



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:54 AM UTC

PDB ID : 3DYU / pdb_00003dyu
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

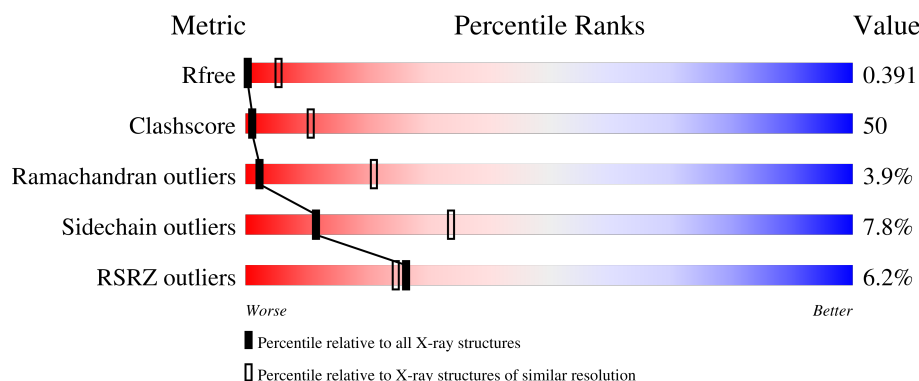
1 Overall quality at a glance

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}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	366	6% 45% 47% 5%
1	B	366	5% 49% 45% 5%
1	C	366	8% 45% 45% 6%

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.

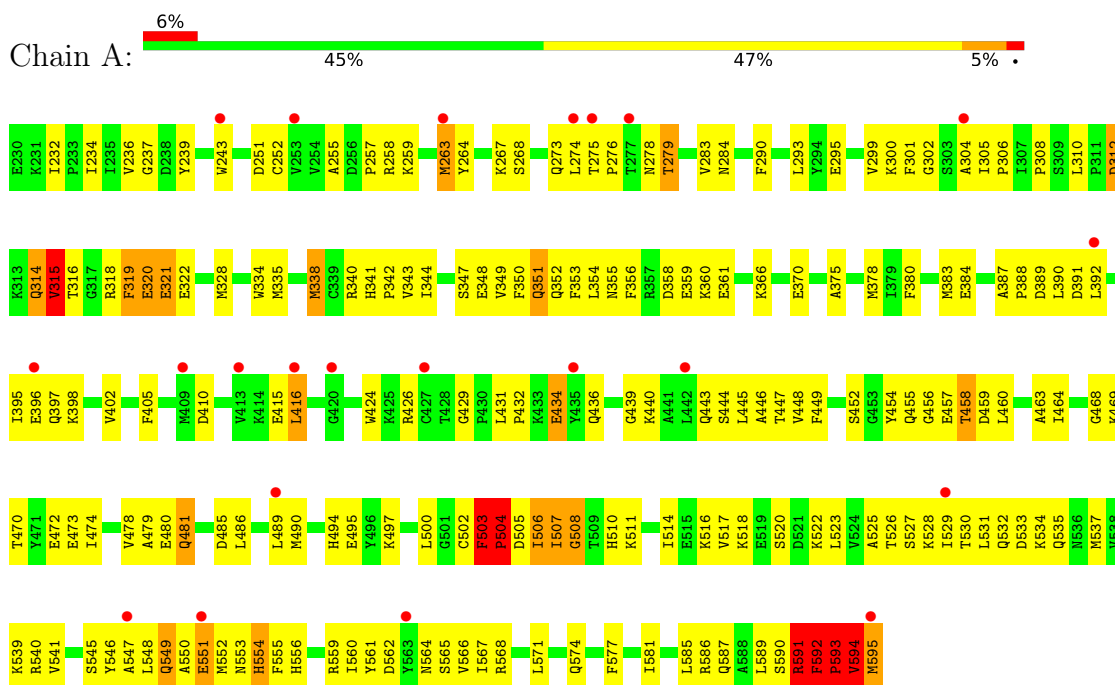
- Molecule 1 is a protein called Sorting nexin-9.

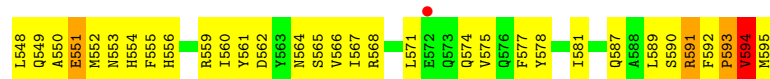
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			
1	B	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			
1	C	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			

3 Residue-property plots

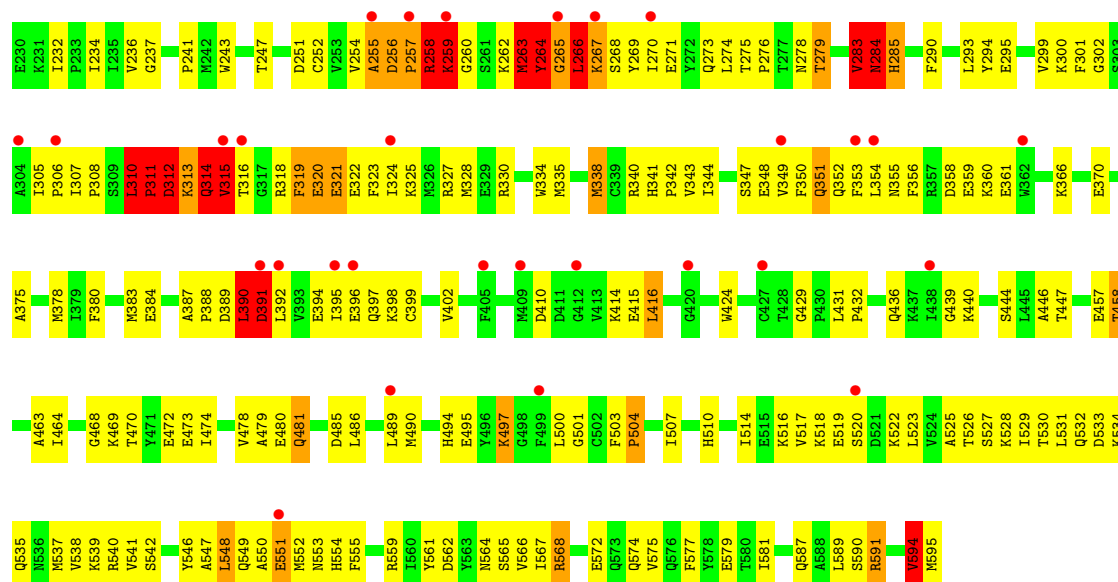
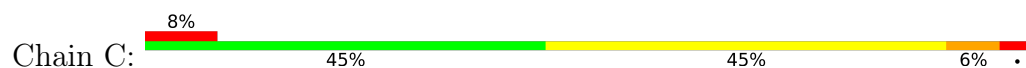
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	131.76 Å 131.76 Å 569.07 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.94 – 4.10 32.94 – 4.10	Depositor EDS
% Data completeness (in resolution range)	89.2 (32.94-4.10) 89.0 (32.94-4.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	129.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.53	0/3044	1.09	14/4100 (0.3%)
1	B	0.52	0/3044	1.01	10/4100 (0.2%)
1	C	0.55	1/3044 (0.0%)	1.04	13/4100 (0.3%)
All	All	0.53	1/9132 (0.0%)	1.05	37/12300 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	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	10.14	1.47	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	LEU	O-C-N	17.16	139.75	122.07
1	A	390	LEU	O-C-N	-16.04	102.84	123.21
1	B	319	PHE	N-CA-C	13.53	130.23	111.56
1	C	319	PHE	N-CA-C	13.47	130.14	111.56
1	A	319	PHE	N-CA-C	13.46	130.13	111.56
1	A	390	LEU	CA-C-N	12.59	143.88	120.97
1	A	390	LEU	C-N-CA	12.59	143.88	120.97
1	B	314	GLN	N-CA-C	9.76	131.59	110.80
1	A	314	GLN	N-CA-C	9.72	131.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	MET	N-CA-C	8.11	128.07	110.80
1	A	310	LEU	N-CA-C	-6.55	101.81	110.07
1	C	390	LEU	N-CA-C	6.55	116.64	108.19
1	B	310	LEU	N-CA-C	-6.54	101.84	110.07
1	A	497	LYS	N-CA-C	-6.27	104.50	111.71
1	C	497	LYS	N-CA-C	-6.24	104.54	111.71
1	A	315	VAL	N-CA-C	6.18	122.20	109.34
1	B	497	LYS	N-CA-C	-6.16	104.63	111.71
1	B	315	VAL	N-CA-C	6.13	122.09	109.34
1	C	315	VAL	N-CA-C	6.09	122.01	109.34
1	B	359	GLU	N-CA-C	-5.98	105.83	113.01
1	C	359	GLU	N-CA-C	-5.95	105.87	113.01
1	A	359	GLU	N-CA-C	-5.92	105.91	113.01
1	B	320	GLU	N-CA-C	5.88	117.53	109.18
1	C	320	GLU	N-CA-C	5.87	117.52	109.18
1	A	320	GLU	N-CA-C	5.85	117.49	109.18
1	C	391	ASP	N-CA-C	5.68	115.74	108.24
1	C	562	ASP	N-CA-C	5.58	117.04	111.07
1	B	562	ASP	N-CA-C	5.53	116.99	111.07
1	A	562	ASP	N-CA-C	5.50	116.95	111.07
1	A	554	HIS	N-CA-C	-5.48	105.33	112.23
1	C	355	ASN	N-CA-C	5.42	117.29	108.63
1	A	355	ASN	N-CA-C	5.39	117.26	108.63
1	B	355	ASN	N-CA-C	5.39	117.25	108.63
1	C	554	HIS	N-CA-C	-5.38	105.45	112.23
1	B	554	HIS	N-CA-C	-5.32	105.53	112.23
1	C	548	LEU	CA-C-N	-5.20	113.32	120.28
1	C	548	LEU	C-N-CA	-5.20	113.32	120.28

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
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	371	0
1	B	2977	0	2958	287	0
1	C	2977	0	2958	386	2
All	All	8931	0	8874	891	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 50.

All (891) 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:283:VAL:HG22	1:C:284:ASN:CG	1.51	1.34
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: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:310:LEU:N	1:C:311:PRO:HD3	1.42	1.16
1:C:395:ILE:CD1	1:C:541:VAL:HG13	1.74	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:324:ILE:HG22	1:C:328:MET:HE2	1.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:523:LEU:HD11	1:C:523:LEU:HD21	1.09	1.06
1:C:312:ASP:HB3	1:C:313:LYS:HA	1.36	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:313:LYS:CB	1:C:327:ARG:HH21	1.69	1.04
1:C:523:LEU:CD1	1:C:528:LYS:HB2	1.83	1.04
1:C:255:ALA:HB1	1:C:256:ASP:CG	1.81	1.04
1:A:264:TYR:CE2	1:A:267:LYS:HD2	1.92	1.04
1:A:454:TYR:CD1	1:B:556:HIS:CD2	2.45	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:B:396:GLU:HA	1:B:514:ILE:HD13	1.37	1.04
1:C:591:ARG:HH11	1:C:591:ARG:HB2	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
1:A:523:LEU:HD11	1:C:523:LEU:CD2	1.89	1.02
1:B:594:VAL:C	1:B:595:MET:HG3	1.82	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:A:457:GLU:HB3	1:B:560:ILE:HD11	1.38	1.01
1:B:392:LEU:HD13	1:B:517:VAL:CG1	1.90	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:255:ALA:HB1	1:C:256:ASP:CB	1.89	1.00
1:C:283:VAL:HG22	1:C:284:ASN:OD1	1.60	1.00
1:C:283:VAL:CG2	1:C:284:ASN:CG	2.35	1.00
1:C:284:ASN:ND2	1:C:285:HIS:CD2	2.30	1.00
1:A:593:PRO:C	1:A:595:MET:H	1.70	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:CG	2.34	0.97
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:523:LEU:CD1	1:C:529:ILE:CG2	2.45	0.94
1:C:294:TYR:CG	1:C:310:LEU:HD22	2.03	0.94
1:C:310:LEU:H	1:C:311:PRO:CD	1.80	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:C:523:LEU:CD2	1:C:529:ILE:HD13	1.98	0.93
1:A:537:MET:HE3	1:C:533:ASP:OD2	1.70	0.92
1:C:319:PHE:CG	1:C:319:PHE:O	2.17	0.92
1:A:568:ARG:HH11	1:B:589:LEU:HD11	0.76	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:266:LEU:HG	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:305:ILE:HA	1:C:551:GLU:HG2	1.58	0.85
1:C:523:LEU:HD21	1:C:529:ILE:CG2	2.06	0.85
1:A:389:ASP:OD1	1:A:539:LYS:HB3	1.77	0.85
1:A:454:TYR:CD1	1:B:556:HIS:CG	2.64	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
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:HB2	1:A:591:ARG:NH1	1.96	0.81
1:C:312:ASP:CA	1:C:313:LYS:CG	2.49	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ARG:HB2	1:B:591:ARG:NH1	1.96	0.80
1:A:264:TYR:HD2	1:A:267:LYS:HB3	1.45	0.80
1:A:452:SER:CB	1:B:405:PHE:CD1	2.63	0.80
1:A:523:LEU:HD21	1:A:529:ILE:N	1.95	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: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:A:537:MET:HG2	1:C:533:ASP:CG	2.08	0.79
1:C:325:LYS:O	1:C:328:MET:HG2	1.82	0.79
1:C:591:ARG:HB2	1:C:591:ARG:NH1	1.96	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:VAL:CG2	1:C:284:ASN:OD1	2.30	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: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:A:516:LYS:HG2	1:C:530:THR:CG2	2.15	0.76
1:B:243:TRP:CD2	1:B:550:ALA:HB1	2.21	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
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:C:312:ASP:C	1:C:313:LYS:HG3	2.11	0.74
1:A:533:ASP:OD2	1:C:537:MET:HE3	1.85	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:B:593:PRO:C	1:B:595:MET:H	1.96	0.74
1:C:284:ASN:CB	1:C:285:HIS:CD2	2.70	0.74
1:A:533:ASP:CG	1:C:537:MET:HG2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:SER:O	1:A:319:PHE:HZ	1.71	0.73
1:A:594:VAL:O	1:A:594:VAL:HG22	1.87	0.73
1:C:262:LYS:O	1:C:264:TYR:HB2	1.89	0.73
1:A:528:LYS:HB3	1:C:523:LEU:HD13	1.71	0.72
1:C:315:VAL:HG12	1:C:315:VAL:O	1.89	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:C:313:LYS:HZ1	1:C:330:ARG:HD3	1.53	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:CD1	1:A:592:PHE:N	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:A:593:PRO:C	1:A:595:MET:N	2.39	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
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:457:GLU:OE2	1:B:559:ARG:NH2	2.22	0.70
1:A:545:SER:HB3	1:A:549:GLN:NE2	2.04	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:502:CYS:C	1:A:504:PRO:CD	2.64	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:C:262:LYS:O	1:C:263:MET:C	2.34	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:TYR:CG	1:B:556:HIS:CB	2.74	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:N	2.51	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:A:530:THR:HG22	1:C:516:LYS:HG2	1.76	0.67
1:C:283:VAL:HG22	1:C:284:ASN:N	2.06	0.67
1:A:316:THR:O	1:A:316:THR:HG22	1.95	0.67
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: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: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:392:LEU:CD2	1:C:518:LYS:CG	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:VAL:HG22	1:C:284:ASN:CA	2.26	0.65
1:C:284:ASN:CG	1:C:285:HIS:CD2	2.74	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:C:316:THR:O	1:C:316:THR:HG22	1.95	0.65
1:A:448:VAL:HG13	1:B:408:ALA:HB1	1.79	0.65
1:A:546:TYR:O	1:A:550:ALA:CB	2.45	0.65
1:C:295:GLU:O	1:C:299:VAL:HG23	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: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:454:TYR:CD1	1:B:556:HIS:HB2	2.31	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: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:A:460:LEU:C	1:A:460:LEU:HD23	2.23	0.64
1:C:324:ILE:C	1:C:328:MET:HE3	2.22	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:A:528:LYS:HG2	1:C:523:LEU:CD1	2.26	0.64
1:C:392:LEU:CD2	1:C:518:LYS:HG3	2.28	0.64
1:C:398:LYS:O	1:C:402:VAL:HG23	1.98	0.63
1:A:239:TYR:CZ	1:B:456:GLY:HA3	2.31	0.63
1:B:398:LYS:O	1:B:402:VAL:HG23	1.98	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:502:CYS:O	1:A:503:PHE:C	2.41	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:HD1	1:A:592:PHE:H	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:CE	1:A:338:MET:HA	2.29	0.63
1:C:338:MET:CE	1:C:338:MET:HA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:O	1:B:263:MET:C	2.42	0.62
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:258:ARG:C	1:C:271:GLU:H	2.06	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:523:LEU:HD21	1:A:528:LYS:C	2.24	0.61
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:B:232:ILE:HD12	1:B:343:VAL:HG13	1.83	0.60
1:C:283:VAL:C	1:C:284:ASN:OD1	2.44	0.60
1:A:537:MET:CG	1:C:533:ASP:OD1	2.42	0.60
1:A:455:GLN:HG3	1:B:239:TYR:C	2.27	0.60
1:A:251:ASP:CG	1:A:252:CYS:H	2.10	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:232:ILE:HD12	1:C:343:VAL:HG13	1.83	0.60
1:C:306:PRO:HD3	1:C:551:GLU:CG	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ARG:HH11	1:C:568:ARG:HG3	1.67	0.59
1:A:503:PHE:HB3	1:A:507:ILE:HD12	1.85	0.59
1:C:251:ASP:CG	1:C:252:CYS:H	2.10	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:HA	1:C:551:GLU:OE1	2.03	0.59
1:A:460:LEU:CD2	1:A:464:ILE:HG13	2.33	0.59
1:B:251:ASP:CG	1:B:252:CYS:H	2.10	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: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:C:232:ILE:HG21	1:C:383:MET:HE2	1.85	0.58
1:B:551:GLU:OE1	1:B:551:GLU:HA	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:502:CYS:C	1:A:504:PRO:HD2	2.29	0.57
1:A:551:GLU:HA	1:A:551:GLU:OE1	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:O	1:C:266:LEU:HD12	2.04	0.57
1:A:232:ILE:HG21	1:A:383:MET:HE2	1.85	0.57
1:A:338:MET:HA	1:A:338:MET:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD23	1:A:460:LEU:O	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:C:262:LYS:HB3	1:C:264:TYR:CD1	2.36	0.57
1:C:480:GLU:O	1:C:480:GLU:HG2	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:B:232:ILE:HG21	1:B:383:MET:HE2	1.85	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:C:258:ARG:O	1:C:270:ILE:C	2.48	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:A:568:ARG:NH1	1:B:589:LEU:HG	2.20	0.56
1:B:470:THR:O	1:B:474:ILE:HG13	2.06	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:338:MET:HA	1:C:338:MET:HE2	1.86	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:A:454:TYR:HD1	1:B:556:HIS:CD2	2.16	0.56
1:B:338:MET:HA	1:B:338:MET:HE2	1.87	0.56
1:B:392:LEU:HD22	1:B:517:VAL:HG12	1.86	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: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:380:PHE:HE2	1:C:547:ALA:HB3	1.71	0.55
1:C:470:THR:O	1:C:474:ILE:HG13	2.06	0.55
1:A:592:PHE:HB2	1:B:568:ARG:HG2	1.88	0.55
1:C:325:LYS:HA	1:C:328:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HA	1:A:566:VAL:HG21	1.89	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: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:A:523:LEU:C	1:A:523:LEU:HD23	2.34	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:556:HIS:HB3	1:B:454:TYR:CD2	2.44	0.53
1:B:589:LEU:C	1:B:591:ARG:H	2.17	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:556:HIS:HB3	1:B:454:TYR:CE2	2.44	0.53
1:A:589:LEU:C	1:A:591:ARG:H	2.17	0.53
1:B:396:GLU:HB3	1:B:514:ILE:CG2	2.37	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:HG12	1:C:594:VAL:O	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:C:490:MET:HA	1:C:490:MET:HE2	1.91	0.52
1:A:460:LEU:CD2	1:A:464:ILE:CG1	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:396:GLU:CB	1:B:514:ILE:HG21	2.38	0.52
1:B:410:ASP:HA	1:B:500:LEU:HD13	1.91	0.52
1:C:306:PRO:HD2	1:C:551:GLU:OE2	2.10	0.52
1:C:410:ASP:HA	1:C:500:LEU:HD13	1.92	0.52
1:A:481:GLN:HG3	1:A:577:PHE:CD1	2.46	0.51
1:A:490:MET:HA	1:A:490:MET:HE2	1.91	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:C:589:LEU:C	1:C:591:ARG:H	2.17	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:C:314:GLN:C	1:C:316:THR:H	2.17	0.51
1:A:523:LEU:HD23	1:A:528:LYS:HB2	1.91	0.51
1:B:490:MET:HE2	1:B:490:MET:HA	1.91	0.51
1:C:232:ILE:O	1:C:383:MET:HA	2.11	0.51
1:A:274:LEU:N	1:A:274:LEU:CD1	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:313:LYS:HB3	1:C:327:ARG:HH21	1.68	0.51
1:C:325:LYS:O	1:C:328:MET:CG	2.57	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:258:ARG:O	1:C:270:ILE:CG2	2.57	0.51
1:C:259:LYS:HB2	1:C:269:TYR:O	2.10	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:B:534:LYS:C	1:B:534:LYS:HD3	2.35	0.51
1:C:294:TYR:CB	1:C:310:LEU:CD2	2.83	0.51
1:C:534:LYS:HD3	1:C:534:LYS:C	2.35	0.51
1:A:232:ILE:O	1:A:383:MET:HA	2.11	0.51
1:A:434:GLU:OE1	1:B:426:ARG:CD	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ARG:HH11	1:C:568:ARG:CG	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: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:523:LEU:CD1	1:C:523:LEU:HD11	2.40	0.50
1:A:534:LYS:HD3	1:A:534:LYS:C	2.35	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:528:LYS:HZ2	1:C:528:LYS:HZ2	1.58	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
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:455:GLN:CB	1:B:239:TYR:HA	2.43	0.49
1:A:474:ILE:O	1:A:478:VAL:HG23	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:503:PHE:N	1:A:504:PRO:HD3	2.28	0.48
1:C:559:ARG:HG2	1:C:559:ARG:HH11	1.78	0.48
1:A:502:CYS:C	1:A:504:PRO:HD3	2.38	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:594:VAL:C	1:B:595:MET:HG2	2.33	0.48
1:A:460:LEU:HD22	1:A:464:ILE:CD1	2.43	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:O	1:A:507:ILE:HG22	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:241:PRO:HG2	1:C:549:GLN:CD	2.39	0.47
1:C:310:LEU:N	1:C:310:LEU:HD12	2.29	0.47
1:A:559:ARG:HG2	1:A:559:ARG:HH11	1.78	0.47
1:A:392:LEU:HD13	1:A:517:VAL:HG11	1.96	0.47
1:B:559:ARG:HH11	1:B:559:ARG:HG2	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
1:A:380:PHE:HB2	1:A:540:ARG:HH22	1.80	0.47
1:C:241:PRO:CG	1:C:549:GLN:CD	2.87	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:A:528:LYS:NZ	1:C:528:LYS:HZ2	2.12	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:243:TRP:CH2	1:C:550:ALA:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TYR:HB2	1:C:310:LEU:CD2	2.45	0.47
1:C:313:LYS:HZ1	1:C:330:ARG:CD	2.21	0.47
1:A:460:LEU:CD2	1:A:460:LEU:C	2.88	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:A:548:LEU:O	1:A:549:GLN:C	2.56	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:239:TYR:CA	1:B:455:GLN:HG3	2.38	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:C:243:TRP:CD2	1:C:550:ALA:HB1	2.50	0.46
1:C:390:LEU:HD11	1:C:394:GLU:OE1	2.15	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:C:290:PHE:HE1	1:C:335:MET:HE3	1.81	0.46
1:A:290:PHE:HE1	1:A:335:MET:HE3	1.81	0.46
1:A:308:PRO:HB2	1:A:334:TRP:CD1	2.50	0.46
1:A:448:VAL:HG11	1:B:409:MET:HA	1.96	0.46
1:A:460:LEU:CD1	1:B:564:ASN:OD1	2.64	0.46
1:C:266:LEU:HD12	1:C:266:LEU:C	2.41	0.46
1:C:306:PRO:CD	1:C:551:GLU:CG	2.90	0.46
1:B:290:PHE:HE1	1:B:335:MET:HE3	1.81	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:396:GLU:HA	1:A:514:ILE:HD13	1.98	0.46
1:A:469:LYS:O	1:A:473:GLU:HG3	2.15	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:B:561:TYR:C	1:B:561:TYR:CD2	2.94	0.46
1:C:273:GLN:HG3	1:C:273:GLN:O	2.14	0.46
1:C:391:ASP:HB3	1:C:538:VAL:HG13	1.34	0.46
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:592:PHE:HB2	1:B:568:ARG:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ALA:C	1:C:527:SER:H	2.24	0.45
1:C:568:ARG:CG	1:C:568:ARG:NH1	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:325:LYS:N	1:C:328:MET:HE3	2.31	0.45
1:C:589:LEU:O	1:C:591:ARG:N	2.47	0.45
1:C:265:GLY:C	1:C:267:LYS:H	2.25	0.45
1:A:525:ALA:C	1:A:527:SER:H	2.24	0.45
1:A:595:MET:HE2	1:A:595:MET:HB2	1.79	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:314:GLN:C	1:C:316:THR:N	2.75	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:B:566:VAL:HG13	1:B:567:ILE:N	2.31	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:B:525:ALA:C	1:B:527:SER:H	2.24	0.45
1:C:265:GLY:C	1:C:267:LYS:N	2.74	0.45
1:A:561:TYR:C	1:A:561:TYR:CD2	2.94	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:C:561:TYR:C	1:C:561:TYR:CD2	2.94	0.45
1:A:439:GLY:HA2	1:A:468:GLY:HA2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ALA:CB	1:C:273:GLN:CG	2.94	0.44
1:C:257:PRO:CB	1:C:324:ILE:HG21	2.47	0.44
1:C:259:LYS:CB	1:C:269:TYR:O	2.65	0.44
1:A:347:SER:O	1:A:351:GLN:HB2	2.18	0.44
1:A:454:TYR:HD1	1:B:556:HIS:HD2	1.60	0.44
1:A:589:LEU:O	1:A:591:ARG:N	2.47	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:448:VAL:HG11	1:B:408:ALA:C	2.43	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:A:415:GLU:O	1:A:416:LEU:C	2.61	0.43
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:C:325:LYS:CA	1:C:328:MET:HE3	2.47	0.43
1:B:347:SER:O	1:B:351:GLN:HB2	2.18	0.43
1:A:494:HIS:O	1:A:495:GLU:C	2.62	0.43
1:B:234:ILE:CD1	1:B:546:TYR:HB3	2.45	0.43
1:B:283:VAL:CG1	1:B:356:PHE:CE2	3.01	0.43
1:C:251:ASP:CG	1:C:252:CYS:N	2.77	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:O	1:C:517:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:CG	1:A:252:CYS:N	2.76	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
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: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:341:HIS:CD2	1:A:554:HIS:CD2	3.07	0.42
1:A:522:LYS:O	1:A:522:LYS:HD3	2.19	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:HG12	1:B:517:VAL:O	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:B:415:GLU:O	1:B:416:LEU:C	2.61	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:C:415:GLU:O	1:C:416:LEU:C	2.61	0.42
1:B:358:ASP:HB2	1:B:361:GLU:HB2	2.00	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:B:251:ASP:CG	1:B:252:CYS:N	2.76	0.42
1:C:399:CYS:SG	1:C:507:ILE:HG23	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:TRP:CD1	1:C:424:TRP:C	2.98	0.42
1:C:259:LYS:HG3	1:C:268:SER:CB	2.50	0.42
1:A:234:ILE:HD13	1:A:546:TYR:C	2.44	0.42
1:A:251:ASP:OD2	1:A:252:CYS:N	2.51	0.41
1:A:338:MET:CE	1:A:338:MET:CA	2.98	0.41
1:A:517:VAL:O	1:A:517:VAL:HG12	2.18	0.41
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:C:324:ILE:CG2	1:C:328:MET:HE2	2.22	0.41
1:A:358:ASP:HB3	1:A:360:LYS:HG2	2.02	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:C:494:HIS:O	1:C:495:GLU:C	2.62	0.41
1:A:290:PHE:CE1	1:A:335:MET:HE3	2.55	0.41
1:A:424:TRP:C	1:A:424:TRP:CD1	2.98	0.41
1:B:424:TRP:CD1	1:B:424:TRP:C	2.98	0.41
1:B:443:GLN:NE2	1:B:472:GLU:OE2	2.54	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:B:494:HIS:O	1:B:495:GLU:C	2.62	0.41
1:C:325:LYS:C	1:C:328:MET:HG2	2.44	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:481:GLN:HG3	1:A:577:PHE:CE1	2.56	0.41
1:A:523:LEU:CD2	1:A:529:ILE:HG23	2.50	0.41
1:B:241:PRO:HG3	1:B:549:GLN:OE1	2.21	0.41
1:B:338:MET:HE1	1:B:344:ILE:HD12	2.03	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:A:338:MET:HE1	1:A:344:ILE:HD12	2.02	0.41
1:A:395:ILE:HG23	1:A:545:SER:OG	2.21	0.41
1:C:314:GLN:OE1	1:C:323:PHE:CD1	2.61	0.41
1:C:392:LEU:HD11	1:C:514:ILE:C	2.46	0.41
1:C:410:ASP:CA	1:C:500:LEU:HD13	2.51	0.41
1:A:529:ILE:CG2	1:C:523:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:264:TYR:HB3	1:C:267:LYS:HB3	2.03	0.41
1:C:290:PHE:CE1	1:C:335:MET:HE3	2.55	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:239:TYR:HA	1:B:455:GLN:CB	2.51	0.40
1:A:338:MET:HE1	1:A:344:ILE:CD1	2.51	0.40
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:C:519:GLU:O	1:C:520:SER:C	2.64	0.40
1:A:243:TRP:CE2	1:A:550:ALA:HB1	2.56	0.40
1:A:397:GLN:HE21	1:A:397:GLN:HB2	1.55	0.40
1:A:455:GLN:HB3	1:B:239:TYR:HA	2.03	0.40
1:B:290:PHE:CE1	1:B:335:MET:HE3	2.55	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:B:243:TRP:CE3	1:B:550:ALA:HB1	2.55	0.40
1:C:338:MET:CE	1:C:338:MET:CA	2.98	0.40
1:C:338:MET:HE1	1:C:344:ILE:CD1	2.51	0.40
1:A:264:TYR:CD2	1:A:267:LYS:CG	2.98	0.40
1:A:523:LEU:CD1	1:C:528:LYS:HB3	2.51	0.40
1:B:355:ASN:OD1	1:B:355:ASN:O	2.40	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:305:ILE:HA	1:A:551:GLU:HG2	2.03	0.40
1:B:338:MET:CE	1:B:338:MET:CA	2.98	0.40
1:C:574:GLN:O	1:C:575:VAL:C	2.64	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

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	364/366 (100%)	313 (86%)	35 (10%)	16 (4%)	2	20
1	B	364/366 (100%)	319 (88%)	34 (9%)	11 (3%)	3	25
1	C	364/366 (100%)	314 (86%)	34 (9%)	16 (4%)	2	20
All	All	1092/1098 (100%)	946 (87%)	103 (9%)	43 (4%)	2	21

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

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Mol	Chain	Res	Type
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
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%)	302 (93%)	24 (7%)	13	35
1	B	326/326 (100%)	304 (93%)	22 (7%)	15	39
1	C	326/326 (100%)	296 (91%)	30 (9%)	8	29
All	All	978/978 (100%)	902 (92%)	76 (8%)	11	34

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	THR
1	A	279	THR
1	A	312	ASP

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Mol	Chain	Res	Type
1	A	322	GLU
1	A	338	MET
1	A	349	VAL
1	A	351	GLN
1	A	384	GLU
1	A	416	LEU
1	A	434	GLU
1	A	458	THR
1	A	481	GLN
1	A	503	PHE
1	A	506	ILE
1	A	507	ILE
1	A	532	GLN
1	A	551	GLU
1	A	553	ASN
1	A	565	SER
1	A	587	GLN
1	A	591	ARG
1	A	592	PHE
1	A	594	VAL
1	A	595	MET
1	B	247	THR
1	B	263	MET
1	B	267	LYS
1	B	275	THR
1	B	312	ASP
1	B	322	GLU
1	B	338	MET
1	B	349	VAL
1	B	351	GLN
1	B	384	GLU
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	553	ASN
1	B	565	SER
1	B	587	GLN

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Mol	Chain	Res	Type
1	B	591	ARG
1	C	247	THR
1	C	258	ARG
1	C	259	LYS
1	C	263	MET
1	C	267	LYS
1	C	275	THR
1	C	279	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	349	VAL
1	C	351	GLN
1	C	384	GLU
1	C	390	LEU
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	553	ASN
1	C	565	SER
1	C	568	ARG
1	C	587	GLN
1	C	591	ARG
1	C	594	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	397	GLN
1	A	443	GLN
1	A	481	GLN
1	A	487	HIS
1	A	535	GLN
1	A	549	GLN

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Mol	Chain	Res	Type
1	A	564	ASN
1	A	573	GLN
1	A	574	GLN
1	B	273	GLN
1	B	397	GLN
1	B	443	GLN
1	B	481	GLN
1	B	535	GLN
1	B	549	GLN
1	B	556	HIS
1	B	573	GLN
1	B	574	GLN
1	C	273	GLN
1	C	397	GLN
1	C	443	GLN
1	C	481	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	366/366 (100%)	0.68	22 (6%)	27 25	153, 153, 153, 153	0
1	B	366/366 (100%)	0.60	17 (4%)	37 30	153, 153, 153, 153	0
1	C	366/366 (100%)	0.72	29 (7%)	18 19	153, 153, 153, 153	0
All	All	1098/1098 (100%)	0.67	68 (6%)	26 25	153, 153, 153, 153	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	392	LEU	8.3
1	C	427	CYS	4.9
1	B	392	LEU	4.9
1	A	547	ALA	4.3
1	A	275	THR	4.3
1	A	392	LEU	3.9
1	A	420	GLY	3.8
1	A	595	MET	3.7
1	A	253	VAL	3.3
1	C	270	ILE	3.3
1	B	514	ILE	3.2
1	B	526	THR	3.2
1	B	395	ILE	3.2
1	A	529	ILE	3.1
1	B	528	LYS	3.1
1	C	551	GLU	3.1
1	C	316	THR	3.0
1	C	349	VAL	3.0
1	C	315	VAL	2.9
1	A	409	MET	2.8
1	A	277	THR	2.8
1	A	263	MET	2.8
1	C	304	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	420	GLY	2.7
1	A	551	GLU	2.7
1	C	353	PHE	2.7
1	C	520	SER	2.6
1	A	563	TYR	2.6
1	C	438	ILE	2.6
1	C	499	PHE	2.6
1	B	412	GLY	2.6
1	A	274	LEU	2.6
1	A	416	LEU	2.6
1	C	324	ILE	2.5
1	C	395	ILE	2.5
1	B	234	ILE	2.5
1	C	257	PRO	2.5
1	A	442	LEU	2.5
1	A	489	LEU	2.5
1	C	409	MET	2.5
1	A	304	ALA	2.3
1	B	374	LEU	2.3
1	C	362	TRP	2.3
1	C	255	ALA	2.3
1	C	267	LYS	2.2
1	B	306	PRO	2.2
1	B	420	GLY	2.2
1	B	489	LEU	2.2
1	B	354	LEU	2.2
1	C	396	GLU	2.2
1	C	405	PHE	2.2
1	A	413	VAL	2.2
1	A	435	TYR	2.1
1	C	259	LYS	2.1
1	C	354	LEU	2.1
1	A	396	GLU	2.1
1	A	243	TRP	2.1
1	B	547	ALA	2.1
1	B	541	VAL	2.1
1	B	572	GLU	2.1
1	B	304	ALA	2.1
1	C	391	ASP	2.1
1	A	427	CYS	2.1
1	C	265	GLY	2.1
1	C	412	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	489	LEU	2.1
1	B	545	SER	2.0
1	C	306	PRO	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 oligosaccharides 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.