1	2.06	0.85
1:B:392:LEU:HD13	1:B:517:VAL:CB	2.05	0.85
1:A:452:SER:CA	1:B:405:PHE:HD1	1.89	0.85
1:C:312:ASP:HB2	1:C:313:LYS:HG2	0.85	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:CD1	1:B:517:VAL:HB	2.06	0.84
1:A:460:LEU:CD2	1:A:464:ILE:CD1	2.56	0.84
1:C:396:GLU:HB2	1:C:514:ILE:HG21	1.59	0.83
1:A:528:LYS:HG2	1:C:523:LEU:HD13	1.57	0.83
1:A:546:TYR:O	1:A:550:ALA:HB2	1.76	0.83
1:C:523:LEU:HD12	1:C:528:LYS:CB	2.00	0.83
1:A:503:PHE:O	1:A:507:ILE:HD12	1.79	0.83
1:C:523:LEU:HD21	1:C:529:ILE:HG23	1.59	0.83
1:C:262:LYS:O	1:C:264:TYR:CD1	2.32	0.83
1:C:390:LEU:HD13	1:C:394:GLU:CB	2.08	0.83
1:A:523:LEU:CD2	1:A:529:ILE:N	2.41	0.82
1:A:523:LEU:HD12	1:C:529:ILE:HG23	1.61	0.82
1:B:396:GLU:CA	1:B:514:ILE:HD13	2.09	0.82
1:C:294:TYR:CD2	1:C:310:LEU:HD22	2.15	0.82
1:A:454:TYR:CZ	1:B:556:HIS:CB	2.62	0.82
1:A:523:LEU:HD13	1:A:529:ILE:HD13	1.60	0.81
1:B:259:LYS:HD2	1:B:268:SER:HB3	1.63	0.81
1:C:523:LEU:CG	1:C:529:ILE:HG12	2.10	0.81
1:A:454:TYR:CD1	1:B:556:HIS:CB	2.64	0.81
1:C:380:PHE:HB2	1:C:540:ARG:HH22	1.44	0.81
1:A:591:ARG:NH1	1:A:591:ARG:HB2	1.96	0.81
1:C:312:ASP:CA	1:C:313:LYS:CG	2.49	0.81
1:B:591:ARG:NH1	1:B:591:ARG:HB2	1.96	0.80
1:A:264:TYR:HD2	1:A:267:LYS:HB3	1.45	0.80
1:A:523:LEU:HD21	1:A:529:ILE:N	1.95	0.80
1:A:452:SER:CB	1:B:405:PHE:CD1	2.63	0.80
1:C:392:LEU:HD21	1:C:518:LYS:HG3	1.64	0.80
1:C:283:VAL:CG1	1:C:284:ASN:OD1	2.30	0.80
1:C:396:GLU:HA	1:C:514:ILE:HD13	1.64	0.80
1:A:589:LEU:HA	1:B:571:LEU:HD13	1.62	0.80
1:C:283:VAL:CG2	1:C:284:ASN:OD1	2.30	0.80
1:C:392:LEU:HD11	1:C:514:ILE:HA	1.64	0.80
1:C:380:PHE:HB2	1:C:540:ARG:NH2	1.96	0.80
1:A:564:ASN:HD22	1:B:595:MET:HA	1.40	0.79
1:B:396:GLU:HB3	1:B:514:ILE:HG21	1.65	0.79
1:A:395:ILE:HD13	1:A:541:VAL:HG13	1.64	0.79
1:A:528:LYS:CG	1:C:523:LEU:HD13	2.11	0.79
1:A:529:ILE:HG23	1:C:523:LEU:CD2	2.13	0.79
1:C:266:LEU:O	1:C:266:LEU:CG	2.30	0.79
1:C:325:LYS:O	1:C:328:MET:HG2	1.82	0.79
1:C:591:ARG:NH1	1:C:591:ARG:HB2	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TRP:CZ2	1:B:550:ALA:HB3	2.18	0.79
1:A:259:LYS:HD2	1:A:268:SER:HB3	1.63	0.79
1:A:454:TYR:CG	1:B:556:HIS:CG	2.71	0.79
1:A:455:GLN:HG3	1:B:239:TYR:O	1.83	0.78
1:A:452:SER:HB2	1:B:405:PHE:CE1	2.17	0.78
1:A:568:ARG:NH1	1:B:589:LEU:CG	2.46	0.78
1:B:395:ILE:HD13	1:B:541:VAL:CG1	2.11	0.78
1:A:387:ALA:HB1	1:A:388:PRO:HD2	1.66	0.78
1:B:392:LEU:HD13	1:B:517:VAL:HB	1.62	0.78
1:A:395:ILE:CD1	1:A:541:VAL:HG13	2.14	0.78
1:C:262:LYS:O	1:C:264:TYR:CG	2.37	0.78
1:B:243:TRP:CE2	1:B:550:ALA:HB1	2.18	0.77
1:B:520:SER:HB2	1:B:534:LYS:HG2	1.66	0.77
1:C:387:ALA:HB1	1:C:388:PRO:HD2	1.66	0.77
1:A:392:LEU:HD21	1:A:518:LYS:HG3	1.67	0.77
1:B:390:LEU:HD13	1:B:394:GLU:OE1	1.85	0.77
1:C:262:LYS:HB3	1:C:264:TYR:HD1	1.50	0.77
1:C:390:LEU:CD1	1:C:394:GLU:HB3	2.13	0.77
1:C:392:LEU:HD21	1:C:514:ILE:O	1.85	0.77
1:B:387:ALA:HB1	1:B:388:PRO:HD2	1.66	0.77
1:C:312:ASP:CB	1:C:313:LYS:CA	2.63	0.77
1:A:592:PHE:CZ	1:B:567:ILE:HG21	2.19	0.77
1:B:396:GLU:HA	1:B:514:ILE:CD1	2.15	0.76
1:C:294:TYR:CE2	1:C:310:LEU:HB2	2.20	0.76
1:C:310:LEU:HG	1:C:311:PRO:HD2	1.66	0.76
1:A:392:LEU:HD21	1:A:518:LYS:CG	2.15	0.76
1:A:445:LEU:CD2	1:B:416:LEU:HD12	2.15	0.76
1:A:510:HIS:CE1	1:A:548:LEU:HB2	2.20	0.76
1:C:283:VAL:CG2	1:C:284:ASN:N	2.48	0.76
1:C:520:SER:HB2	1:C:534:LYS:HG2	1.67	0.76
1:A:520:SER:HB2	1:A:534:LYS:HG2	1.67	0.76
1:A:593:PRO:C	1:A:595:MET:N	2.39	0.76
1:C:306:PRO:CD	1:C:551:GLU:HG3	2.15	0.76
1:A:592:PHE:HZ	1:B:567:ILE:HG21	1.49	0.76
1:B:243:TRP:CD2	1:B:550:ALA:HB1	2.21	0.76
1:A:516:LYS:HG2	1:C:530:THR:CG2	2.15	0.76
1:B:564:ASN:O	1:B:568:ARG:CG	2.34	0.76
1:C:294:TYR:CD1	1:C:310:LEU:HD13	2.21	0.76
1:C:283:VAL:CG2	1:C:284:ASN:HB3	2.15	0.75
1:A:529:ILE:CG2	1:C:523:LEU:CD2	2.64	0.75
1:A:405:PHE:HD1	1:B:452:SER:HA	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:CD2	1:A:464:ILE:HD11	2.16	0.75
1:B:594:VAL:O	1:B:595:MET:CG	2.30	0.75
1:A:392:LEU:CD2	1:A:518:LYS:HG2	2.17	0.75
1:A:392:LEU:HD13	1:A:517:VAL:CG1	2.16	0.75
1:B:268:SER:O	1:B:319:PHE:HZ	1.70	0.75
1:C:255:ALA:HB3	1:C:273:GLN:HE21	1.48	0.75
1:A:395:ILE:HG22	1:A:514:ILE:HD11	1.67	0.74
1:B:234:ILE:HD13	1:B:546:TYR:HB3	1.69	0.74
1:A:454:TYR:CE2	1:B:556:HIS:CB	2.70	0.74
1:C:312:ASP:CB	1:C:313:LYS:HA	2.17	0.74
1:C:255:ALA:HB1	1:C:273:GLN:HE21	1.50	0.74
1:A:537:MET:HG2	1:C:533:ASP:CG	2.08	0.74
1:C:284:ASN:CB	1:C:285:HIS:CD2	2.70	0.74
1:C:396:GLU:CA	1:C:514:ILE:HD13	2.17	0.74
1:A:523:LEU:HD21	1:A:528:LYS:HB3	1.68	0.74
1:A:239:TYR:CE2	1:B:456:GLY:CA	2.70	0.73
1:A:395:ILE:HG22	1:A:514:ILE:CD1	2.17	0.73
1:A:548:LEU:O	1:A:551:GLU:N	2.20	0.73
1:C:255:ALA:HB3	1:C:273:GLN:HG2	1.70	0.73
1:A:268:SER:O	1:A:319:PHE:HZ	1.71	0.73
1:A:594:VAL:HG22	1:A:594:VAL:O	1.87	0.73
1:C:262:LYS:O	1:C:264:TYR:HB2	1.89	0.73
1:C:315:VAL:HG12	1:C:315:VAL:O	1.89	0.72
1:A:528:LYS:HB3	1:C:523:LEU:HD13	1.71	0.72
1:C:523:LEU:CD2	1:C:529:ILE:CD1	2.55	0.72
1:A:523:LEU:CD2	1:A:528:LYS:CB	2.67	0.72
1:B:315:VAL:HG12	1:B:315:VAL:O	1.89	0.72
1:C:314:GLN:OE1	1:C:323:PHE:HD1	1.72	0.72
1:C:594:VAL:HG13	1:C:595:MET:CG	2.17	0.72
1:A:503:PHE:HB3	1:A:507:ILE:CD1	2.19	0.72
1:A:592:PHE:N	1:A:592:PHE:CD1	2.55	0.72
1:A:460:LEU:HG	1:B:564:ASN:OD1	1.88	0.72
1:A:396:GLU:OE1	1:A:518:LYS:NZ	2.15	0.72
1:A:454:TYR:CG	1:B:556:HIS:HB3	2.25	0.72
1:B:262:LYS:O	1:B:264:TYR:CD1	2.43	0.72
1:B:306:PRO:HD3	1:B:551:GLU:HG3	1.70	0.72
1:C:523:LEU:HD23	1:C:529:ILE:CG1	2.19	0.72
1:B:393:VAL:O	1:B:396:GLU:HG2	1.89	0.71
1:A:315:VAL:HG12	1:A:315:VAL:O	1.89	0.71
1:A:416:LEU:HD12	1:B:445:LEU:HD22	1.72	0.71
1:A:405:PHE:CD1	1:B:452:SER:HA	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:LEU:HA	1:B:571:LEU:CD1	2.21	0.71
1:C:258:ARG:HB2	1:C:271:GLU:O	1.90	0.71
1:A:510:HIS:HE1	1:A:548:LEU:HB2	1.55	0.70
1:B:305:ILE:HA	1:B:551:GLU:HG2	1.73	0.70
1:A:545:SER:HB3	1:A:549:GLN:NE2	2.04	0.70
1:A:457:GLU:OE2	1:B:559:ARG:NH2	2.22	0.70
1:A:594:VAL:O	1:A:595:MET:CB	2.40	0.70
1:A:523:LEU:CD2	1:A:529:ILE:H	2.03	0.70
1:C:262:LYS:O	1:C:264:TYR:CB	2.39	0.70
1:C:283:VAL:HG21	1:C:356:PHE:CE2	2.26	0.70
1:A:564:ASN:ND2	1:B:595:MET:CA	2.53	0.70
1:C:390:LEU:CD1	1:C:394:GLU:CB	2.67	0.70
1:C:523:LEU:CD2	1:C:529:ILE:HG12	2.22	0.70
1:A:274:LEU:HD12	1:A:274:LEU:N	2.07	0.70
1:A:508:GLY:HA2	1:A:511:LYS:HB2	1.71	0.70
1:A:454:TYR:CG	1:B:556:HIS:CB	2.74	0.70
1:C:312:ASP:C	1:C:313:LYS:HG3	2.11	0.70
1:A:523:LEU:HD21	1:A:528:LYS:CB	2.22	0.70
1:B:300:LYS:HD3	1:B:301:PHE:CZ	2.27	0.70
1:C:300:LYS:HD3	1:C:301:PHE:CZ	2.27	0.70
1:C:395:ILE:HG22	1:C:514:ILE:CD1	2.20	0.69
1:B:510:HIS:CE1	1:B:548:LEU:HB2	2.27	0.69
1:B:274:LEU:N	1:B:274:LEU:HD12	2.07	0.69
1:B:391:ASP:O	1:B:395:ILE:HG13	1.93	0.69
1:B:593:PRO:C	1:B:595:MET:H	1.96	0.69
1:A:533:ASP:CG	1:C:537:MET:HG2	2.13	0.69
1:A:456:GLY:CA	1:B:239:TYR:CE2	2.76	0.69
1:B:545:SER:O	1:B:549:GLN:N	2.22	0.69
1:C:523:LEU:CD2	1:C:529:ILE:CG1	2.71	0.69
1:A:300:LYS:HD3	1:A:301:PHE:CZ	2.27	0.68
1:A:392:LEU:HD13	1:A:517:VAL:HB	1.73	0.68
1:A:528:LYS:CB	1:C:523:LEU:HD13	2.23	0.68
1:A:592:PHE:CZ	1:B:567:ILE:CG2	2.76	0.68
1:A:593:PRO:HB2	1:A:595:MET:OXT	1.93	0.68
1:A:239:TYR:CZ	1:B:456:GLY:CA	2.76	0.68
1:C:258:ARG:HB3	1:C:271:GLU:HB2	1.74	0.68
1:C:243:TRP:CZ2	1:C:550:ALA:HB3	2.29	0.67
1:A:434:GLU:OE1	1:B:426:ARG:NE	2.27	0.67
1:C:283:VAL:HG22	1:C:284:ASN:N	2.06	0.67
1:A:530:THR:HG22	1:C:516:LYS:HG2	1.76	0.67
1:A:316:THR:O	1:A:316:THR:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD21	1:A:464:ILE:CD1	2.19	0.67
1:B:243:TRP:CZ2	1:B:550:ALA:CB	2.78	0.67
1:C:316:THR:HG22	1:C:316:THR:O	1.95	0.67
1:A:529:ILE:CG2	1:C:523:LEU:HD22	2.23	0.67
1:C:392:LEU:HD23	1:C:518:LYS:HG2	1.75	0.67
1:B:564:ASN:O	1:B:568:ARG:CD	2.42	0.66
1:C:256:ASP:HB2	1:C:273:GLN:NE2	2.11	0.66
1:A:571:LEU:HB2	1:B:589:LEU:HD13	1.77	0.66
1:C:392:LEU:HD13	1:C:517:VAL:CG1	2.25	0.66
1:B:546:TYR:O	1:B:550:ALA:N	2.29	0.66
1:A:295:GLU:O	1:A:299:VAL:HG23	1.96	0.66
1:A:523:LEU:HD13	1:A:529:ILE:CD1	2.26	0.66
1:A:391:ASP:O	1:A:395:ILE:HG13	1.96	0.66
1:C:258:ARG:O	1:C:270:ILE:HG23	1.96	0.66
1:B:316:THR:HG22	1:B:316:THR:O	1.95	0.66
1:A:502:CYS:C	1:A:504:PRO:CD	2.64	0.65
1:B:243:TRP:CH2	1:B:550:ALA:HB3	2.31	0.65
1:C:284:ASN:CB	1:C:285:HIS:CG	2.68	0.65
1:C:262:LYS:O	1:C:263:MET:C	2.34	0.65
1:C:392:LEU:CD2	1:C:518:LYS:CG	2.75	0.65
1:C:283:VAL:HG22	1:C:284:ASN:CA	2.26	0.65
1:C:243:TRP:CE2	1:C:550:ALA:HB1	2.32	0.65
1:A:239:TYR:CG	1:B:455:GLN:HB2	2.32	0.65
1:A:546:TYR:O	1:A:550:ALA:CB	2.45	0.65
1:A:448:VAL:HG13	1:B:408:ALA:HB1	1.79	0.65
1:C:295:GLU:O	1:C:299:VAL:HG23	1.96	0.65
1:C:324:ILE:O	1:C:328:MET:HE2	1.96	0.65
1:A:556:HIS:HB2	1:B:454:TYR:CE1	2.32	0.65
1:C:310:LEU:HG	1:C:311:PRO:CD	2.27	0.65
1:B:593:PRO:C	1:B:595:MET:N	2.51	0.64
1:C:294:TYR:CZ	1:C:310:LEU:HB2	2.31	0.64
1:B:295:GLU:O	1:B:299:VAL:HG23	1.96	0.64
1:A:523:LEU:HD13	1:C:529:ILE:CG2	2.27	0.64
1:B:545:SER:O	1:B:549:GLN:HG3	1.98	0.64
1:A:454:TYR:CD1	1:B:556:HIS:HB2	2.31	0.64
1:C:396:GLU:N	1:C:514:ILE:HD13	2.12	0.64
1:C:285:HIS:CD2	1:C:353:PHE:CZ	2.85	0.64
1:C:255:ALA:HB3	1:C:273:GLN:CG	2.27	0.64
1:A:398:LYS:O	1:A:402:VAL:HG23	1.98	0.64
1:C:284:ASN:HB2	1:C:285:HIS:ND1	2.13	0.64
1:C:392:LEU:CD2	1:C:518:LYS:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LYS:HG2	1:C:523:LEU:CD1	2.26	0.64
1:C:398:LYS:O	1:C:402:VAL:HG23	1.98	0.63
1:B:398:LYS:O	1:B:402:VAL:HG23	1.98	0.63
1:A:239:TYR:CZ	1:B:456:GLY:HA3	2.31	0.63
1:C:510:HIS:CE1	1:C:548:LEU:HB2	2.33	0.63
1:A:358:ASP:HB2	1:A:361:GLU:H	1.63	0.63
1:A:405:PHE:CE1	1:B:452:SER:CB	2.82	0.63
1:A:264:TYR:CD2	1:A:267:LYS:HB3	2.25	0.63
1:A:436:GLN:O	1:A:440:LYS:HG2	1.99	0.63
1:A:460:LEU:HD23	1:A:464:ILE:HG13	1.80	0.63
1:A:592:PHE:H	1:A:592:PHE:HD1	1.46	0.63
1:A:594:VAL:O	1:A:595:MET:HB3	1.98	0.63
1:C:390:LEU:O	1:C:542:SER:HB2	1.98	0.63
1:C:436:GLN:O	1:C:440:LYS:HG2	1.99	0.63
1:B:436:GLN:O	1:B:440:LYS:HG2	1.99	0.63
1:A:338:MET:HA	1:A:338:MET:CE	2.29	0.63
1:C:338:MET:HA	1:C:338:MET:CE	2.29	0.63
1:C:358:ASP:HB2	1:C:361:GLU:H	1.64	0.62
1:A:589:LEU:CA	1:B:571:LEU:HD13	2.30	0.62
1:C:392:LEU:HD11	1:C:514:ILE:CA	2.28	0.62
1:B:392:LEU:HD11	1:B:517:VAL:HB	1.80	0.62
1:B:338:MET:HA	1:B:338:MET:CE	2.29	0.62
1:B:358:ASP:HB2	1:B:361:GLU:H	1.63	0.62
1:C:313:LYS:HZ1	1:C:330:ARG:HD3	1.64	0.62
1:C:396:GLU:HA	1:C:514:ILE:CD1	2.28	0.62
1:A:523:LEU:HD21	1:A:529:ILE:HG23	1.80	0.62
1:C:255:ALA:HB3	1:C:273:GLN:NE2	2.07	0.62
1:A:454:TYR:CD2	1:B:556:HIS:CB	2.75	0.62
1:A:523:LEU:CD2	1:A:528:LYS:HB2	2.29	0.62
1:A:392:LEU:HD23	1:A:518:LYS:HG2	1.82	0.62
1:A:264:TYR:CG	1:A:267:LYS:HD3	2.34	0.61
1:A:267:LYS:O	1:A:267:LYS:HG2	2.01	0.61
1:A:392:LEU:CD2	1:A:518:LYS:CG	2.76	0.61
1:A:568:ARG:HH12	1:B:589:LEU:HD21	1.63	0.61
1:C:259:LYS:HG3	1:C:268:SER:OG	2.00	0.61
1:A:392:LEU:HD13	1:A:517:VAL:CB	2.30	0.61
1:A:589:LEU:HD13	1:B:571:LEU:CB	2.24	0.61
1:C:313:LYS:NZ	1:C:330:ARG:HD3	2.16	0.61
1:B:255:ALA:HA	1:B:328:MET:SD	2.41	0.61
1:C:284:ASN:CG	1:C:285:HIS:CD2	2.74	0.60
1:B:232:ILE:HD12	1:B:343:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:MET:CG	1:C:533:ASP:OD1	2.42	0.60
1:B:243:TRP:CE2	1:B:550:ALA:CB	2.84	0.60
1:C:510:HIS:HE1	1:C:548:LEU:HB2	1.67	0.60
1:A:239:TYR:HA	1:B:455:GLN:CG	2.32	0.60
1:C:306:PRO:HD3	1:C:551:GLU:CG	2.30	0.60
1:C:232:ILE:HD12	1:C:343:VAL:HG13	1.83	0.60
1:A:255:ALA:HA	1:A:328:MET:SD	2.41	0.60
1:A:506:ILE:HG22	1:A:507:ILE:HG13	1.84	0.60
1:C:356:PHE:HA	1:C:361:GLU:OE2	2.02	0.60
1:A:356:PHE:HA	1:A:361:GLU:OE2	2.02	0.60
1:B:356:PHE:HA	1:B:361:GLU:OE2	2.02	0.60
1:A:460:LEU:HD23	1:A:460:LEU:C	2.23	0.59
1:A:392:LEU:CD1	1:A:517:VAL:HB	2.31	0.59
1:B:429:GLY:O	1:B:432:PRO:HD2	2.02	0.59
1:C:568:ARG:HG3	1:C:568:ARG:HH11	1.67	0.59
1:A:503:PHE:HB3	1:A:507:ILE:HD12	1.85	0.59
1:C:283:VAL:HG11	1:C:354:LEU:O	2.03	0.59
1:A:560:ILE:HD11	1:B:457:GLU:HB3	1.85	0.59
1:C:429:GLY:O	1:C:432:PRO:HD2	2.02	0.59
1:A:239:TYR:HE2	1:B:456:GLY:HA3	1.55	0.59
1:A:366:LYS:O	1:A:370:GLU:HG3	2.02	0.59
1:C:366:LYS:O	1:C:370:GLU:HG3	2.02	0.59
1:A:283:VAL:HG21	1:A:354:LEU:O	2.03	0.59
1:C:551:GLU:OE1	1:C:551:GLU:HA	2.03	0.59
1:A:460:LEU:CD2	1:A:464:ILE:HG13	2.33	0.59
1:B:306:PRO:HD2	1:B:551:GLU:OE2	2.03	0.59
1:B:283:VAL:HG21	1:B:354:LEU:O	2.03	0.59
1:A:232:ILE:HD12	1:A:343:VAL:HG13	1.83	0.59
1:A:522:LYS:O	1:A:526:THR:HG23	2.03	0.58
1:B:510:HIS:HE1	1:B:548:LEU:HB2	1.67	0.58
1:C:266:LEU:O	1:C:266:LEU:CD1	2.51	0.58
1:A:502:CYS:O	1:A:503:PHE:C	2.41	0.58
1:C:243:TRP:CZ2	1:C:550:ALA:CB	2.85	0.58
1:B:366:LYS:O	1:B:370:GLU:HG3	2.02	0.58
1:B:480:GLU:O	1:B:480:GLU:HG2	2.03	0.58
1:A:507:ILE:O	1:A:511:LYS:HG3	2.03	0.58
1:C:294:TYR:CD2	1:C:310:LEU:HB2	2.39	0.58
1:A:429:GLY:O	1:A:432:PRO:HD2	2.02	0.58
1:C:255:ALA:HB2	1:C:273:GLN:NE2	2.04	0.58
1:A:405:PHE:HE1	1:B:452:SER:HB3	1.68	0.58
1:B:262:LYS:O	1:B:263:MET:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:GLU:HA	1:B:551:GLU:OE1	2.03	0.58
1:C:311:PRO:HB2	1:C:312:ASP:HA	1.85	0.58
1:C:522:LYS:O	1:C:526:THR:HG23	2.03	0.58
1:C:312:ASP:N	1:C:312:ASP:OD1	2.35	0.57
1:A:405:PHE:CE1	1:B:452:SER:HB3	2.39	0.57
1:A:551:GLU:OE1	1:A:551:GLU:HA	2.03	0.57
1:A:239:TYR:OH	1:B:456:GLY:HA2	2.04	0.57
1:A:454:TYR:CD1	1:B:556:HIS:HD2	2.11	0.57
1:C:236:VAL:HG12	1:C:237:GLY:N	2.20	0.57
1:C:266:LEU:HD12	1:C:266:LEU:O	2.04	0.57
1:A:460:LEU:O	1:A:460:LEU:HD23	2.05	0.57
1:B:522:LYS:O	1:B:526:THR:HG23	2.03	0.57
1:A:480:GLU:O	1:A:480:GLU:HG2	2.03	0.57
1:C:390:LEU:HD13	1:C:394:GLU:HB2	1.87	0.57
1:A:523:LEU:HD21	1:A:528:LYS:C	2.24	0.57
1:C:262:LYS:HB3	1:C:264:TYR:CD1	2.36	0.57
1:C:480:GLU:HG2	1:C:480:GLU:O	2.03	0.57
1:A:460:LEU:CG	1:B:564:ASN:OD1	2.53	0.57
1:C:395:ILE:HD13	1:C:541:VAL:CG1	2.24	0.57
1:A:236:VAL:HG12	1:A:237:GLY:N	2.19	0.56
1:A:236:VAL:HG12	1:A:237:GLY:H	1.71	0.56
1:B:236:VAL:HG12	1:B:237:GLY:N	2.20	0.56
1:B:593:PRO:O	1:B:595:MET:N	2.39	0.56
1:A:470:THR:O	1:A:474:ILE:HG13	2.06	0.56
1:A:529:ILE:HG21	1:C:529:ILE:HG21	1.86	0.56
1:A:535:GLN:O	1:A:539:LYS:HG2	2.06	0.56
1:B:470:THR:O	1:B:474:ILE:HG13	2.06	0.56
1:A:568:ARG:NH1	1:B:589:LEU:HG	2.20	0.56
1:A:531:LEU:HG	1:A:535:GLN:HE21	1.71	0.56
1:C:283:VAL:CB	1:C:284:ASN:OD1	2.52	0.56
1:C:531:LEU:HG	1:C:535:GLN:HE21	1.71	0.56
1:B:236:VAL:HG12	1:B:237:GLY:H	1.71	0.56
1:C:258:ARG:C	1:C:271:GLU:H	2.06	0.56
1:B:392:LEU:HD22	1:B:517:VAL:HG12	1.86	0.56
1:A:454:TYR:HD1	1:B:556:HIS:CD2	2.16	0.56
1:C:283:VAL:C	1:C:284:ASN:OD1	2.44	0.56
1:C:392:LEU:HD11	1:C:514:ILE:O	2.06	0.56
1:C:523:LEU:HD21	1:C:529:ILE:HG21	1.87	0.56
1:B:260:GLY:HA3	1:B:271:GLU:OE1	2.05	0.55
1:A:530:THR:CG2	1:C:516:LYS:HG2	2.36	0.55
1:A:455:GLN:HG3	1:B:239:TYR:C	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:PRO:HB2	1:C:312:ASP:CA	2.36	0.55
1:C:432:PRO:HG2	1:C:479:ALA:HB2	1.88	0.55
1:C:535:GLN:O	1:C:539:LYS:HG2	2.06	0.55
1:B:531:LEU:HG	1:B:535:GLN:HE21	1.71	0.55
1:B:535:GLN:O	1:B:539:LYS:HG2	2.06	0.55
1:B:432:PRO:HG2	1:B:479:ALA:HB2	1.88	0.55
1:C:470:THR:O	1:C:474:ILE:HG13	2.06	0.55
1:C:380:PHE:HE2	1:C:547:ALA:HB3	1.71	0.55
1:A:592:PHE:HB2	1:B:568:ARG:HG2	1.88	0.55
1:A:489:LEU:HA	1:A:566:VAL:HG21	1.89	0.55
1:C:251:ASP:CG	1:C:252:CYS:H	2.10	0.55
1:A:556:HIS:CD2	1:B:454:TYR:CD1	2.95	0.55
1:C:232:ILE:CG2	1:C:383:MET:HG2	2.37	0.54
1:A:251:ASP:CG	1:A:252:CYS:H	2.10	0.54
1:B:251:ASP:CG	1:B:252:CYS:H	2.10	0.54
1:A:318:ARG:HD2	1:A:319:PHE:CE1	2.43	0.54
1:A:432:PRO:HG2	1:A:479:ALA:HB2	1.88	0.54
1:A:232:ILE:CG2	1:A:383:MET:HG2	2.38	0.54
1:B:395:ILE:HD11	1:B:541:VAL:HG13	1.77	0.54
1:A:523:LEU:HD11	1:C:529:ILE:CG2	2.26	0.54
1:C:390:LEU:HD13	1:C:394:GLU:CG	2.37	0.54
1:B:318:ARG:HD2	1:B:319:PHE:CE1	2.43	0.53
1:B:489:LEU:HA	1:B:566:VAL:HG21	1.89	0.53
1:C:236:VAL:HG12	1:C:237:GLY:H	1.71	0.53
1:A:234:ILE:HG21	1:A:546:TYR:HB3	1.90	0.53
1:A:268:SER:O	1:A:319:PHE:CZ	2.58	0.53
1:A:454:TYR:CG	1:B:556:HIS:CD2	2.89	0.53
1:B:348:GLU:OE1	1:B:352:GLN:NE2	2.42	0.53
1:C:259:LYS:O	1:C:259:LYS:HG2	2.08	0.53
1:B:232:ILE:CG2	1:B:383:MET:HG2	2.37	0.53
1:C:546:TYR:O	1:C:550:ALA:N	2.41	0.53
1:C:391:ASP:CB	1:C:538:VAL:HG11	2.24	0.53
1:C:262:LYS:HD3	1:C:264:TYR:HE1	1.74	0.53
1:A:306:PRO:HD2	1:A:551:GLU:OE2	2.09	0.53
1:A:502:CYS:C	1:A:504:PRO:HD2	2.29	0.53
1:A:556:HIS:HB3	1:B:454:TYR:CD2	2.44	0.53
1:A:452:SER:HB2	1:B:405:PHE:CD1	2.41	0.53
1:C:258:ARG:CB	1:C:271:GLU:O	2.56	0.53
1:C:390:LEU:CD1	1:C:394:GLU:CG	2.87	0.53
1:C:489:LEU:HA	1:C:566:VAL:HG21	1.89	0.53
1:A:338:MET:HA	1:A:338:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLU:HB3	1:B:514:ILE:CG2	2.37	0.53
1:A:556:HIS:HB3	1:B:454:TYR:CE2	2.44	0.53
1:A:258:ARG:HH22	1:A:273:GLN:NE2	2.07	0.52
1:A:348:GLU:OE1	1:A:352:GLN:NE2	2.42	0.52
1:C:594:VAL:O	1:C:594:VAL:HG12	2.09	0.52
1:A:410:ASP:HA	1:A:500:LEU:HD13	1.92	0.52
1:C:348:GLU:OE1	1:C:352:GLN:NE2	2.42	0.52
1:A:395:ILE:CD1	1:A:541:VAL:CG1	2.86	0.52
1:A:528:LYS:NZ	1:C:528:LYS:NZ	2.57	0.52
1:A:460:LEU:CD2	1:A:464:ILE:CG1	2.88	0.52
1:C:444:SER:O	1:C:447:THR:HB	2.10	0.52
1:B:258:ARG:HH22	1:B:273:GLN:NE2	2.08	0.52
1:B:485:ASP:OD2	1:B:486:LEU:N	2.40	0.52
1:C:257:PRO:HB3	1:C:324:ILE:HG21	1.91	0.52
1:A:306:PRO:HD3	1:A:551:GLU:HG3	1.90	0.52
1:B:410:ASP:HA	1:B:500:LEU:HD13	1.91	0.52
1:B:396:GLU:CB	1:B:514:ILE:HG21	2.38	0.52
1:C:410:ASP:HA	1:C:500:LEU:HD13	1.92	0.52
1:C:306:PRO:HD2	1:C:551:GLU:OE2	2.10	0.52
1:A:481:GLN:HG3	1:A:577:PHE:CD1	2.46	0.51
1:A:594:VAL:CG2	1:A:594:VAL:O	2.58	0.51
1:B:268:SER:O	1:B:319:PHE:CZ	2.58	0.51
1:B:444:SER:O	1:B:447:THR:HB	2.10	0.51
1:C:256:ASP:CB	1:C:273:GLN:NE2	2.72	0.51
1:C:391:ASP:HB2	1:C:538:VAL:CG1	2.20	0.51
1:B:243:TRP:CH2	1:B:550:ALA:CB	2.94	0.51
1:A:592:PHE:HB2	1:B:568:ARG:CG	2.41	0.51
1:A:523:LEU:HD23	1:A:528:LYS:HB2	1.91	0.51
1:C:232:ILE:O	1:C:383:MET:HA	2.11	0.51
1:C:338:MET:HA	1:C:338:MET:HE3	1.92	0.51
1:A:274:LEU:CD1	1:A:274:LEU:N	2.74	0.51
1:A:432:PRO:CG	1:A:479:ALA:HB2	2.41	0.51
1:A:449:PHE:HE2	1:B:409:MET:HG3	1.75	0.51
1:A:560:ILE:CD1	1:B:457:GLU:HB3	2.41	0.51
1:B:432:PRO:CG	1:B:479:ALA:HB2	2.41	0.51
1:B:560:ILE:O	1:B:564:ASN:ND2	2.44	0.51
1:C:325:LYS:O	1:C:328:MET:CG	2.57	0.51
1:C:313:LYS:HB3	1:C:327:ARG:HH21	1.68	0.51
1:B:232:ILE:O	1:B:383:MET:HA	2.11	0.51
1:B:481:GLN:HG3	1:B:577:PHE:CD1	2.45	0.51
1:C:259:LYS:HB2	1:C:269:TYR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:O	1:C:270:ILE:CG2	2.57	0.51
1:A:444:SER:O	1:A:447:THR:HB	2.10	0.51
1:B:274:LEU:N	1:B:274:LEU:CD1	2.74	0.51
1:C:258:ARG:O	1:C:270:ILE:C	2.48	0.51
1:C:294:TYR:CB	1:C:310:LEU:CD2	2.83	0.51
1:A:232:ILE:O	1:A:383:MET:HA	2.11	0.51
1:B:338:MET:HE3	1:B:338:MET:HA	1.92	0.51
1:A:434:GLU:OE1	1:B:426:ARG:CD	2.59	0.51
1:C:568:ARG:CG	1:C:568:ARG:HH11	2.24	0.51
1:C:305:ILE:HA	1:C:551:GLU:CG	2.37	0.51
1:A:503:PHE:O	1:A:507:ILE:CD1	2.54	0.50
1:A:537:MET:CE	1:C:533:ASP:OD2	2.59	0.50
1:C:320:GLU:HG2	1:C:321:GLU:H	1.76	0.50
1:C:392:LEU:HA	1:C:395:ILE:HD12	1.93	0.50
1:A:568:ARG:HD3	1:B:592:PHE:HB2	1.94	0.50
1:C:481:GLN:HG3	1:C:577:PHE:CD1	2.45	0.50
1:A:523:LEU:CD1	1:C:523:LEU:HD11	2.40	0.50
1:B:320:GLU:HG2	1:B:321:GLU:H	1.76	0.50
1:C:284:ASN:ND2	1:C:353:PHE:O	2.45	0.50
1:A:547:ALA:O	1:A:550:ALA:HB3	2.12	0.50
1:A:585:LEU:HD13	1:B:574:GLN:HB3	1.94	0.50
1:C:432:PRO:CG	1:C:479:ALA:HB2	2.41	0.50
1:C:546:TYR:O	1:C:550:ALA:HB2	2.10	0.50
1:C:294:TYR:CG	1:C:310:LEU:HD13	2.47	0.50
1:B:501:GLY:O	1:B:504:PRO:HD2	2.11	0.50
1:C:256:ASP:OD2	1:C:273:GLN:NE2	2.45	0.50
1:A:485:ASP:OD2	1:A:486:LEU:N	2.40	0.50
1:A:574:GLN:O	1:A:577:PHE:HB3	2.12	0.50
1:B:392:LEU:HA	1:B:395:ILE:HD12	1.93	0.50
1:A:431:LEU:HB3	1:A:432:PRO:HD3	1.94	0.50
1:B:391:ASP:OD1	1:B:393:VAL:HB	2.12	0.50
1:C:501:GLY:O	1:C:504:PRO:HD2	2.11	0.50
1:A:320:GLU:HG2	1:A:321:GLU:H	1.76	0.49
1:A:264:TYR:HB3	1:A:267:LYS:HB3	1.94	0.49
1:A:568:ARG:HD2	1:B:589:LEU:CD1	2.42	0.49
1:C:574:GLN:O	1:C:577:PHE:HB3	2.12	0.49
1:A:446:ALA:HB2	1:A:464:ILE:CG2	2.42	0.49
1:B:431:LEU:HB3	1:B:432:PRO:HD3	1.94	0.49
1:B:574:GLN:O	1:B:577:PHE:HB3	2.12	0.49
1:C:241:PRO:CG	1:C:549:GLN:NE2	2.75	0.49
1:A:392:LEU:HA	1:A:395:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:TYR:CE2	1:C:271:GLU:OE2	2.65	0.49
1:C:431:LEU:HB3	1:C:432:PRO:HD3	1.95	0.49
1:A:474:ILE:O	1:A:478:VAL:HG23	2.13	0.49
1:A:455:GLN:CB	1:B:239:TYR:HA	2.43	0.49
1:C:254:VAL:HG22	1:C:274:LEU:HD21	1.80	0.49
1:B:306:PRO:CD	1:B:551:GLU:HG3	2.40	0.49
1:A:556:HIS:CB	1:B:454:TYR:CE1	2.95	0.49
1:A:593:PRO:O	1:A:595:MET:N	2.42	0.48
1:B:446:ALA:HB2	1:B:464:ILE:CG2	2.43	0.48
1:A:283:VAL:HG11	1:A:356:PHE:CE2	2.49	0.48
1:A:503:PHE:N	1:A:504:PRO:HD3	2.28	0.48
1:A:342:PRO:HD2	1:A:554:HIS:CE1	2.48	0.48
1:A:454:TYR:HB2	1:B:556:HIS:CD2	2.48	0.48
1:C:559:ARG:HH11	1:C:559:ARG:HG2	1.78	0.48
1:B:283:VAL:HG11	1:B:356:PHE:CE2	2.48	0.48
1:B:474:ILE:O	1:B:478:VAL:HG23	2.13	0.48
1:C:446:ALA:HB2	1:C:464:ILE:CG2	2.42	0.48
1:A:523:LEU:CD2	1:A:528:LYS:HB3	2.34	0.48
1:A:455:GLN:HB2	1:B:239:TYR:HB3	1.95	0.48
1:A:523:LEU:HD12	1:C:528:LYS:HB3	1.96	0.48
1:B:589:LEU:C	1:B:591:ARG:H	2.17	0.48
1:A:460:LEU:HD22	1:A:464:ILE:CD1	2.43	0.48
1:A:589:LEU:C	1:A:591:ARG:H	2.17	0.48
1:C:474:ILE:O	1:C:478:VAL:HG23	2.13	0.48
1:B:395:ILE:HG22	1:B:514:ILE:HD11	1.95	0.48
1:A:459:ASP:OD2	1:A:593:PRO:CG	2.53	0.48
1:A:507:ILE:HG22	1:A:507:ILE:O	2.13	0.48
1:B:258:ARG:HH22	1:B:273:GLN:HE22	1.62	0.48
1:C:264:TYR:O	1:C:267:LYS:CB	2.43	0.48
1:C:312:ASP:CB	1:C:313:LYS:CB	2.90	0.48
1:C:324:ILE:HG22	1:C:328:MET:HE1	1.87	0.48
1:A:523:LEU:C	1:A:523:LEU:HD23	2.34	0.47
1:C:310:LEU:HD12	1:C:310:LEU:N	2.29	0.47
1:A:559:ARG:HH11	1:A:559:ARG:HG2	1.78	0.47
1:A:392:LEU:HD13	1:A:517:VAL:HG11	1.96	0.47
1:B:559:ARG:HG2	1:B:559:ARG:HH11	1.78	0.47
1:C:293:LEU:HD22	1:C:353:PHE:CD2	2.49	0.47
1:A:567:ILE:HG21	1:B:592:PHE:CZ	2.50	0.47
1:C:390:LEU:HD13	1:C:394:GLU:HG3	1.95	0.47
1:C:523:LEU:CD2	1:C:529:ILE:CG2	2.87	0.47
1:C:568:ARG:HD3	1:C:572:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PHE:HB2	1:A:540:ARG:HH22	1.80	0.47
1:C:534:LYS:HD3	1:C:534:LYS:C	2.35	0.47
1:C:243:TRP:CH2	1:C:550:ALA:HB3	2.50	0.47
1:A:293:LEU:HD22	1:A:353:PHE:CD2	2.49	0.47
1:A:463:ALA:HA	1:A:591:ARG:HG2	1.96	0.47
1:B:308:PRO:HB2	1:B:334:TRP:CD1	2.50	0.47
1:B:380:PHE:HE2	1:B:547:ALA:HB3	1.80	0.47
1:C:273:GLN:O	1:C:273:GLN:HG3	2.14	0.47
1:C:294:TYR:HB2	1:C:310:LEU:CD2	2.45	0.47
1:B:564:ASN:O	1:B:568:ARG:HD3	2.14	0.47
1:C:308:PRO:HB2	1:C:334:TRP:CD1	2.50	0.47
1:C:589:LEU:C	1:C:591:ARG:H	2.17	0.47
1:A:568:ARG:HH12	1:B:589:LEU:CD2	2.27	0.47
1:B:267:LYS:HG3	1:B:318:ARG:HH22	1.80	0.47
1:A:528:LYS:HZ2	1:C:528:LYS:HZ2	1.61	0.47
1:A:239:TYR:CA	1:B:455:GLN:HG3	2.38	0.47
1:C:314:GLN:C	1:C:316:THR:H	2.17	0.47
1:C:463:ALA:HA	1:C:591:ARG:HG2	1.97	0.47
1:A:234:ILE:HD13	1:A:546:TYR:HB3	1.97	0.46
1:A:593:PRO:HB2	1:A:595:MET:N	2.31	0.46
1:B:293:LEU:HD22	1:B:353:PHE:CD2	2.49	0.46
1:B:396:GLU:OE1	1:B:518:LYS:NZ	2.44	0.46
1:C:390:LEU:HD11	1:C:394:GLU:OE1	2.15	0.46
1:C:243:TRP:CD2	1:C:550:ALA:HB1	2.50	0.46
1:B:469:LYS:O	1:B:473:GLU:HG3	2.15	0.46
1:C:283:VAL:HG23	1:C:284:ASN:N	2.30	0.46
1:C:392:LEU:CD2	1:C:518:LYS:HG2	2.37	0.46
1:A:426:ARG:HD2	1:B:434:GLU:OE1	2.16	0.46
1:B:463:ALA:HA	1:B:591:ARG:HG2	1.97	0.46
1:A:308:PRO:HB2	1:A:334:TRP:CD1	2.50	0.46
1:A:460:LEU:CD1	1:B:564:ASN:OD1	2.64	0.46
1:A:448:VAL:HG11	1:B:409:MET:HA	1.96	0.46
1:C:306:PRO:CD	1:C:551:GLU:CG	2.90	0.46
1:B:534:LYS:C	1:B:534:LYS:HD3	2.35	0.46
1:C:267:LYS:HG3	1:C:318:ARG:HH22	1.80	0.46
1:C:469:LYS:O	1:C:473:GLU:HG3	2.15	0.46
1:A:469:LYS:O	1:A:473:GLU:HG3	2.15	0.46
1:A:396:GLU:HA	1:A:514:ILE:HD13	1.98	0.46
1:A:568:ARG:HD2	1:B:589:LEU:HD12	1.98	0.46
1:A:566:VAL:HG13	1:A:567:ILE:N	2.31	0.46
1:C:391:ASP:HB3	1:C:538:VAL:HG13	1.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:HH22	1:A:273:GLN:HE22	1.62	0.46
1:B:526:THR:OG1	1:B:528:LYS:HG2	2.16	0.46
1:C:285:HIS:CD2	1:C:353:PHE:CE2	3.04	0.46
1:A:534:LYS:C	1:A:534:LYS:HD3	2.35	0.46
1:A:592:PHE:HB2	1:B:568:ARG:CD	2.46	0.46
1:C:568:ARG:NH1	1:C:568:ARG:CG	2.78	0.45
1:A:239:TYR:CZ	1:B:456:GLY:HA2	2.50	0.45
1:A:434:GLU:OE1	1:B:426:ARG:HD2	2.17	0.45
1:B:395:ILE:HD12	1:B:541:VAL:CG1	2.42	0.45
1:C:589:LEU:O	1:C:591:ARG:N	2.47	0.45
1:C:338:MET:HE2	1:C:338:MET:HA	1.97	0.45
1:B:566:VAL:HG13	1:B:567:ILE:N	2.31	0.45
1:A:564:ASN:HD21	1:B:595:MET:CA	2.27	0.45
1:C:566:VAL:HG13	1:C:567:ILE:N	2.31	0.45
1:A:533:ASP:OD1	1:C:537:MET:CG	2.54	0.45
1:C:294:TYR:HB3	1:C:310:LEU:HD22	1.90	0.45
1:C:350:PHE:O	1:C:353:PHE:HB3	2.17	0.45
1:C:503:PHE:N	1:C:504:PRO:CD	2.79	0.45
1:B:350:PHE:O	1:B:353:PHE:HB3	2.17	0.45
1:B:503:PHE:N	1:B:504:PRO:CD	2.79	0.45
1:C:312:ASP:HA	1:C:313:LYS:CG	2.25	0.45
1:C:375:ALA:O	1:C:378:MET:HB2	2.16	0.45
1:A:571:LEU:HD13	1:B:589:LEU:HA	1.99	0.45
1:A:577:PHE:CZ	1:A:581:ILE:HD11	2.52	0.45
1:B:439:GLY:HA2	1:B:468:GLY:HA2	1.98	0.45
1:C:439:GLY:HA2	1:C:468:GLY:HA2	1.98	0.45
1:A:439:GLY:HA2	1:A:468:GLY:HA2	1.98	0.45
1:B:338:MET:HE2	1:B:338:MET:HA	1.98	0.45
1:C:324:ILE:O	1:C:328:MET:HG2	2.17	0.45
1:A:585:LEU:HD11	1:B:578:TYR:HE1	1.82	0.44
1:B:594:VAL:C	1:B:595:MET:HG2	2.33	0.44
1:C:284:ASN:HB2	1:C:285:HIS:CE1	2.52	0.44
1:B:546:TYR:HA	1:B:549:GLN:HB2	1.99	0.44
1:A:283:VAL:CG1	1:A:356:PHE:CE2	3.01	0.44
1:A:395:ILE:HD13	1:A:541:VAL:CG1	2.41	0.44
1:A:375:ALA:O	1:A:378:MET:HB2	2.17	0.44
1:B:262:LYS:O	1:B:263:MET:O	2.35	0.44
1:B:503:PHE:HB3	1:B:507:ILE:CD1	2.47	0.44
1:C:243:TRP:CE2	1:C:550:ALA:CB	3.00	0.44
1:C:259:LYS:CB	1:C:269:TYR:O	2.65	0.44
1:C:255:ALA:CB	1:C:273:GLN:CG	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:PRO:CB	1:C:324:ILE:HG21	2.47	0.44
1:A:347:SER:O	1:A:351:GLN:HB2	2.18	0.44
1:A:528:LYS:NZ	1:C:528:LYS:HZ2	2.14	0.44
1:A:589:LEU:O	1:A:591:ARG:N	2.47	0.44
1:A:454:TYR:HD1	1:B:556:HIS:HD2	1.60	0.44
1:C:523:LEU:HD23	1:C:529:ILE:HD11	1.81	0.44
1:C:313:LYS:NZ	1:C:330:ARG:CD	2.81	0.44
1:A:315:VAL:O	1:A:315:VAL:CG1	2.60	0.44
1:A:545:SER:CB	1:A:549:GLN:HE21	2.14	0.44
1:B:396:GLU:N	1:B:514:ILE:HD13	2.33	0.44
1:C:485:ASP:OD2	1:C:486:LEU:N	2.40	0.44
1:B:358:ASP:HB2	1:B:361:GLU:CB	2.48	0.44
1:C:347:SER:O	1:C:351:GLN:HB2	2.17	0.44
1:A:350:PHE:O	1:A:353:PHE:HB3	2.17	0.44
1:A:358:ASP:HB2	1:A:361:GLU:CB	2.48	0.44
1:A:502:CYS:C	1:A:504:PRO:HD3	2.38	0.44
1:A:502:CYS:O	1:A:504:PRO:HD2	2.18	0.44
1:B:375:ALA:O	1:B:378:MET:HB2	2.18	0.44
1:B:577:PHE:CZ	1:B:581:ILE:HD11	2.52	0.44
1:C:392:LEU:HD23	1:C:518:LYS:CG	2.41	0.44
1:C:284:ASN:ND2	1:C:285:HIS:NE2	2.34	0.43
1:C:523:LEU:CD1	1:C:528:LYS:CG	2.94	0.43
1:A:338:MET:HA	1:A:338:MET:HE3	1.99	0.43
1:B:347:SER:O	1:B:351:GLN:HB2	2.18	0.43
1:B:283:VAL:CG1	1:B:356:PHE:CE2	3.01	0.43
1:B:234:ILE:CD1	1:B:546:TYR:HB3	2.45	0.43
1:C:440:LYS:HD3	1:C:472:GLU:OE2	2.19	0.43
1:A:251:ASP:HB2	1:A:340:ARG:HH12	1.83	0.43
1:A:440:LYS:HD3	1:A:472:GLU:OE2	2.19	0.43
1:A:502:CYS:O	1:A:504:PRO:CD	2.66	0.43
1:C:517:VAL:HG12	1:C:517:VAL:O	2.18	0.43
1:C:577:PHE:CZ	1:C:581:ILE:HD11	2.52	0.43
1:A:278:ASN:OD1	1:A:279:THR:N	2.52	0.43
1:A:455:GLN:HB2	1:B:239:TYR:CB	2.48	0.43
1:B:274:LEU:O	1:B:276:PRO:HD3	2.19	0.43
1:B:589:LEU:O	1:B:591:ARG:N	2.47	0.43
1:C:358:ASP:HB2	1:C:361:GLU:CB	2.48	0.43
1:A:460:LEU:CD2	1:A:464:ILE:HD12	2.44	0.43
1:A:564:ASN:HD22	1:B:595:MET:CA	2.19	0.43
1:B:251:ASP:HB2	1:B:340:ARG:HH12	1.83	0.43
1:C:294:TYR:HB2	1:C:310:LEU:HD22	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ARG:HD3	1:C:340:ARG:HA	1.85	0.43
1:A:586:ARG:NH2	1:B:575:VAL:CG1	2.81	0.43
1:B:503:PHE:HB3	1:B:507:ILE:HD12	1.99	0.43
1:C:251:ASP:HB2	1:C:340:ARG:HH12	1.83	0.43
1:C:306:PRO:HD2	1:C:551:GLU:HG3	2.00	0.43
1:C:241:PRO:HG2	1:C:549:GLN:CD	2.39	0.43
1:C:522:LYS:O	1:C:522:LYS:HD3	2.19	0.43
1:C:552:MET:O	1:C:555:PHE:N	2.52	0.43
1:A:274:LEU:O	1:A:276:PRO:HD3	2.19	0.42
1:A:522:LYS:HD3	1:A:522:LYS:O	2.19	0.42
1:A:341:HIS:CD2	1:A:554:HIS:CD2	3.07	0.42
1:B:546:TYR:O	1:B:550:ALA:HB2	2.18	0.42
1:C:564:ASN:O	1:C:568:ARG:HB2	2.18	0.42
1:A:502:CYS:O	1:A:506:ILE:HB	2.19	0.42
1:B:517:VAL:O	1:B:517:VAL:HG12	2.18	0.42
1:C:278:ASN:OD1	1:C:279:THR:N	2.52	0.42
1:A:405:PHE:CE1	1:B:452:SER:HB2	2.53	0.42
1:A:552:MET:O	1:A:555:PHE:N	2.52	0.42
1:C:274:LEU:O	1:C:276:PRO:HD3	2.19	0.42
1:C:358:ASP:HB2	1:C:361:GLU:HB2	2.00	0.42
1:B:358:ASP:HB2	1:B:361:GLU:HB2	2.00	0.42
1:C:241:PRO:CG	1:C:549:GLN:CD	2.87	0.42
1:C:234:ILE:HD13	1:C:546:TYR:HB3	2.02	0.42
1:B:251:ASP:OD2	1:B:252:CYS:N	2.50	0.42
1:B:552:MET:O	1:B:555:PHE:N	2.52	0.42
1:C:232:ILE:HG21	1:C:383:MET:HG2	2.02	0.42
1:A:358:ASP:HB2	1:A:361:GLU:HB2	2.00	0.42
1:B:278:ASN:OD1	1:B:279:THR:N	2.52	0.42
1:B:522:LYS:O	1:B:522:LYS:HD3	2.19	0.42
1:C:310:LEU:CG	1:C:311:PRO:HD2	2.43	0.42
1:A:392:LEU:HD11	1:A:514:ILE:O	2.20	0.42
1:B:305:ILE:HA	1:B:551:GLU:CG	2.46	0.42
1:B:440:LYS:HD3	1:B:472:GLU:OE2	2.19	0.42
1:C:241:PRO:HG2	1:C:549:GLN:NE2	2.34	0.42
1:A:460:LEU:CD2	1:A:460:LEU:C	2.88	0.42
1:A:548:LEU:O	1:A:549:GLN:C	2.56	0.42
1:C:399:CYS:SG	1:C:507:ILE:HG23	2.60	0.42
1:C:259:LYS:HG3	1:C:268:SER:CB	2.50	0.42
1:A:251:ASP:OD2	1:A:252:CYS:N	2.51	0.41
1:A:338:MET:CA	1:A:338:MET:CE	2.98	0.41
1:A:517:VAL:O	1:A:517:VAL:HG12	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ILE:O	1:A:511:LYS:CG	2.68	0.41
1:C:306:PRO:HG2	1:C:503:PHE:CZ	2.56	0.41
1:A:340:ARG:HD3	1:A:340:ARG:HA	1.85	0.41
1:A:341:HIS:CD2	1:A:554:HIS:NE2	2.88	0.41
1:A:358:ASP:HB3	1:A:360:LYS:HG2	2.02	0.41
1:C:266:LEU:C	1:C:266:LEU:HD12	2.41	0.41
1:C:324:ILE:C	1:C:328:MET:HE2	2.39	0.41
1:A:592:PHE:HB2	1:B:568:ARG:HD2	2.01	0.41
1:B:283:VAL:HG12	1:B:284:ASN:N	2.36	0.41
1:B:443:GLN:NE2	1:B:472:GLU:OE2	2.54	0.41
1:B:561:TYR:CD2	1:B:561:TYR:C	2.94	0.41
1:A:304:ALA:O	1:A:551:GLU:HG2	2.20	0.41
1:A:410:ASP:CA	1:A:500:LEU:HD13	2.50	0.41
1:B:306:PRO:HD3	1:B:551:GLU:CG	2.44	0.41
1:B:340:ARG:HD3	1:B:340:ARG:HA	1.85	0.41
1:C:358:ASP:HB3	1:C:360:LYS:HG2	2.02	0.41
1:C:390:LEU:CD1	1:C:394:GLU:HG3	2.50	0.41
1:A:283:VAL:HG12	1:A:284:ASN:N	2.36	0.41
1:A:523:LEU:CD2	1:A:529:ILE:HG23	2.50	0.41
1:A:481:GLN:HG3	1:A:577:PHE:CE1	2.56	0.41
1:B:241:PRO:HG3	1:B:549:GLN:OE1	2.21	0.41
1:B:481:GLN:HG3	1:B:577:PHE:CE1	2.56	0.41
1:C:307:ILE:HA	1:C:308:PRO:HD2	1.95	0.41
1:C:341:HIS:HA	1:C:342:PRO:HD2	1.88	0.41
1:C:525:ALA:C	1:C:527:SER:H	2.24	0.41
1:A:395:ILE:HG23	1:A:545:SER:OG	2.21	0.41
1:C:410:ASP:CA	1:C:500:LEU:HD13	2.51	0.41
1:C:314:GLN:OE1	1:C:323:PHE:CD1	2.61	0.41
1:A:529:ILE:CG2	1:C:523:LEU:HD21	2.50	0.41
1:A:556:HIS:CB	1:B:454:TYR:CD1	3.03	0.41
1:B:392:LEU:HD11	1:B:514:ILE:HA	2.03	0.41
1:C:265:GLY:C	1:C:267:LYS:H	2.25	0.41
1:C:264:TYR:HB3	1:C:267:LYS:HB3	2.03	0.41
1:C:294:TYR:CG	1:C:310:LEU:CD2	2.91	0.41
1:C:481:GLN:HG3	1:C:577:PHE:CE1	2.56	0.41
1:A:443:GLN:NE2	1:A:472:GLU:OE2	2.54	0.40
1:B:234:ILE:HG21	1:B:546:TYR:HB3	2.02	0.40
1:B:358:ASP:HB3	1:B:360:LYS:HG2	2.02	0.40
1:A:239:TYR:HA	1:B:455:GLN:CB	2.51	0.40
1:A:243:TRP:CE2	1:A:550:ALA:HB1	2.56	0.40
1:A:397:GLN:HB2	1:A:397:GLN:HE21	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLN:HB3	1:B:239:TYR:HA	2.03	0.40
1:B:410:ASP:CA	1:B:500:LEU:HD13	2.50	0.40
1:C:274:LEU:HD12	1:C:285:HIS:HD2	1.86	0.40
1:A:525:ALA:C	1:A:527:SER:H	2.24	0.40
1:B:243:TRP:CE3	1:B:550:ALA:HB1	2.55	0.40
1:C:314:GLN:C	1:C:316:THR:N	2.75	0.40
1:C:338:MET:CE	1:C:338:MET:CA	2.98	0.40
1:A:264:TYR:CD2	1:A:267:LYS:CG	2.98	0.40
1:B:355:ASN:OD1	1:B:355:ASN:O	2.40	0.40
1:B:525:ALA:C	1:B:527:SER:H	2.24	0.40
1:C:294:TYR:CE2	1:C:310:LEU:CB	2.98	0.40
1:C:397:GLN:HE21	1:C:397:GLN:HB2	1.56	0.40
1:A:523:LEU:CD1	1:C:528:LYS:HB3	2.51	0.40
1:A:305:ILE:HA	1:A:551:GLU:HG2	2.03	0.40
1:B:338:MET:CA	1:B:338:MET:CE	2.98	0.40
1:C:265:GLY:C	1:C:267:LYS:N	2.74	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:GLU:OE2	1:C:579:GLU:OE2[10_455]	1.88	0.32
1:C:457:GLU:OE2	1:C:559:ARG:NH2[10_455]	2.07	0.13

## 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	364/366 (100%)	313 (86%)	35 (10%)	16 (4%)	<b>2</b> 24
1	B	364/366 (100%)	319 (88%)	34 (9%)	11 (3%)	<b>4</b> 31
1	C	364/366 (100%)	314 (86%)	34 (9%)	16 (4%)	<b>2</b> 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1092/1098 (100%)	946 (87%)	103 (9%)	43 (4%)	3	26

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	MET
1	A	314	GLN
1	A	315	VAL
1	A	503	PHE
1	A	504	PRO
1	A	505	ASP
1	A	592	PHE
1	A	594	VAL
1	B	314	GLN
1	B	315	VAL
1	B	594	VAL
1	C	256	ASP
1	C	266	LEU
1	C	284	ASN
1	C	310	LEU
1	C	311	PRO
1	C	313	LYS
1	C	314	GLN
1	C	315	VAL
1	A	458	THR
1	A	549	GLN
1	A	590	SER
1	B	263	MET
1	B	391	ASP
1	B	458	THR
1	B	590	SER
1	C	263	MET
1	C	458	THR
1	C	590	SER
1	C	257	PRO
1	A	312	ASP
1	B	312	ASP
1	C	264	TYR
1	A	257	PRO
1	A	321	GLU
1	A	593	PRO
1	B	257	PRO

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Mol	Chain	Res	Type
1	B	321	GLU
1	C	321	GLU
1	A	302	GLY
1	B	302	GLY
1	C	302	GLY
1	C	594	VAL

### 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	326/326 (100%)	308 (94%)	18 (6%)	21	50
1	B	326/326 (100%)	308 (94%)	18 (6%)	21	50
1	C	326/326 (100%)	301 (92%)	25 (8%)	13	40
All	All	978/978 (100%)	917 (94%)	61 (6%)	18	46

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	THR
1	A	312	ASP
1	A	322	GLU
1	A	338	MET
1	A	351	GLN
1	A	357	ARG
1	A	416	LEU
1	A	434	GLU
1	A	458	THR
1	A	481	GLN
1	A	503	PHE
1	A	532	GLN
1	A	551	GLU
1	A	565	SER
1	A	587	GLN
1	A	591	ARG

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Mol	Chain	Res	Type
1	A	592	PHE
1	A	594	VAL
1	B	263	MET
1	B	275	THR
1	B	312	ASP
1	B	322	GLU
1	B	338	MET
1	B	351	GLN
1	B	357	ARG
1	B	390	LEU
1	B	391	ASP
1	B	416	LEU
1	B	434	GLU
1	B	458	THR
1	B	481	GLN
1	B	504	PRO
1	B	551	GLU
1	B	565	SER
1	B	587	GLN
1	B	591	ARG
1	C	247	THR
1	C	258	ARG
1	C	259	LYS
1	C	263	MET
1	C	264	TYR
1	C	275	THR
1	C	283	VAL
1	C	285	HIS
1	C	310	LEU
1	C	312	ASP
1	C	314	GLN
1	C	322	GLU
1	C	338	MET
1	C	351	GLN
1	C	357	ARG
1	C	416	LEU
1	C	458	THR
1	C	481	GLN
1	C	504	PRO
1	C	532	GLN
1	C	551	GLU
1	C	565	SER

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Mol	Chain	Res	Type
1	C	568	ARG
1	C	587	GLN
1	C	591	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	355	ASN
1	A	397	GLN
1	A	443	GLN
1	A	481	GLN
1	A	510	HIS
1	A	535	GLN
1	A	549	GLN
1	A	564	ASN
1	A	573	GLN
1	B	273	GLN
1	B	355	ASN
1	B	397	GLN
1	B	443	GLN
1	B	481	GLN
1	B	510	HIS
1	B	535	GLN
1	B	549	GLN
1	B	556	HIS
1	B	573	GLN
1	C	273	GLN
1	C	355	ASN
1	C	397	GLN
1	C	443	GLN
1	C	481	GLN
1	C	510	HIS
1	C	535	GLN
1	C	549	GLN
1	C	573	GLN

### 5.3.3 RNA ⓘ

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	366/366 (100%)	0.36	14 (3%)	40	32	153, 153, 153, 153	0
1	B	366/366 (100%)	0.35	14 (3%)	40	32	153, 153, 153, 153	0
1	C	366/366 (100%)	0.57	40 (10%)	5	6	153, 153, 153, 153	0
All	All	1098/1098 (100%)	0.43	68 (6%)	20	17	153, 153, 153, 153	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	392	LEU	5.7
1	C	316	THR	5.4
1	C	267	LYS	5.2
1	C	258	ARG	5.1
1	B	318	ARG	4.9
1	B	317	GLY	4.7
1	C	391	ASP	4.7
1	C	315	VAL	4.6
1	A	529	ILE	4.2
1	C	317	GLY	4.2
1	C	312	ASP	4.1
1	C	427	CYS	4.0
1	A	265	GLY	4.0
1	C	318	ARG	4.0
1	C	257	PRO	3.7
1	B	230	GLU	3.6
1	B	313	LYS	3.6
1	C	266	LEU	3.5
1	C	268	SER	3.5
1	C	529	ILE	3.5
1	B	316	THR	3.4
1	A	396	GLU	3.3
1	C	311	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	265	GLY	3.3
1	C	230	GLU	3.2
1	C	321	GLU	3.2
1	B	265	GLY	3.2
1	C	528	LYS	3.2
1	A	455	GLN	3.2
1	A	264	TYR	3.2
1	C	282	SER	3.1
1	C	256	ASP	3.0
1	B	312	ASP	3.0
1	C	259	LYS	2.9
1	B	315	VAL	2.9
1	A	528	LYS	2.9
1	C	396	GLU	2.8
1	C	260	GLY	2.8
1	B	266	LEU	2.7
1	C	520	SER	2.7
1	C	249	THR	2.7
1	A	436	GLN	2.6
1	C	238	ASP	2.6
1	C	359	GLU	2.6
1	C	384	GLU	2.6
1	C	363	LYS	2.6
1	A	312	ASP	2.5
1	A	457	GLU	2.4
1	C	360	LYS	2.4
1	C	255	ALA	2.4
1	C	314	GLN	2.4
1	C	313	LYS	2.3
1	A	315	VAL	2.3
1	A	454	TYR	2.3
1	B	267	LYS	2.3
1	A	427	CYS	2.3
1	B	359	GLU	2.2
1	B	356	PHE	2.2
1	C	461	ASN	2.2
1	B	392	LEU	2.2
1	B	314	GLN	2.2
1	C	251	ASP	2.1
1	C	264	TYR	2.1
1	A	263	MET	2.1
1	C	320	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	271	GLU	2.1
1	C	324	ILE	2.1
1	A	595	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.