Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:16 AM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

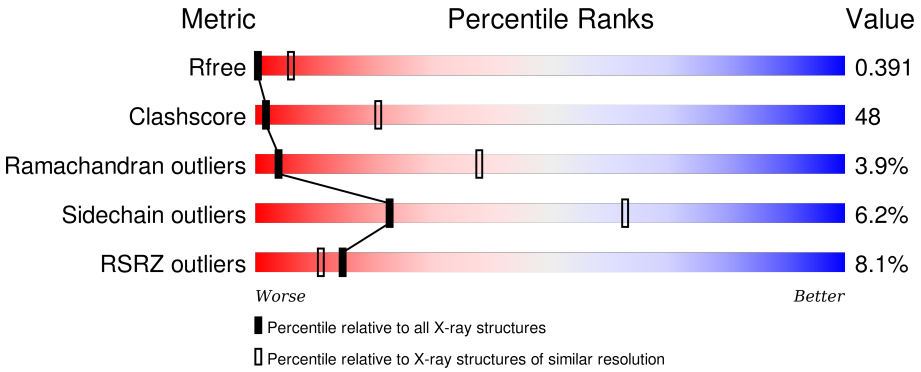
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	5% 50% 45%
1	B	366	6% 53% 42% 5%
1	C	366	13% 49% 42% 5%

2 Entry composition (i)

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.

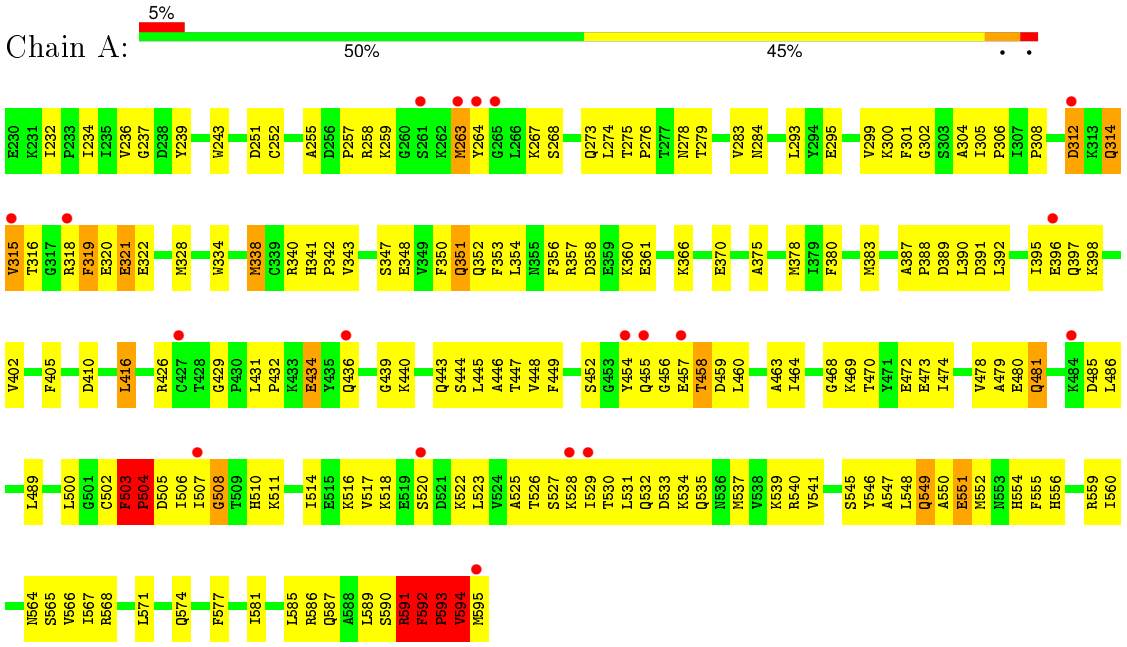
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			
1	B	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			
1	C	366	Total	C	N	O	S	0	0	0
			2977	1898	503	556	20			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

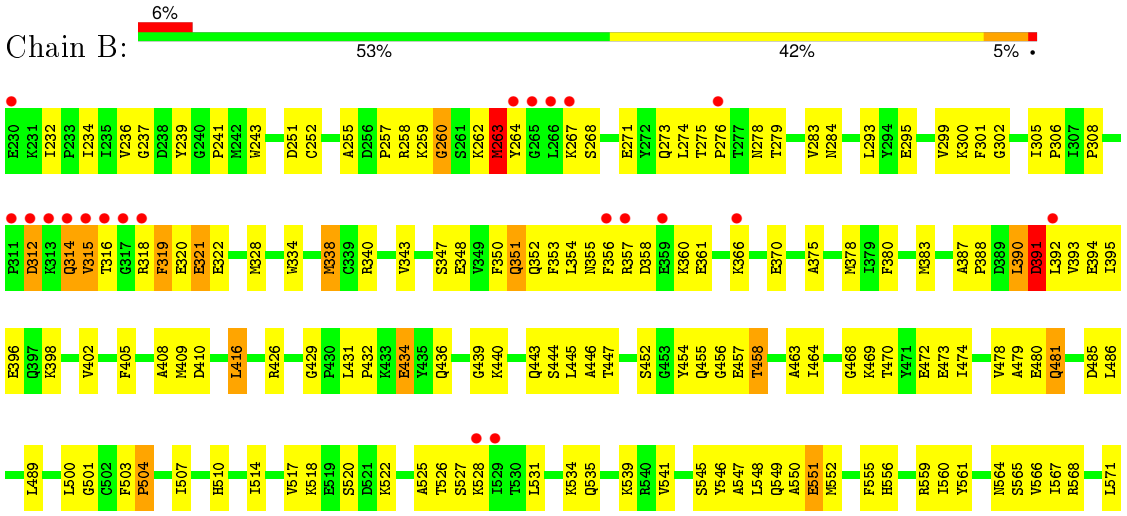
- Molecule 1: Sorting nexin-9

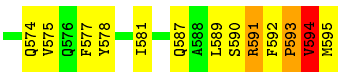
Chain A:



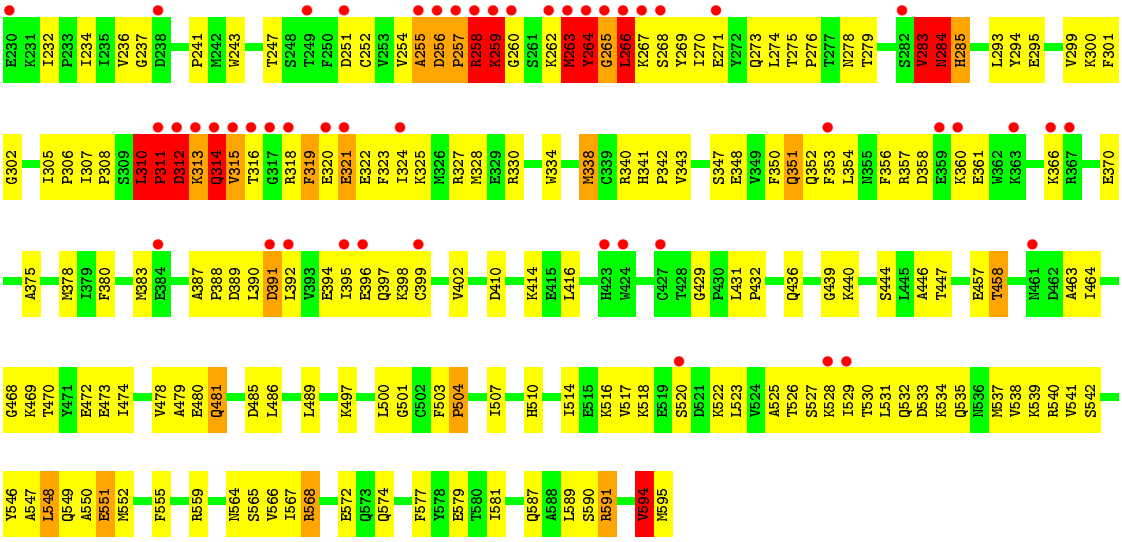
- Molecule 1: Sorting nexin-9

Chain B:





- Molecule 1: Sorting nexin-9



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	131.76Å 131.76Å 569.07Å 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
$< I/\sigma(I) >$ [1]	5.24 (at 4.14Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.388 , 0.403 0.391 , 0.391	Depositor DCC
R_{free} test set	682 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	129.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 15467 reflections (0.006%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:310:LEU:N	1:C:311:PRO:HD3	1.42	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:452:SER:CB	1:B:405:PHE:CE1	2.34	1.11
1:A:264:TYR:HD2	1:A:267:LYS:CB	1.63	1.11
1:C:324:ILE:HG22	1:C:328:MET:HE2	1.34	1.10
1:C:523:LEU:HD12	1:C:528:LYS:HB2	1.29	1.09
1:C:312:ASP:CB	1:C:313:LYS:HG2	1.78	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:C:312:ASP:HA	1:C:313:LYS:HG3	1.34	1.07
1:A:454:TYR:CD2	1:B:556:HIS:HB3	1.89	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: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:B:591:ARG:HH11	1:B:591:ARG:HB2	1.17	1.04
1:A:454:TYR:CD1	1:B:556:HIS:CD2	2.45	1.04
1:A:264:TYR:CE2	1:A:267:LYS:HD2	1.92	1.04
1:C:324:ILE:HG22	1:C:328:MET:CE	1.86	1.04
1:A:589:LEU:HD13	1:B:571:LEU:HB2	1.39	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:C:255:ALA:HB1	1:C:256:ASP:CB	1.89	1.01
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: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:C:255:ALA:CB	1:C:256:ASP:CB	2.42	0.97
1:A:545:SER:HB3	1:A:549:GLN:HE21	1.28	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: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: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:C:523:LEU:CD1	1:C:528:LYS:HB3	1.90	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:HH11	1:B:589:LEU:HD11	0.76	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:C:306:PRO:HD3	1:C:551:GLU:HG3	1.53	0.90
1:A:456:GLY:HA3	1:B:239:TYR:CE2	2.07	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:523:LEU:CD1	1:C:523:LEU:HD21	2.01	0.88
1:A:459:ASP:OD2	1:A:593:PRO:HG3	1.70	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:C:523:LEU:HD21	1:C:529:ILE:CG2	2.06	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: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:C:312:ASP:HB2	1:C:313:LYS:HG2	0.85	0.85
1:A:452:SER:CA	1:B:405:PHE:HD1	1.89	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:C:523:LEU:HD21	1:C:529:ILE:HG23	1.59	0.83
1:A:503:PHE:O	1:A:507:ILE:HD12	1.79	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:C:523:LEU:CG	1:C:529:ILE:HG12	2.10	0.81
1:B:259:LYS:HD2	1:B:268:SER:HB3	1.63	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: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:A:589:LEU:HA	1:B:571:LEU:HD13	1.62	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:528:LYS:CG	1:C:523:LEU:HD13	2.11	0.79
1:A:395:ILE:HD13	1:A:541:VAL:HG13	1.64	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:454:TYR:CG	1:B:556:HIS:CG	2.71	0.79
1:A:259:LYS:HD2	1:A:268:SER:HB3	1.63	0.79
1:A:455:GLN:HG3	1:B:239:TYR:O	1.83	0.78
1:A:568:ARG:NH1	1:B:589:LEU:CG	2.46	0.78
1:A:452:SER:HB2	1:B:405:PHE:CE1	2.17	0.78
1:B:395:ILE:HD13	1:B:541:VAL:CG1	2.11	0.78
1:B:392:LEU:HD13	1:B:517:VAL:HB	1.62	0.78
1:A:387:ALA:HB1	1:A:388:PRO:HD2	1.66	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:C:387:ALA:HB1	1:C:388:PRO:HD2	1.66	0.77
1:B:520:SER:HB2	1:B:534:LYS:HG2	1.66	0.77
1:C:262:LYS:HB3	1:C:264:TYR:HD1	1.50	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:392:LEU:HD21	1:C:514:ILE:O	1.85	0.77
1:C:390:LEU:CD1	1:C:394:GLU:HB3	2.13	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:C:294:TYR:CE2	1:C:310:LEU:HB2	2.20	0.76
1:B:396:GLU:HA	1:B:514:ILE:CD1	2.15	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:510:HIS:CE1	1:A:548:LEU:HB2	2.20	0.76
1:A:445:LEU:CD2	1:B:416:LEU:HD12	2.15	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: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:520:SER:HB2	1:A:534:LYS:HG2	1.67	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:C:294:TYR:CD1	1:C:310:LEU:HD13	2.21	0.76
1:B:564:ASN:O	1:B:568:ARG:CG	2.34	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:B:594:VAL:O	1:B:595:MET:CG	2.30	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:A:405:PHE:HD1	1:B:452:SER:HA	1.52	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:C:255:ALA:HB3	1:C:273:GLN:HE21	1.48	0.75
1:B:268:SER:O	1:B:319:PHE:HZ	1.70	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:CB	1:C:313:LYS:HA	2.17	0.74
1:A:454:TYR:CE2	1:B:556:HIS:CB	2.70	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:C:255:ALA:HB3	1:C:273:GLN:HG2	1.70	0.73
1:A:548:LEU:O	1:A:551:GLU:N	2.20	0.73
1:C:262:LYS:O	1:C:264:TYR:HB2	1.89	0.73
1:A:594:VAL:HG22	1:A:594:VAL:O	1.87	0.73
1:A:268:SER:O	1:A:319:PHE:HZ	1.71	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:594:VAL:HG13	1:C:595:MET:CG	2.17	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:A:592:PHE:N	1:A:592:PHE:CD1	2.55	0.72
1:A:503:PHE:HB3	1:A:507:ILE:CD1	2.19	0.72
1:A:460:LEU:HG	1:B:564:ASN:OD1	1.88	0.72
1:A:454:TYR:CG	1:B:556:HIS:HB3	2.25	0.72
1:A:396:GLU:OE1	1:A:518:LYS:NZ	2.15	0.72
1:C:523:LEU:HD23	1:C:529:ILE:CG1	2.19	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: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:589:LEU:HA	1:B:571:LEU:CD1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:HB2	1:C:271:GLU:O	1.90	0.71
1:A:405:PHE:CD1	1:B:452:SER:HA	2.25	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:283:VAL:HG21	1:C:356:PHE:CE2	2.26	0.70
1:C:262:LYS:O	1:C:264:TYR:CB	2.39	0.70
1:C:523:LEU:CD2	1:C:529:ILE:HG12	2.22	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:A:508:GLY:HA2	1:A:511:LYS:HB2	1.71	0.70
1:A:274:LEU:HD12	1:A:274:LEU:N	2.07	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:391:ASP:O	1:B:395:ILE:HG13	1.93	0.69
1:B:274:LEU:N	1:B:274:LEU:HD12	2.07	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:392:LEU:HD13	1:A:517:VAL:HB	1.73	0.68
1:A:300:LYS:HD3	1:A:301:PHE:CZ	2.27	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:460:LEU:HD21	1:A:464:ILE:CD1	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TRP:CZ2	1:B:550:ALA:CB	2.78	0.67
1:A:316:THR:O	1:A:316:THR:HG22	1.95	0.67
1:A:529:ILE:CG2	1:C:523:LEU:HD22	2.23	0.67
1:C:316:THR:O	1:C:316:THR:HG22	1.95	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:523:LEU:HD13	1:A:529:ILE:CD1	2.26	0.66
1:A:295:GLU:O	1:A:299:VAL:HG23	1.96	0.66
1:C:258:ARG:O	1:C:270:ILE:HG23	1.96	0.66
1:A:391:ASP:O	1:A:395:ILE:HG13	1.96	0.66
1:B:316:THR:HG22	1:B:316:THR:O	1.95	0.66
1:C:284:ASN:CB	1:C:285:HIS:CG	2.68	0.65
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:392:LEU:CD2	1:C:518:LYS:CG	2.75	0.65
1:C:262:LYS:O	1:C:263:MET:C	2.34	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:C:295:GLU:O	1:C:299:VAL:HG23	1.96	0.65
1:A:448:VAL:HG13	1:B:408:ALA:HB1	1.79	0.65
1:C:324:ILE:O	1:C:328:MET:HE2	1.96	0.65
1:C:310:LEU:HG	1:C:311:PRO:CD	2.27	0.65
1:A:556:HIS:HB2	1:B:454:TYR:CE1	2.32	0.65
1:C:294:TYR:CZ	1:C:310:LEU:HB2	2.31	0.64
1:B:593:PRO:C	1:B:595:MET:N	2.51	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:C:396:GLU:N	1:C:514:ILE:HD13	2.12	0.64
1:A:454:TYR:CD1	1:B:556:HIS:HB2	2.31	0.64
1:B:545:SER:O	1:B:549:GLN:HG3	1.98	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:C:284:ASN:HB2	1:C:285:HIS:ND1	2.13	0.64
1:A:398:LYS:O	1:A:402:VAL:HG23	1.98	0.64
1:A:528:LYS:HG2	1:C:523:LEU:CD1	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:510:HIS:CE1	1:C:548:LEU:HB2	2.33	0.63
1:B:398:LYS:O	1:B:402:VAL:HG23	1.98	0.63
1:A:405:PHE:CE1	1:B:452:SER:CB	2.82	0.63
1:A:358:ASP:HB2	1:A:361:GLU:H	1.63	0.63
1:A:264:TYR:CD2	1:A:267:LYS:HB3	2.25	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:A:436:GLN:O	1:A:440:LYS:HG2	1.99	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: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:C:392:LEU:HD11	1:C:514:ILE:CA	2.28	0.62
1:A:589:LEU:CA	1:B:571:LEU:HD13	2.30	0.62
1:B:392:LEU:HD11	1:B:517:VAL:HB	1.80	0.62
1:B:358:ASP:HB2	1:B:361:GLU:H	1.63	0.62
1:B:338:MET:CE	1:B:338:MET:HA	2.29	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:523:LEU:CD2	1:A:528:LYS:HB2	2.29	0.62
1:A:454:TYR:CD2	1:B:556:HIS:CB	2.75	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:HG2	1:A:267:LYS:O	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:589:LEU:HD13	1:B:571:LEU:CB	2.24	0.61
1:A:392:LEU:HD13	1:A:517:VAL:CB	2.30	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:C:356:PHE:HA	1:C:361:GLU:OE2	2.02	0.60
1:A:506:ILE:HG22	1:A:507:ILE:HG13	1.84	0.60
1:A:255:ALA:HA	1:A:328:MET:SD	2.41	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:C:568:ARG:HH11	1:C:568:ARG:HG3	1.67	0.59
1:B:429:GLY:O	1:B:432:PRO:HD2	2.02	0.59
1:C:283:VAL:HG11	1:C:354:LEU:O	2.03	0.59
1:A:503:PHE:HB3	1:A:507:ILE:HD12	1.85	0.59
1:C:429:GLY:O	1:C:432:PRO:HD2	2.02	0.59
1:A:560:ILE:HD11	1:B:457:GLU:HB3	1.85	0.59
1:A:239:TYR:HE2	1:B:456:GLY:HA3	1.55	0.59
1:C:366:LYS:O	1:C:370:GLU:HG3	2.02	0.59
1:A:366:LYS:O	1:A:370:GLU:HG3	2.02	0.59
1:C:551:GLU:OE1	1:C:551:GLU:HA	2.03	0.59
1:A:283:VAL:HG21	1:A:354:LEU:O	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:C:266:LEU:O	1:C:266:LEU:CD1	2.51	0.58
1:B:510:HIS:HE1	1:B:548:LEU:HB2	1.67	0.58
1:A:522:LYS:O	1:A:526:THR:HG23	2.03	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:HG2	1:B:480:GLU:O	2.03	0.58
1:C:294:TYR:CD2	1:C:310:LEU:HB2	2.39	0.58
1:A:507:ILE:O	1:A:511:LYS:HG3	2.03	0.58
1:C:255:ALA:HB2	1:C:273:GLN:NE2	2.04	0.58
1:A:429:GLY:O	1:A:432:PRO:HD2	2.02	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: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:551:GLU:OE1	1:A:551:GLU:HA	2.03	0.57
1:A:405:PHE:CE1	1:B:452:SER:HB3	2.39	0.57
1:A:454:TYR:CD1	1:B:556:HIS:HD2	2.11	0.57
1:A:239:TYR:OH	1:B:456:GLY:HA2	2.04	0.57
1:C:266:LEU:HD12	1:C:266:LEU:O	2.04	0.57
1:C:236:VAL:HG12	1:C:237:GLY:N	2.20	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:C:390:LEU:HD13	1:C:394:GLU:HB2	1.87	0.57
1:A:480:GLU:O	1:A:480:GLU:HG2	2.03	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:C:395:ILE:HD13	1:C:541:VAL:CG1	2.24	0.57
1:A:460:LEU:CG	1:B:564:ASN:OD1	2.53	0.57
1:A:236:VAL:HG12	1:A:237:GLY:N	2.19	0.56
1:B:593:PRO:O	1:B:595:MET:N	2.39	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:A:529:ILE:HG21	1:C:529:ILE:HG21	1.86	0.56
1:A:470:THR:O	1:A:474:ILE:HG13	2.06	0.56
1:A:568:ARG:NH1	1:B:589:LEU:HG	2.20	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: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:C:258:ARG:C	1:C:271:GLU:H	2.06	0.56
1:B:236:VAL:HG12	1:B:237:GLY:H	1.71	0.56
1:C:523:LEU:HD21	1:C:529:ILE:HG21	1.87	0.56
1:C:283:VAL:C	1:C:284:ASN:OD1	2.44	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:A:454:TYR:HD1	1:B:556:HIS:CD2	2.16	0.56
1:B:260:GLY:HA3	1:B:271:GLU:OE1	2.05	0.55
1:C:311:PRO:HB2	1:C:312:ASP:CA	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:A:530:THR:CG2	1:C:516:LYS:HG2	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:C:380:PHE:HE2	1:C:547:ALA:HB3	1.71	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: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:B:395:ILE:HD11	1:B:541:VAL:HG13	1.77	0.54
1:A:232:ILE:CG2	1:A:383:MET:HG2	2.38	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:489:LEU:HA	1:B:566:VAL:HG21	1.89	0.53
1:B:318:ARG:HD2	1:B:319:PHE:CE1	2.43	0.53
1:C:236:VAL:HG12	1:C:237:GLY:H	1.71	0.53
1:A:454:TYR:CG	1:B:556:HIS:CD2	2.89	0.53
1:C:259:LYS:O	1:C:259:LYS:HG2	2.08	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:B:348:GLU:OE1	1:B:352:GLN:NE2	2.42	0.53
1:C:546:TYR:O	1:C:550:ALA:N	2.41	0.53
1:B:232:ILE:CG2	1:B:383:MET:HG2	2.37	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:502:CYS:C	1:A:504:PRO:HD2	2.29	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: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:B:396:GLU:HB3	1:B:514:ILE:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:HIS:HB3	1:B:454:TYR:CE2	2.44	0.53
1:A:338:MET:HA	1:A:338:MET:HE2	1.91	0.53
1:A:258:ARG:HH22	1:A:273:GLN:NE2	2.07	0.52
1:C:594:VAL:O	1:C:594:VAL:HG12	2.09	0.52
1:A:348:GLU:OE1	1:A:352:GLN:NE2	2.42	0.52
1:C:348:GLU:OE1	1:C:352:GLN:NE2	2.42	0.52
1:A:410:ASP:HA	1:A:500:LEU:HD13	1.92	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:C:257:PRO:HB3	1:C:324:ILE:HG21	1.91	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:B:396:GLU:CB	1:B:514:ILE:HG21	2.38	0.52
1:A:306:PRO:HD3	1:A:551:GLU:HG3	1.90	0.52
1:C:306:PRO:HD2	1:C:551:GLU:OE2	2.10	0.52
1:B:410:ASP:HA	1:B:500:LEU:HD13	1.91	0.52
1:C:410:ASP:HA	1:C:500:LEU:HD13	1.92	0.52
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: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:A:481:GLN:HG3	1:A:577:PHE:CD1	2.46	0.51
1:B:444:SER:O	1:B:447:THR:HB	2.10	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:338:MET:HA	1:C:338:MET:HE3	1.92	0.51
1:C:232:ILE:O	1:C:383:MET:HA	2.11	0.51
1:A:274:LEU:CD1	1:A:274:LEU:N	2.74	0.51
1:A:449:PHE:HE2	1:B:409:MET:HG3	1.75	0.51
1:A:432:PRO:CG	1:A:479:ALA:HB2	2.41	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:560:ILE:O	1:B:564:ASN:ND2	2.44	0.51
1:B:432:PRO:CG	1:B:479:ALA:HB2	2.41	0.51
1:A:560:ILE:CD1	1:B:457:GLU:HB3	2.41	0.51
1:C:259:LYS:HB2	1:C:269:TYR:O	2.10	0.51
1:C:258:ARG:O	1:C:270:ILE:CG2	2.57	0.51
1:B:232:ILE:O	1:B:383:MET:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:GLN:HG3	1:B:577:PHE:CD1	2.45	0.51
1:C:294:TYR:CB	1:C:310:LEU:CD2	2.83	0.51
1:C:258:ARG:O	1:C:270:ILE:C	2.48	0.51
1:B:274:LEU:N	1:B:274:LEU:CD1	2.74	0.51
1:A:444:SER:O	1:A:447:THR:HB	2.10	0.51
1:A:434:GLU:OE1	1:B:426:ARG:CD	2.59	0.51
1:B:338:MET:HE3	1:B:338:MET:HA	1.92	0.51
1:C:568:ARG:HH11	1:C:568:ARG:CG	2.24	0.51
1:A:232:ILE:O	1:A:383:MET:HA	2.11	0.51
1:C:305:ILE:HA	1:C:551:GLU:CG	2.37	0.51
1:C:392:LEU:HA	1:C:395:ILE:HD12	1.93	0.50
1:A:537:MET:CE	1:C:533:ASP:OD2	2.59	0.50
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:A:523:LEU:CD1	1:C:523:LEU:HD11	2.40	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:C:284:ASN:ND2	1:C:353:PHE:O	2.45	0.50
1:B:320:GLU:HG2	1:B:321:GLU:H	1.76	0.50
1:A:547:ALA:O	1:A:550:ALA:HB3	2.12	0.50
1:C:546:TYR:O	1:C:550:ALA:HB2	2.10	0.50
1:C:432:PRO:CG	1:C:479:ALA:HB2	2.41	0.50
1:A:585:LEU:HD13	1:B:574:GLN:HB3	1.94	0.50
1:C:294:TYR:CG	1:C:310:LEU:HD13	2.47	0.50
1:C:256:ASP:OD2	1:C:273:GLN:NE2	2.45	0.50
1:B:501:GLY:O	1:B:504:PRO:HD2	2.11	0.50
1:B:392:LEU:HA	1:B:395:ILE:HD12	1.93	0.50
1:A:574:GLN:O	1:A:577:PHE:HB3	2.12	0.50
1:A:485:ASP:OD2	1:A:486:LEU:N	2.40	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:431:LEU:HB3	1:A:432:PRO:HD3	1.94	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:C:269:TYR:CE2	1:C:271:GLU:OE2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:HA	1:A:395:ILE:HD12	1.93	0.49
1:C:431:LEU:HB3	1:C:432:PRO:HD3	1.95	0.49
1:C:254:VAL:HG22	1:C:274:LEU:HD21	1.80	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: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: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:HH11	1:C:559:ARG:HG2	1.78	0.48
1:A:342:PRO:HD2	1:A:554:HIS:CE1	2.48	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: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:455:GLN:HB2	1:B:239:TYR:HB3	1.95	0.48
1:A:589:LEU:C	1:A:591:ARG:H	2.17	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: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:C:264:TYR:O	1:C:267:LYS:CB	2.43	0.48
1:A:507:ILE:HG22	1:A:507:ILE:O	2.13	0.48
1:A:459:ASP:OD2	1:A:593:PRO:CG	2.53	0.48
1:B:258:ARG:HH22	1:B:273:GLN:HE22	1.62	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:C:293:LEU:HD22	1:C:353:PHE:CD2	2.49	0.47
1:B:559:ARG:HG2	1:B:559:ARG:HH11	1.78	0.47
1:A:392:LEU:HD13	1:A:517:VAL:HG11	1.96	0.47
1:C:523:LEU:CD2	1:C:529:ILE:CG2	2.87	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: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:C:534:LYS:HD3	1:C:534:LYS:C	2.35	0.47
1:A:380:PHE:HB2	1:A:540:ARG:HH22	1.80	0.47
1:C:294:TYR:HB2	1:C:310:LEU:CD2	2.45	0.47
1:C:273:GLN:O	1:C:273:GLN:HG3	2.14	0.47
1:A:463:ALA:HA	1:A:591:ARG:HG2	1.96	0.47
1:C:243:TRP:CH2	1:C:550:ALA:HB3	2.50	0.47
1:B:380:PHE:HE2	1:B:547:ALA:HB3	1.80	0.47
1:B:308:PRO:HB2	1:B:334:TRP:CD1	2.50	0.47
1:A:293:LEU:HD22	1:A:353:PHE:CD2	2.49	0.47
1:C:589:LEU:C	1:C:591:ARG:H	2.17	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: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:463:ALA:HA	1:C:591:ARG:HG2	1.97	0.47
1:C:314:GLN:C	1:C:316:THR:H	2.17	0.47
1:B:396:GLU:OE1	1:B:518:LYS:NZ	2.44	0.46
1:A:593:PRO:HB2	1:A:595:MET:N	2.31	0.46
1:A:234:ILE:HD13	1:A:546:TYR:HB3	1.97	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:293:LEU:HD22	1:B:353:PHE:CD2	2.49	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:B:469:LYS:O	1:B:473:GLU:HG3	2.15	0.46
1:B:463:ALA:HA	1:B:591:ARG:HG2	1.97	0.46
1:A:426:ARG:HD2	1:B:434:GLU:OE1	2.16	0.46
1:A:460:LEU:CD1	1:B:564:ASN:OD1	2.64	0.46
1:C:306:PRO:CD	1:C:551:GLU:CG	2.90	0.46
1:A:448:VAL:HG11	1:B:409:MET:HA	1.96	0.46
1:A:308:PRO:HB2	1:A:334:TRP:CD1	2.50	0.46
1:C:267:LYS:HG3	1:C:318:ARG:HH22	1.80	0.46
1:B:534:LYS:C	1:B:534:LYS:HD3	2.35	0.46
1:C:469:LYS:O	1:C:473:GLU:HG3	2.15	0.46
1:A:568:ARG:HD2	1:B:589:LEU:HD12	1.98	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:C:391:ASP:HB3	1:C:538:VAL:HG13	1.34	0.46
1:A:566:VAL:HG13	1:A:567:ILE:N	2.31	0.46

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ALA:O	1:A:378:MET:HB2	2.17	0.44
1:A:528:LYS:NZ	1:C:528:LYS:HZ2	2.14	0.44
1:C:523:LEU:HD23	1:C:529:ILE:HD11	1.81	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:A:347:SER:O	1:A:351:GLN:HB2	2.18	0.44
1:C:313:LYS:NZ	1:C:330:ARG:CD	2.81	0.44
1:B:396:GLU:N	1:B:514:ILE:HD13	2.33	0.44
1:A:545:SER:CB	1:A:549:GLN:HE21	2.14	0.44
1:A:315:VAL:O	1:A:315:VAL:CG1	2.60	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:C:392:LEU:HD23	1:C:518:LYS:CG	2.41	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:A:358:ASP:HB2	1:A:361:GLU:CB	2.48	0.44
1:B:577:PHE:CZ	1:B:581:ILE:HD11	2.52	0.44
1:A:350:PHE:O	1:A:353:PHE:HB3	2.17	0.44
1:B:375:ALA:O	1:B:378:MET:HB2	2.18	0.44
1:C:523:LEU:CD1	1:C:528:LYS:CG	2.94	0.43
1:C:284:ASN:ND2	1:C:285:HIS:NE2	2.34	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: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:B:283:VAL:CG1	1:B:356:PHE:CE2	3.01	0.43
1:C:517:VAL:HG12	1:C:517:VAL:O	2.18	0.43
1:A:502:CYS:O	1:A:504:PRO:CD	2.66	0.43
1:A:440:LYS:HD3	1:A:472:GLU:OE2	2.19	0.43
1:A:251:ASP:HB2	1:A:340:ARG:HH12	1.83	0.43
1:C:577:PHE:CZ	1:C:581:ILE:HD11	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:A:278:ASN:OD1	1:A:279:THR:N	2.52	0.43
1:C:358:ASP:HB2	1:C:361:GLU:CB	2.48	0.43
1:B:589:LEU:O	1:B:591:ARG:N	2.47	0.43
1:C:294:TYR:HB2	1:C:310:LEU:HD22	1.89	0.43
1:A:564:ASN:HD22	1:B:595:MET:CA	2.19	0.43
1:A:460:LEU:CD2	1:A:464:ILE:HD12	2.44	0.43
1:C:340:ARG:HD3	1:C:340:ARG:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASP:HB2	1:B:340:ARG:HH12	1.83	0.43
1:C:306:PRO:HD2	1:C:551:GLU:HG3	2.00	0.43
1:C:251:ASP:HB2	1:C:340:ARG:HH12	1.83	0.43
1:B:503:PHE:HB3	1:B:507:ILE:HD12	1.99	0.43
1:A:586:ARG:NH2	1:B:575:VAL:CG1	2.81	0.43
1:C:522:LYS:O	1:C:522:LYS:HD3	2.19	0.43
1:C:241:PRO:HG2	1:C:549:GLN:CD	2.39	0.43
1:C:552:MET:O	1:C:555:PHE:N	2.52	0.43
1:B:546:TYR:O	1:B:550:ALA:HB2	2.18	0.42
1:A:274:LEU:O	1:A:276:PRO:HD3	2.19	0.42
1:C:564:ASN:O	1:C:568:ARG:HB2	2.18	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:517:VAL:O	1:B:517:VAL:HG12	2.18	0.42
1:A:502:CYS:O	1:A:506:ILE:HB	2.19	0.42
1:C:278:ASN:OD1	1:C:279:THR: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: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:234:ILE:HD13	1:C:546:TYR:HB3	2.02	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:232:ILE:HG21	1:C:383:MET:HG2	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:310:LEU:CG	1:C:311:PRO:HD2	2.43	0.42
1:A:358:ASP:HB2	1:A:361:GLU:HB2	2.00	0.42
1:B:522:LYS:O	1:B:522:LYS:HD3	2.19	0.42
1:B:278:ASN:OD1	1:B:279:THR:N	2.52	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:517:VAL:O	1:A:517:VAL:HG12	2.18	0.41
1:A:338:MET:CE	1:A:338:MET:CA	2.98	0.41
1:A:251:ASP:OD2	1:A:252:CYS:N	2.51	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:C:324:ILE:C	1:C:328:MET:HE2	2.39	0.41
1:C:266:LEU:C	1:C:266:LEU:HD12	2.41	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: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:C:358:ASP:HB3	1:C:360:LYS:HG2	2.02	0.41
1:A:304:ALA:O	1:A:551:GLU:HG2	2.20	0.41
1:C:390:LEU:CD1	1:C:394:GLU:HG3	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:A:410:ASP:CA	1:A:500:LEU:HD13	2.50	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: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: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:525:ALA:C	1:C:527:SER:H	2.24	0.41
1:C:341:HIS:HA	1:C:342:PRO:HD2	1.88	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: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
1:C:294:TYR:CG	1:C:310:LEU:CD2	2.91	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:A:556:HIS:CB	1:B:454:TYR:CD1	3.03	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:B:234:ILE:HG21	1:B:546:TYR:HB3	2.02	0.40
1:A:443:GLN:NE2	1:A:472:GLU:OE2	2.54	0.40
1:B:358:ASP:HB3	1:B:360:LYS:HG2	2.02	0.40
1:C:274:LEU:HD12	1:C:285:HIS:HD2	1.86	0.40
1:A:455:GLN:HB3	1:B:239:TYR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TRP:CE2	1:A:550:ALA:HB1	2.56	0.40
1:B:410:ASP:CA	1:B:500:LEU:HD13	2.50	0.40
1:A:397:GLN:HB2	1:A:397:GLN:HE21	1.55	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:CA	1:C:338:MET:CE	2.98	0.40
1:A:525:ALA:C	1:A:527:SER:H	2.24	0.40
1:A:523:LEU:CD1	1:C:528:LYS:HB3	2.51	0.40
1:C:294:TYR:CE2	1:C:310:LEU:CB	2.98	0.40
1:A:264:TYR:CD2	1:A:267:LYS:CG	2.98	0.40
1:C:397:GLN:HE21	1:C:397:GLN:HB2	1.56	0.40
1:B:355:ASN:O	1:B:355:ASN:OD1	2.40	0.40
1:B:525:ALA:C	1:B:527:SER:H	2.24	0.40
1:C:265:GLY:C	1:C:267:LYS:N	2.74	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

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%)	3 35
1	B	364/366 (100%)	319 (88%)	34 (9%)	11 (3%)	5 45
1	C	364/366 (100%)	314 (86%)	34 (9%)	16 (4%)	3 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1092/1098 (100%)	946 (87%)	103 (9%)	43 (4%)	4 38

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 (i)

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%)	27	67
1	B	326/326 (100%)	308 (94%)	18 (6%)	27	67
1	C	326/326 (100%)	301 (92%)	25 (8%)	16	55
All	All	978/978 (100%)	917 (94%)	61 (6%)	23	63

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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^{th} 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%)	0.45	19 (5%) 31 23	153, 153, 153, 153	0
1	B	366/366 (100%)	0.44	21 (5%) 27 20	153, 153, 153, 153	0
1	C	366/366 (100%)	0.69	49 (13%) 4 5	153, 153, 153, 153	0
All	All	1098/1098 (100%)	0.53	89 (8%) 15 11	153, 153, 153, 153	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	392	LEU	6.4
1	C	316	THR	6.3
1	C	315	VAL	5.7
1	B	317	GLY	5.5
1	B	318	ARG	5.5
1	C	258	ARG	5.4
1	C	267	LYS	5.2
1	C	317	GLY	5.0
1	C	312	ASP	4.9
1	C	391	ASP	4.8
1	A	529	ILE	4.6
1	C	318	ARG	4.4
1	C	257	PRO	4.2
1	C	427	CYS	4.1
1	C	266	LEU	4.0
1	B	313	LYS	3.9
1	A	265	GLY	3.8
1	C	311	PRO	3.8
1	C	321	GLU	3.7
1	A	396	GLU	3.7
1	B	316	THR	3.7
1	C	529	ILE	3.7
1	A	455	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	3.6
1	B	315	VAL	3.5
1	C	268	SER	3.5
1	B	230	GLU	3.4
1	B	312	ASP	3.4
1	B	265	GLY	3.4
1	C	259	LYS	3.3
1	C	230	GLU	3.3
1	C	260	GLY	3.3
1	C	282	SER	3.3
1	C	528	LYS	3.2
1	A	264	TYR	3.2
1	C	238	ASP	3.2
1	C	265	GLY	3.1
1	C	384	GLU	3.1
1	B	266	LEU	3.1
1	C	396	GLU	3.1
1	C	249	THR	3.0
1	C	359	GLU	3.0
1	C	255	ALA	3.0
1	C	520	SER	2.9
1	A	315	VAL	2.9
1	A	528	LYS	2.9
1	A	312	ASP	2.9
1	C	363	LYS	2.8
1	C	314	GLN	2.8
1	C	313	LYS	2.7
1	A	454	TYR	2.7
1	C	360	LYS	2.6
1	A	436	GLN	2.6
1	A	457	GLU	2.5
1	B	267	LYS	2.5
1	C	251	ASP	2.4
1	B	356	PHE	2.4
1	A	595	MET	2.4
1	C	320	GLU	2.4
1	C	461	ASN	2.4
1	A	427	CYS	2.4
1	B	392	LEU	2.3
1	C	264	TYR	2.3
1	B	314	GLN	2.3
1	C	262	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	263	MET	2.3
1	A	261	SER	2.3
1	C	271	GLU	2.2
1	B	264	TYR	2.2
1	B	366	LYS	2.2
1	C	324	ILE	2.2
1	C	366	LYS	2.2
1	B	276	PRO	2.1
1	B	528	LYS	2.1
1	B	359	GLU	2.1
1	A	318	ARG	2.1
1	C	353	PHE	2.1
1	C	395	ILE	2.1
1	B	357	ARG	2.1
1	A	263	MET	2.1
1	C	399	CYS	2.1
1	C	367	ARG	2.1
1	B	529	ILE	2.1
1	C	424	TRP	2.1
1	A	520	SER	2.0
1	B	311	PRO	2.0
1	C	423	HIS	2.0
1	A	507	ILE	2.0
1	A	484	LYS	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.