



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:20 pm BST

PDB ID : 3LWW
Title : Structure of an open and closed conformation of Human Importin Beta bound to the Snurportin1 IBB-domain trapped in the same crystallographic asymmetric unit
Authors : Bhardwaj, A.; Cingolani, G.
Deposited on : 2010-02-24
Resolution : 3.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

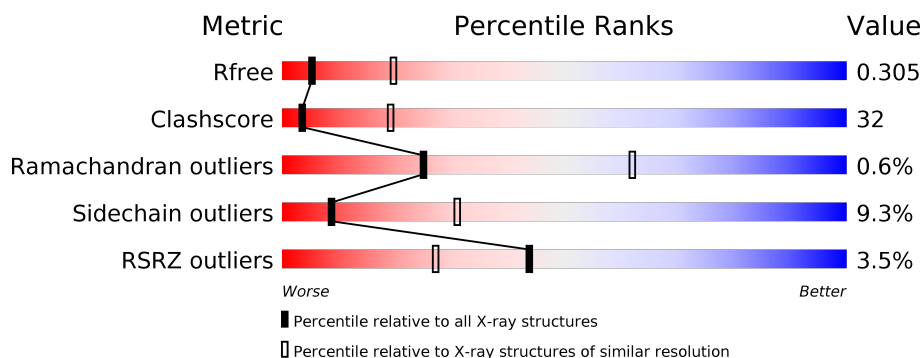
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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	876	<div> <div>4%</div> <div> <div>54%</div> <div>40%</div> <div>6%</div> </div> </div>
1	C	876	<div> <div>3%</div> <div> <div>54%</div> <div>39%</div> <div>6%</div> </div> </div>
2	B	40	<div> <div>5%</div> <div> <div>60%</div> <div>35%</div> </div> </div>
2	D	40	<div> <div> <div>38%</div> <div>23%</div> <div>5%</div> <div>35%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14127 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 Importin subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	873	Total	C	N	O	S	0	0	0
			6782	4273	1136	1326	47			
1	C	871	Total	C	N	O	S	0	0	0
			6766	4263	1134	1322	47			

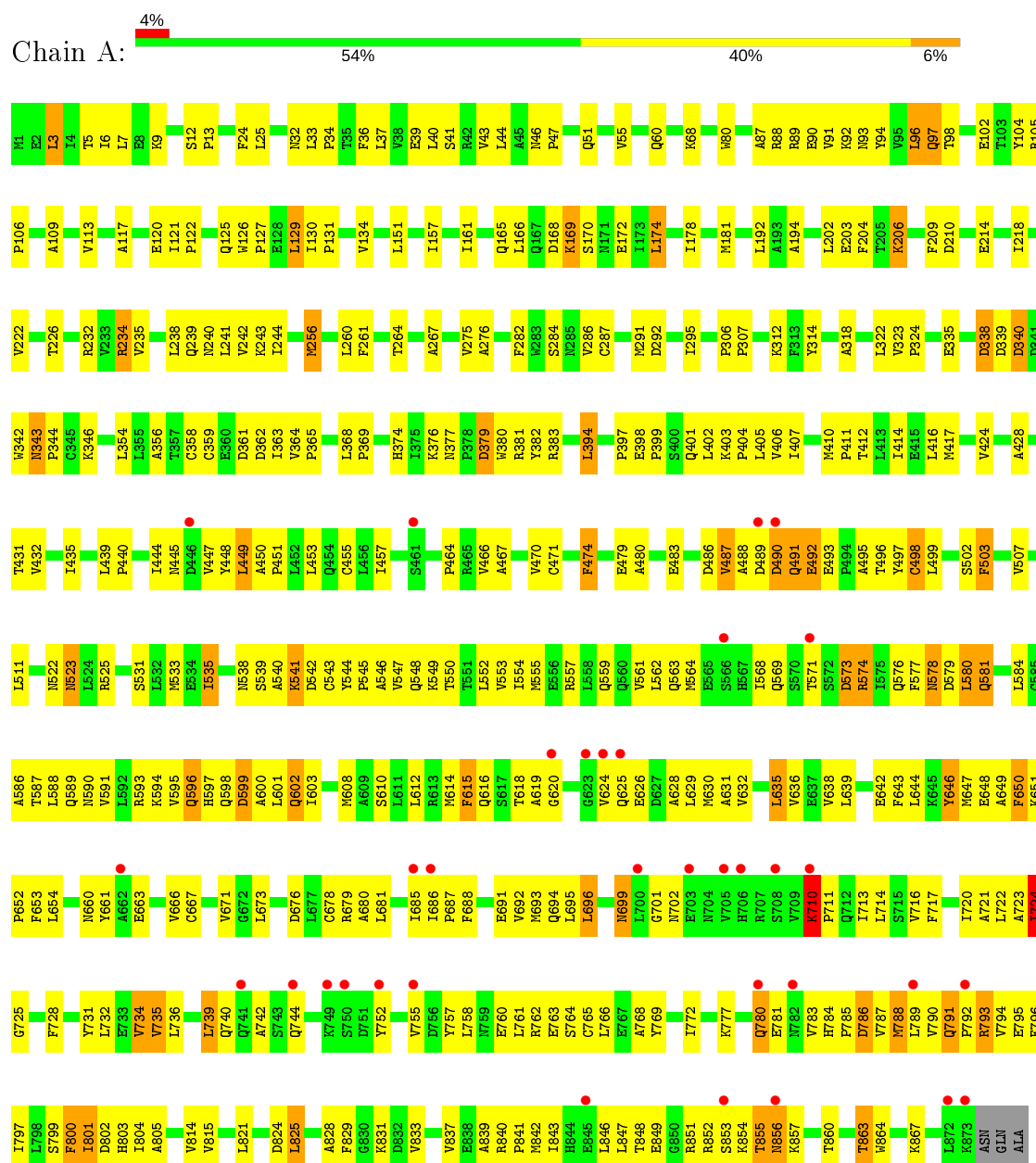
- Molecule 2 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	0	0	0
			344	210	73	61			
2	D	26	Total	C	N	O	0	0	0
			235	140	54	41			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Importin subunit beta-1



- Molecule 1: Importin subunit beta-1

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.65Å 101.73Å 101.96Å 90.00° 110.88° 90.00°	Depositor
Resolution (Å)	14.96 – 3.15 14.96 – 3.15	Depositor EDS
% Data completeness (in resolution range)	91.2 (14.96-3.15) 90.2 (14.96-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.264 , 0.313 0.253 , 0.305	Depositor DCC
R_{free} test set	1707 reflections (5.61%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 14.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14127	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.47% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/6893	0.40	0/9360
1	C	0.26	0/6875	0.46	5/9333 (0.1%)
2	B	0.19	0/348	0.33	0/458
2	D	0.19	0/236	0.32	0/309
All	All	0.26	0/14352	0.42	5/19460 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	545	PRO	N-CA-C	-9.06	88.56	112.10
1	C	496	THR	N-CA-C	5.72	126.44	111.00
1	C	446	ASP	N-CA-C	-5.46	96.25	111.00
1	C	543	CYS	CB-CA-C	-5.19	100.02	110.40
1	C	497	TYR	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6782	0	6781	414	0
1	C	6766	0	6767	478	0
2	B	344	0	359	24	0
2	D	235	0	244	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14127	0	14151	898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (898) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:HIS:CG	1:C:785:PRO:O	1.87	1.27
1:C:784:HIS:CD2	1:C:785:PRO:O	1.92	1.22
1:A:203:GLU:O	1:A:206:LYS:HE2	1.40	1.18
1:C:784:HIS:HB2	1:C:785:PRO:C	1.64	1.16
1:A:722:LEU:CD1	2:B:58:TYR:HE1	1.59	1.16
1:A:784:HIS:HE1	1:A:829:PHE:CZ	1.64	1.15
1:C:442:ALA:N	1:C:443:ALA:HB3	1.59	1.14
1:A:488:ALA:HB3	1:A:489:ASP:HA	1.17	1.13
1:C:442:ALA:H	1:C:443:ALA:HB3	1.00	1.12
1:A:722:LEU:CD1	2:B:58:TYR:CE1	2.32	1.11
1:A:487:VAL:N	1:A:488:ALA:HA	1.55	1.10
1:C:441:GLU:HA	1:C:444:ILE:HB	1.23	1.10
1:A:97:GLN:HE21	1:A:97:GLN:N	1.49	1.10
1:C:546:ALA:O	1:C:549:LYS:HB3	1.57	1.04
1:C:488:ALA:HB1	1:C:489:ASP:HB3	1.39	1.00
1:C:784:HIS:HB2	1:C:786:ASP:HB2	1.43	1.00
1:C:471:CYS:HA	1:C:474:PHE:CE1	1.97	0.99
1:A:784:HIS:CE1	1:A:829:PHE:CE2	2.50	0.98
1:C:544:TYR:HA	1:C:547:VAL:HB	1.47	0.97
1:A:495:ALA:HA	1:A:541:LYS:HG3	1.46	0.97
1:C:701:GLY:HA2	1:C:702:ASN:HB3	1.44	0.96
1:A:784:HIS:CE1	1:A:829:PHE:CZ	2.53	0.96
1:C:504:GLU:HA	1:C:507:VAL:HG22	1.45	0.96
1:C:429:ALA:HB1	1:C:477:LEU:HD11	1.45	0.96
1:C:433:GLY:HA3	1:C:477:LEU:CD2	1.96	0.96
1:A:722:LEU:HD13	2:B:58:TYR:CE1	1.98	0.95
1:C:429:ALA:HB1	1:C:477:LEU:CD1	1.97	0.95
1:C:784:HIS:CB	1:C:785:PRO:C	2.33	0.95
1:C:543:CYS:HB3	1:C:547:VAL:HG21	1.47	0.94
1:C:334:ASP:OD1	1:C:336:ASN:HB3	1.66	0.94
1:A:105:ARG:HB3	1:A:106:PRO:HD3	1.49	0.93
1:A:602:GLN:H	1:A:602:GLN:HE21	1.01	0.93
1:C:781:GLU:HG2	1:C:784:HIS:ND1	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:HIS:CB	1:C:785:PRO:O	2.16	0.93
1:A:90:GLU:O	1:A:94:TYR:HD2	1.51	0.93
1:A:488:ALA:CB	1:A:489:ASP:HA	1.85	0.93
1:A:780:GLN:HE21	1:A:780:GLN:H	1.10	0.92
1:A:722:LEU:HD12	2:B:58:TYR:HE1	1.31	0.92
1:C:543:CYS:O	1:C:547:VAL:HG23	1.67	0.92
1:C:596:GLN:HE21	1:C:596:GLN:H	1.11	0.91
1:C:105:ARG:HH21	1:C:189:ASN:HD22	1.14	0.91
1:C:702:ASN:CG	1:C:703:GLU:H	1.74	0.91
1:C:853:SER:HA	1:C:854:LYS:C	1.92	0.90
1:A:90:GLU:O	1:A:94:TYR:CD2	2.25	0.90
1:C:377:ASN:HD22	1:C:379:ASP:H	1.21	0.89
1:C:486:ASP:HB3	1:C:494:PRO:HG3	1.54	0.89
1:A:781:GLU:HG2	1:A:784:HIS:HA	1.55	0.88
1:C:596:GLN:NE2	1:C:596:GLN:H	1.69	0.88
1:C:433:GLY:CA	1:C:477:LEU:CD2	2.51	0.88
1:A:488:ALA:HB3	1:A:489:ASP:CA	2.04	0.87
1:A:854:LYS:HB3	1:A:855:THR:HA	1.57	0.87
1:C:543:CYS:O	1:C:547:VAL:CG2	2.22	0.86
1:C:784:HIS:CB	1:C:786:ASP:HB2	2.05	0.86
1:C:497:TYR:CD1	1:C:497:TYR:N	2.33	0.86
1:A:97:GLN:HE21	1:A:97:GLN:H	1.23	0.85
1:A:839:ALA:HB1	1:C:105:ARG:HG2	1.57	0.85
1:A:574:ARG:HA	1:A:574:ARG:HE	1.41	0.85
1:A:374:HIS:HA	1:A:377:ASN:HB2	1.58	0.84
1:C:442:ALA:CA	1:C:443:ALA:HB3	2.08	0.84
1:A:849:GLU:HA	1:A:852:ARG:HE	1.43	0.83
1:A:544:TYR:N	1:A:545:PRO:HD2	1.92	0.83
1:C:784:HIS:HB2	1:C:785:PRO:O	1.72	0.82
1:C:474:PHE:HA	1:C:477:LEU:HD12	1.61	0.82
1:C:781:GLU:HG3	1:C:782:ASN:H	1.45	0.82
1:C:433:GLY:HA3	1:C:477:LEU:HD23	1.59	0.81
1:A:722:LEU:HD13	2:B:58:TYR:CZ	2.14	0.81
1:C:701:GLY:CA	1:C:702:ASN:HB3	2.10	0.81
1:C:27:ARG:HG3	1:C:28:ALA:N	1.96	0.81
1:A:533:MET:HB2	1:A:590:ASN:HD22	1.46	0.81
1:A:399:PRO:HB3	1:A:403:LYS:HE3	1.63	0.80
1:C:527:SER:O	1:C:530:GLU:HG3	1.81	0.80
1:A:794:VAL:HA	1:A:797:ILE:HB	1.63	0.80
1:C:460:LEU:HA	1:C:474:PHE:CZ	2.17	0.80
1:A:97:GLN:NE2	1:A:97:GLN:N	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:LEU:HB3	1:C:532:LEU:HD21	1.64	0.78
1:A:671:VAL:HG12	1:A:716:VAL:HG21	1.65	0.78
1:C:450:ALA:HB3	1:C:451:PRO:HD3	1.64	0.78
1:C:495:ALA:O	1:C:540:ALA:HB1	1.83	0.77
1:A:786:ASP:HA	1:A:789:LEU:HD12	1.65	0.77
1:C:441:GLU:HA	1:C:444:ILE:CB	2.11	0.77
1:C:449:LEU:H	1:C:449:LEU:HD22	1.49	0.77
1:A:780:GLN:HE21	1:A:780:GLN:N	1.83	0.77
1:C:497:TYR:HD1	1:C:497:TYR:N	1.80	0.77
1:C:433:GLY:CA	1:C:477:LEU:HD22	2.16	0.76
1:C:784:HIS:HD2	1:C:785:PRO:HA	1.49	0.76
1:C:540:ALA:HB3	1:C:543:CYS:SG	2.25	0.76
1:A:488:ALA:CB	1:A:489:ASP:CA	2.64	0.76
1:C:445:ASN:O	1:C:447:VAL:HG23	1.86	0.75
1:A:97:GLN:NE2	1:A:97:GLN:H	1.82	0.75
1:C:433:GLY:N	1:C:477:LEU:HD22	2.01	0.75
1:C:448:TYR:C	1:C:451:PRO:HD2	2.07	0.75
1:C:503:PHE:HE2	1:C:547:VAL:HG21	1.51	0.75
1:C:784:HIS:CD2	1:C:785:PRO:HA	2.21	0.75
1:C:561:VAL:HG11	1:C:584:LEU:HD13	1.69	0.75
1:C:531:SER:O	1:C:535:ILE:HG22	1.86	0.75
1:C:488:ALA:HB1	1:C:489:ASP:CB	2.14	0.75
1:A:602:GLN:H	1:A:602:GLN:NE2	1.82	0.74
1:C:784:HIS:HB2	1:C:786:ASP:CB	2.17	0.74
1:C:445:ASN:ND2	1:C:448:TYR:HE2	1.86	0.74
1:C:442:ALA:H	1:C:443:ALA:CB	1.91	0.74
1:A:487:VAL:H	1:A:488:ALA:HA	1.48	0.73
1:A:781:GLU:CG	1:A:784:HIS:HA	2.17	0.73
1:A:361:ASP:HB2	1:A:401:GLN:HE22	1.54	0.73
1:C:449:LEU:O	1:C:453:LEU:HB2	1.87	0.73
1:C:442:ALA:N	1:C:443:ALA:CB	2.48	0.73
1:A:525:ARG:HH22	1:A:579:ASP:HB3	1.52	0.73
1:C:619:ALA:HB1	1:C:620:GLY:HA2	1.70	0.73
1:C:27:ARG:HG3	1:C:28:ALA:H	1.53	0.73
1:C:702:ASN:OD1	1:C:705:VAL:HB	1.89	0.73
1:C:785:PRO:HG2	1:C:786:ASP:H	1.54	0.72
1:C:105:ARG:HB3	1:C:106:PRO:HD3	1.71	0.72
1:C:447:VAL:HG12	1:C:448:TYR:H	1.54	0.72
1:C:543:CYS:O	1:C:547:VAL:CB	2.37	0.72
1:A:87:ALA:O	1:A:91:VAL:HG23	1.88	0.72
1:A:589:GLN:HB3	1:A:593:ARG:HH12	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ARG:HD3	1:A:804:ILE:HG12	1.70	0.71
1:C:588:LEU:HD21	1:C:611:LEU:HD11	1.72	0.71
1:A:650:PHE:CZ	1:A:673:LEU:HD11	2.25	0.71
1:A:649:ALA:O	1:A:653:PHE:HD2	1.73	0.71
1:C:419:ASP:O	1:C:425:ARG:HD2	1.90	0.71
1:A:497:TYR:CE2	1:A:499:LEU:HB2	2.24	0.71
1:C:395:GLU:HB2	1:C:438:LEU:HD13	1.71	0.71
1:C:784:HIS:CD2	1:C:785:PRO:C	2.63	0.71
1:A:854:LYS:HD2	1:A:854:LYS:H	1.55	0.71
1:C:589:GLN:HG3	1:C:590:ASN:H	1.55	0.71
1:A:788:MET:SD	1:A:791:GLN:HG2	2.30	0.71
1:C:163:PRO:HA	1:C:204:PHE:HE2	1.54	0.71
1:C:360:GLU:O	1:C:363:ILE:HG22	1.90	0.71
1:C:534:GLU:HA	1:C:537:LYS:HB2	1.72	0.71
1:A:487:VAL:N	1:A:488:ALA:CA	2.46	0.70
1:C:589:GLN:HA	1:C:634:THR:HG21	1.74	0.70
1:C:784:HIS:CG	1:C:785:PRO:C	2.62	0.70
1:C:445:ASN:C	1:C:446:ASP:OD2	2.30	0.70
1:C:702:ASN:CG	1:C:703:GLU:N	2.45	0.70
1:C:785:PRO:CG	1:C:786:ASP:H	2.05	0.70
1:C:403:LYS:HZ2	1:C:441:GLU:HG3	1.56	0.70
1:A:523:ASN:O	1:A:523:ASN:CG	2.30	0.70
1:C:130:ILE:HD12	1:C:130:ILE:H	1.56	0.70
1:A:650:PHE:HE2	1:A:673:LEU:HD21	1.56	0.70
1:A:90:GLU:CG	1:A:94:TYR:HE2	2.05	0.69
1:C:336:ASN:OD1	1:C:336:ASN:C	2.30	0.69
1:C:784:HIS:HB2	1:C:786:ASP:N	2.07	0.69
1:A:497:TYR:HE2	1:A:499:LEU:HB2	1.56	0.69
1:C:444:ILE:C	1:C:446:ASP:OD2	2.30	0.69
1:A:732:LEU:O	1:A:736:LEU:HG	1.92	0.69
1:A:555:MET:O	1:A:559:GLN:HG2	1.93	0.69
1:C:417:MET:HE1	1:C:429:ALA:HB2	1.75	0.69
1:A:594:LYS:O	1:A:595:VAL:HG13	1.92	0.69
1:C:702:ASN:HA	1:C:705:VAL:HG23	1.75	0.69
1:C:429:ALA:CB	1:C:477:LEU:HD11	2.19	0.69
1:C:781:GLU:HG3	1:C:782:ASN:N	2.08	0.68
1:A:632:VAL:HG11	1:A:650:PHE:CE2	2.28	0.68
1:C:333:GLN:HG3	1:C:345:CYS:SG	2.34	0.68
1:C:624:VAL:H	1:C:656:ILE:HD11	1.59	0.68
1:A:589:GLN:NE2	1:A:630:MET:HB3	2.08	0.68
1:A:795:GLU:HB2	1:C:104:TYR:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:GLU:O	1:C:534:GLU:HG2	1.94	0.68
1:A:723:ALA:O	1:A:724:ILE:HG13	1.93	0.68
1:C:457:ILE:HA	1:C:460:LEU:HB2	1.74	0.68
1:C:503:PHE:HE2	1:C:547:VAL:CG2	2.07	0.67
1:C:700:LEU:O	1:C:702:ASN:HB3	1.93	0.67
1:C:697:LEU:HD23	1:C:700:LEU:CD1	2.24	0.67
1:A:134:VAL:HG21	1:A:172:GLU:HG3	1.76	0.67
1:A:161:ILE:HG12	1:A:166:LEU:HG	1.76	0.67
1:C:785:PRO:HG2	1:C:786:ASP:N	2.08	0.67
1:A:780:GLN:NE2	1:A:780:GLN:H	1.87	0.67
1:C:377:ASN:ND2	1:C:379:ASP:H	1.93	0.66
1:A:589:GLN:HB3	1:A:593:ARG:NH1	2.11	0.66
1:C:442:ALA:HB3	1:C:443:ALA:CB	2.25	0.66
1:C:544:TYR:CA	1:C:547:VAL:HB	2.25	0.66
1:A:93:ASN:OD1	1:A:93:ASN:C	2.34	0.66
1:C:526:SER:H	1:C:529:TYR:HB2	1.60	0.66
1:C:460:LEU:HA	1:C:474:PHE:CE2	2.31	0.66
1:C:751:ASP:O	1:C:755:VAL:HG23	1.96	0.66
1:C:79:ARG:O	1:C:83:ILE:HG13	1.95	0.66
1:A:624:VAL:HG12	1:A:626:GLU:H	1.61	0.65
1:A:97:GLN:HE21	1:A:97:GLN:CA	2.08	0.65
1:A:93:ASN:O	1:A:97:GLN:NE2	2.29	0.65
1:A:824:ASP:HB3	2:B:63:ARG:HD3	1.78	0.65
1:A:90:GLU:HG2	1:A:94:TYR:HE2	1.60	0.65
1:C:453:LEU:HG	1:C:498:CYS:SG	2.37	0.65
1:C:546:ALA:C	1:C:549:LYS:HB3	2.15	0.65
1:C:784:HIS:CD2	1:C:785:PRO:CA	2.79	0.65
1:C:445:ASN:OD1	1:C:446:ASP:N	2.30	0.65
1:A:491:GLN:HG2	1:A:492:GLU:HG2	1.79	0.65
1:A:710:LYS:HB3	1:A:761:LEU:HD13	1.77	0.65
1:C:359:CYS:SG	1:C:362:ASP:HB2	2.37	0.65
1:A:440:PRO:HB3	1:A:480:ALA:HB1	1.77	0.65
1:C:445:ASN:ND2	1:C:446:ASP:O	2.30	0.65
1:C:543:CYS:O	1:C:547:VAL:HB	1.95	0.65
1:C:446:ASP:N	1:C:446:ASP:OD2	2.29	0.65
1:C:550:THR:O	1:C:554:ILE:HB	1.97	0.65
1:A:840:ARG:HH11	1:A:843:ILE:HD11	1.61	0.65
1:A:722:LEU:HD13	2:B:58:TYR:OH	1.96	0.64
1:A:632:VAL:HG11	1:A:650:PHE:CZ	2.32	0.64
1:A:562:LEU:HD22	1:A:614:MET:HG3	1.79	0.64
1:A:736:LEU:HD23	1:A:769:TYR:OH	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ALA:CB	1:A:490:ASP:H	2.10	0.64
1:C:452:LEU:O	1:C:456:LEU:N	2.27	0.64
1:A:710:LYS:HD3	1:A:757:TYR:OH	1.97	0.64
1:A:856:ASN:O	1:A:857:LYS:HB3	1.96	0.64
1:C:442:ALA:CA	1:C:443:ALA:CB	2.76	0.64
1:A:722:LEU:HD12	2:B:58:TYR:CE1	2.20	0.64
1:C:785:PRO:CG	1:C:786:ASP:N	2.61	0.64
1:A:523:ASN:O	1:A:523:ASN:ND2	2.30	0.63
1:A:790:VAL:O	1:A:794:VAL:HG23	1.98	0.63
1:A:801:ILE:HD13	1:A:804:ILE:HD12	1.79	0.63
1:C:455:CYS:HA	1:C:458:GLU:HB2	1.80	0.63
1:C:468:SER:O	1:C:471:CYS:HB2	1.98	0.63
1:C:493:GLU:OE2	1:C:540:ALA:HA	1.99	0.63
1:A:792:PRO:HG2	1:C:11:VAL:HG11	1.81	0.63
1:C:356:ALA:O	1:C:360:GLU:HG2	1.99	0.63
1:A:394:LEU:HD11	1:A:435:ILE:HG12	1.80	0.63
1:C:185:GLU:O	1:C:191:LYS:HD2	1.99	0.62
1:C:697:LEU:HD23	1:C:700:LEU:HD12	1.80	0.62
1:C:537:LYS:HD3	1:C:538:ASN:HB2	1.81	0.62
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.82	0.62
1:A:612:LEU:HA	1:A:615:PHE:HB2	1.80	0.62
1:C:395:GLU:HB2	1:C:438:LEU:CD1	2.28	0.62
1:C:442:ALA:HB3	1:C:443:ALA:HB2	1.82	0.62
1:A:569:GLN:HB2	1:A:573:ASP:CG	2.20	0.62
1:C:105:ARG:HH21	1:C:189:ASN:ND2	1.93	0.62
1:C:785:PRO:CD	1:C:786:ASP:H	2.12	0.62
1:A:784:HIS:ND1	1:A:829:PHE:CE2	2.66	0.62
1:C:72:ILE:HD12	1:C:76:TYR:CD1	2.35	0.62
1:A:383:ARG:NH1	1:A:424:VAL:HG21	2.15	0.62
1:C:510:LEU:HD23	1:C:532:LEU:HG	1.81	0.62
1:C:784:HIS:HD2	1:C:785:PRO:CA	2.12	0.62
1:A:679:ARG:HH21	2:B:55:ARG:HG2	1.65	0.61
1:C:454:GLN:O	1:C:458:GLU:HB2	1.99	0.61
1:A:731:TYR:O	1:A:734:VAL:HG22	2.00	0.61
1:C:554:ILE:HG12	1:C:591:VAL:HB	1.81	0.61
1:C:807:ASP:HB3	1:C:809:ASP:OD1	2.00	0.61
1:A:151:LEU:HD13	1:A:194:ALA:HB2	1.82	0.61
1:A:574:ARG:HE	1:A:574:ARG:CA	2.12	0.61
1:C:360:GLU:O	1:C:397:PRO:HG3	2.01	0.61
1:A:450:ALA:HB3	1:A:451:PRO:HD3	1.83	0.61
1:A:805:ALA:HB2	1:A:846:LEU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ALA:O	1:C:477:LEU:HG	2.00	0.61
1:A:649:ALA:O	1:A:652:PRO:HD2	2.01	0.61
1:A:449:LEU:HG	1:A:498:CYS:SG	2.41	0.61
2:B:60:ASN:ND2	2:B:63:ARG:HH21	1.99	0.61
1:C:749:LYS:HD3	1:C:749:LYS:H	1.65	0.61
2:D:41:SER:HA	2:D:44:ARG:HD2	1.81	0.61
2:B:60:ASN:HD21	2:B:63:ARG:HH21	1.48	0.60
1:C:372:LYS:HA	1:C:372:LYS:HE2	1.82	0.60
1:A:410:MET:O	1:A:414:ILE:HG13	2.01	0.60
1:A:488:ALA:HB3	1:A:490:ASP:H	1.67	0.60
1:A:685:ILE:HG23	1:A:688:PHE:HD1	1.66	0.60
1:A:728:PHE:HD1	1:A:731:TYR:HE1	1.49	0.60
1:C:256:MET:HA	1:C:260:LEU:HB2	1.83	0.60
1:C:343:ASN:HB2	1:C:344:PRO:HD2	1.82	0.60
1:C:399:PRO:O	1:C:403:LYS:HG3	2.02	0.60
1:C:762:ARG:HB3	1:C:804:ILE:HD11	1.84	0.60
1:A:651:LYS:HB3	1:A:652:PRO:HD3	1.82	0.60
1:A:5:THR:O	1:A:9:LYS:HG2	2.02	0.60
1:C:595:VAL:HG12	1:C:597:HIS:HD2	1.67	0.60
1:A:343:ASN:ND2	1:A:346:LYS:H	2.00	0.60
1:A:544:TYR:N	1:A:545:PRO:CD	2.63	0.60
1:C:208:ASN:N	1:C:208:ASN:HD22	2.00	0.60
1:C:586:ALA:C	1:C:588:LEU:H	2.05	0.60
1:A:650:PHE:O	1:A:654:LEU:HB3	2.02	0.59
1:A:568:ILE:HG21	1:A:574:ARG:HG2	1.84	0.59
1:A:104:TYR:HD2	1:A:106:PRO:O	1.86	0.59
1:A:802:ASP:OD2	1:A:842:MET:HB2	2.03	0.59
1:C:541:LYS:O	1:C:545:PRO:HD2	2.01	0.59
1:A:847:LEU:O	1:A:851:ARG:HG3	2.02	0.59
1:C:397:PRO:HB2	1:C:402:LEU:CD2	2.31	0.59
1:A:736:LEU:HD13	1:A:793:ARG:HG3	1.83	0.59
1:C:374:HIS:HB3	1:C:382:TYR:HB3	1.83	0.59
1:C:503:PHE:HE1	1:C:536:VAL:HG12	1.68	0.59
1:C:596:GLN:N	1:C:596:GLN:HE21	1.93	0.59
1:A:593:ARG:HH21	2:B:47:LEU:HD23	1.67	0.59
1:C:539:SER:H	1:C:594:LYS:HE3	1.68	0.59
1:A:374:HIS:O	1:A:383:ARG:HA	2.03	0.59
1:A:735:VAL:O	1:A:739:LEU:HD22	2.02	0.59
1:A:829:PHE:O	1:A:833:VAL:HG21	2.03	0.59
1:C:72:ILE:HD12	1:C:76:TYR:HD1	1.67	0.59
1:C:174:LEU:HD12	1:C:208:ASN:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ALA:O	1:A:635:LEU:HD22	2.04	0.58
1:C:500:SER:HA	1:C:543:CYS:SG	2.42	0.58
1:A:696:LEU:HD13	1:A:713:ILE:HG23	1.84	0.58
1:A:593:ARG:NH2	2:B:47:LEU:HD23	2.18	0.58
1:C:105:ARG:NH2	1:C:189:ASN:HD22	1.93	0.58
1:A:777:LYS:NZ	1:A:829:PHE:CE2	2.71	0.58
1:C:588:LEU:HD11	1:C:607:VAL:HG11	1.86	0.58
1:C:506:ILE:O	1:C:510:LEU:HB2	2.03	0.58
1:A:784:HIS:CE1	1:A:829:PHE:HE2	2.19	0.58
1:C:161:ILE:HG21	1:C:166:LEU:HG	1.86	0.58
1:C:759:ASN:N	1:C:759:ASN:HD22	2.02	0.58
1:A:588:LEU:HA	1:A:591:VAL:HG22	1.85	0.58
1:A:591:VAL:O	1:A:595:VAL:HG22	2.03	0.58
1:C:573:ASP:O	1:C:577:PHE:HB2	2.03	0.58
1:C:685:ILE:HD13	1:C:685:ILE:O	2.04	0.58
1:A:335:GLU:HG2	1:A:380:TRP:HH2	1.69	0.58
1:A:600:ALA:HB1	1:A:638:VAL:HG11	1.85	0.58
1:C:334:ASP:CG	1:C:336:ASN:HB3	2.24	0.58
1:A:497:TYR:CD1	1:A:540:ALA:HB2	2.38	0.57
1:C:543:CYS:HB3	1:C:547:VAL:CG2	2.28	0.57
1:A:787:VAL:HG23	1:A:788:MET:H	1.69	0.57
1:C:439:LEU:C	1:C:441:GLU:H	2.07	0.57
1:C:483:GLU:O	1:C:487:VAL:HG22	2.04	0.57
1:A:555:MET:HE1	1:A:603:ILE:HG13	1.87	0.57
1:C:548:GLN:O	1:C:552:LEU:HG	2.05	0.57
1:C:580:LEU:O	1:C:584:LEU:HB2	2.04	0.57
1:C:336:ASN:CG	1:C:337:ASP:N	2.57	0.57
1:C:397:PRO:HB2	1:C:402:LEU:HD23	1.85	0.57
1:C:442:ALA:CB	1:C:443:ALA:HB3	2.33	0.57
1:C:504:GLU:O	1:C:508:GLN:HG2	2.04	0.57
1:C:506:ILE:HA	1:C:509:LYS:HB3	1.86	0.57
1:A:711:PRO:HG2	1:A:760:GLU:OE1	2.04	0.57
1:A:121:ILE:HD11	1:A:129:LEU:HD23	1.87	0.57
1:A:562:LEU:HD12	1:A:610:SER:HB3	1.85	0.57
1:C:503:PHE:O	1:C:507:VAL:HG13	2.05	0.57
1:A:412:THR:O	1:A:416:LEU:HG	2.05	0.57
1:C:72:ILE:HG23	1:C:76:TYR:CD1	2.40	0.57
1:C:445:ASN:O	1:C:447:VAL:CG2	2.53	0.56
1:A:486:ASP:C	1:A:488:ALA:HA	2.24	0.56
1:A:511:LEU:HD22	1:A:557:ARG:HH12	1.70	0.56
1:A:736:LEU:HD22	1:A:793:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:SER:HA	1:A:854:LYS:C	2.25	0.56
1:C:403:LYS:HB2	1:C:404:PRO:HD3	1.87	0.56
1:A:202:LEU:HD12	1:A:243:LYS:HD3	1.87	0.56
1:A:681:LEU:HD12	1:A:685:ILE:HG12	1.86	0.56
1:C:445:ASN:C	1:C:447:VAL:HG23	2.25	0.56
1:A:596:GLN:HG2	1:A:598:GLN:HG3	1.88	0.56
1:A:857:LYS:HA	1:A:860:THR:HG23	1.88	0.56
1:C:332:LYS:HA	1:C:381:ARG:HH21	1.70	0.56
1:C:445:ASN:ND2	1:C:448:TYR:CE2	2.65	0.56
1:C:807:ASP:O	1:C:810:HIS:HD2	1.88	0.56
1:A:728:PHE:HA	1:A:731:TYR:CD1	2.40	0.56
1:C:28:ALA:HA	1:C:31:GLU:HB3	1.87	0.56
1:A:784:HIS:HB2	1:A:785:PRO:HA	1.88	0.56
1:A:343:ASN:HB2	1:A:344:PRO:HD2	1.87	0.56
1:C:497:TYR:CD1	1:C:498:CYS:N	2.75	0.55
1:A:740:GLN:HB2	1:A:793:ARG:NH2	2.22	0.55
1:A:691:GLU:O	1:A:695:LEU:HB2	2.06	0.55
1:A:643:PHE:O	1:A:647:MET:HG2	2.06	0.55
1:C:403:LYS:HZ2	1:C:441:GLU:CG	2.19	0.55
1:C:482:TYR:CE1	1:C:494:PRO:HD2	2.42	0.55
1:A:466:VAL:O	1:A:470:VAL:HG23	2.07	0.55
1:A:511:LEU:HD13	1:A:553:VAL:HG11	1.87	0.55
1:A:554:ILE:HG23	1:A:584:LEU:HD22	1.89	0.55
1:A:837:VAL:HG13	1:A:843:ILE:HG21	1.87	0.55
1:A:41:SER:HB2	1:A:94:TYR:HB2	1.88	0.55
1:A:676:ASP:HA	1:A:679:ARG:NH1	2.22	0.55
1:C:545:PRO:O	1:C:546:ALA:HB3	2.05	0.55
1:A:667:CYS:O	1:A:671:VAL:HG23	2.06	0.55
1:A:716:VAL:O	1:A:716:VAL:HG12	2.07	0.55
1:C:449:LEU:HD12	1:C:453:LEU:HD23	1.88	0.55
1:C:849:GLU:HA	1:C:852:ARG:NH2	2.21	0.55
1:A:55:VAL:HG21	1:A:104:TYR:CD1	2.42	0.55
1:A:591:VAL:O	1:A:595:VAL:HG13	2.07	0.55
1:C:414:ILE:HG12	1:C:452:LEU:HG	1.89	0.54
1:C:488:ALA:CB	1:C:489:ASP:HB3	2.25	0.54
1:A:762:ARG:O	1:A:766:LEU:HG	2.06	0.54
1:A:856:ASN:ND2	1:A:856:ASN:H	2.03	0.54
1:C:331:THR:HG21	1:C:382:TYR:CZ	2.42	0.54
1:C:495:ALA:HB1	1:C:541:LYS:HG3	1.88	0.54
1:C:547:VAL:C	1:C:550:THR:H	2.11	0.54
1:A:364:VAL:HB	1:A:365:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:O	1:C:157:ILE:HG13	2.07	0.54
1:A:88:ARG:HH22	1:A:125:GLN:NE2	2.04	0.54
1:C:182:ARG:HG3	1:C:184:GLU:HG2	1.87	0.54
1:C:496:THR:HB	1:C:542:ASP:HB2	1.89	0.54
1:C:774:GLN:NE2	2:D:63:ARG:HG2	2.23	0.54
1:A:323:VAL:HB	1:A:324:PRO:HD3	1.89	0.54
1:A:495:ALA:O	1:A:540:ALA:HB1	2.07	0.54
1:A:711:PRO:HA	1:A:764:SER:HB3	1.90	0.54
1:C:433:GLY:N	1:C:477:LEU:CD2	2.68	0.54
1:A:226:THR:O	1:A:234:ARG:HD2	2.07	0.54
1:C:429:ALA:HB1	1:C:477:LEU:HD12	1.87	0.54
1:C:563:GLN:HG3	1:C:564:MET:N	2.23	0.54
1:C:702:ASN:HA	1:C:705:VAL:CG2	2.38	0.54
1:C:791:GLN:HB3	1:C:792:PRO:HD3	1.89	0.54
1:A:356:ALA:HB2	1:A:363:ILE:HD13	1.89	0.54
1:C:403:LYS:HZ2	1:C:441:GLU:CB	2.21	0.54
1:A:444:ILE:HG22	1:A:444:ILE:O	2.07	0.53
1:A:648:GLU:O	1:A:652:PRO:HD3	2.09	0.53
1:C:543:CYS:C	1:C:547:VAL:HB	2.28	0.53
1:C:651:LYS:HB3	1:C:652:PRO:HD3	1.90	0.53
1:C:702:ASN:O	1:C:703:GLU:HB2	2.08	0.53
1:C:847:LEU:O	1:C:851:ARG:HG3	2.08	0.53
1:C:534:GLU:HA	1:C:537:LYS:CB	2.38	0.53
1:C:134:VAL:HG22	1:C:176:ALA:HB2	1.89	0.53
1:A:444:ILE:HG23	1:A:449:LEU:HD21	1.90	0.53
1:A:569:GLN:OE1	1:A:573:ASP:HB3	2.08	0.53
1:A:636:VAL:CG1	1:A:680:ALA:HB2	2.39	0.53
1:C:438:LEU:O	1:C:440:PRO:HD3	2.09	0.53
1:C:452:LEU:O	1:C:452:LEU:HD23	2.09	0.53
1:C:462:ALA:C	1:C:467:ALA:HB1	2.29	0.53
1:A:157:ILE:O	1:A:161:ILE:HB	2.09	0.53
1:A:203:GLU:O	1:A:206:LYS:CE	2.34	0.53
1:C:516:ARG:HD3	1:C:524:LEU:HD11	1.91	0.53
1:C:853:SER:HA	1:C:854:LYS:O	2.09	0.53
1:A:51:GLN:O	1:A:55:VAL:HG23	2.09	0.53
1:A:763:GLU:HB2	1:A:814:VAL:HG22	1.91	0.53
1:A:589:GLN:HE22	1:A:630:MET:HB3	1.74	0.53
1:C:429:ALA:C	1:C:477:LEU:HD11	2.29	0.53
1:A:256:MET:HA	1:A:260:LEU:HB2	1.92	0.52
1:A:860:THR:O	1:A:863:THR:HG22	2.09	0.52
1:C:699:ASN:O	1:C:702:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:ALA:O	1:C:822:ILE:HG12	2.10	0.52
1:A:130:ILE:HG13	1:A:169:LYS:HG2	1.90	0.52
1:A:264:THR:HG21	1:A:282:PHE:CE2	2.44	0.52
1:C:433:GLY:CA	1:C:477:LEU:HD23	2.29	0.52
1:C:529:TYR:CD2	1:C:583:LEU:HD11	2.44	0.52
1:C:531:SER:C	1:C:533:MET:H	2.13	0.52
1:A:453:LEU:O	1:A:457:ILE:HG12	2.08	0.52
1:A:599:ASP:O	1:A:603:ILE:HD13	2.10	0.52
1:A:848:THR:O	1:A:852:ARG:HG3	2.10	0.52
1:C:449:LEU:CA	1:C:453:LEU:HB2	2.39	0.52
1:C:531:SER:O	1:C:535:ILE:N	2.36	0.52
1:A:491:GLN:HG2	1:A:492:GLU:N	2.24	0.52
1:A:784:HIS:HE1	1:A:829:PHE:HZ	1.40	0.52
1:C:181:MET:CE	1:C:198:LEU:HD22	2.40	0.52
1:A:721:ALA:HA	1:A:728:PHE:CZ	2.44	0.52
1:C:40:LEU:HB2	1:C:61:ILE:HD11	1.92	0.52
1:C:445:ASN:CG	1:C:446:ASP:N	2.63	0.52
1:A:503:PHE:CZ	1:A:546:ALA:HB3	2.45	0.52
1:C:488:ALA:HB1	1:C:489:ASP:CA	2.39	0.52
1:C:502:SER:O	1:C:506:ILE:HD11	2.09	0.52
1:C:781:GLU:HG2	1:C:784:HIS:CE1	2.45	0.52
1:C:700:LEU:C	1:C:702:ASN:HB3	2.30	0.51
1:A:453:LEU:HD21	1:A:499:LEU:HD22	1.92	0.51
1:A:608:MET:HG2	1:A:646:TYR:CD2	2.46	0.51
1:A:768:ALA:O	1:A:772:ILE:HG13	2.10	0.51
1:A:713:ILE:HB	1:A:714:LEU:HD12	1.92	0.51
1:C:375:ILE:HD11	1:C:416:LEU:HD11	1.92	0.51
1:C:61:ILE:HG22	1:C:65:LEU:HD11	1.92	0.51
1:C:686:ILE:HD13	1:C:727:GLU:HG3	1.92	0.51
1:C:710:LYS:HB3	1:C:711:PRO:HD3	1.92	0.51
1:A:368:LEU:HB2	1:A:369:PRO:HD3	1.93	0.51
1:C:364:VAL:HB	1:C:365:PRO:HD3	1.93	0.51
1:C:442:ALA:HB3	1:C:443:ALA:HB3	1.91	0.51
1:A:571:THR:C	1:A:573:ASP:H	2.14	0.51
1:A:92:LYS:O	1:A:96:LEU:HD22	2.10	0.51
1:C:248:TYR:O	1:C:252:MET:HG2	2.10	0.51
1:A:6:ILE:HG21	1:A:24:PHE:HD1	1.75	0.51
1:C:137:VAL:HG11	1:C:176:ALA:O	2.10	0.51
1:C:449:LEU:HA	1:C:453:LEU:HD23	1.92	0.51
1:C:645:LYS:HD3	1:C:645:LYS:C	2.31	0.51
1:C:701:GLY:CA	1:C:702:ASN:CB	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:ILE:HG22	1:A:728:PHE:CZ	2.46	0.51
1:C:222:VAL:O	1:C:226:THR:HG23	2.10	0.51
1:C:399:PRO:HB3	1:C:403:LYS:NZ	2.26	0.51
1:C:80:TRP:CE2	1:C:88:ARG:HD2	2.46	0.51
1:A:444:ILE:HG23	1:A:449:LEU:CD2	2.41	0.51
1:A:784:HIS:ND1	1:A:829:PHE:HE2	2.07	0.51
1:A:805:ALA:CB	1:A:846:LEU:HB2	2.40	0.51
1:C:450:ALA:N	1:C:451:PRO:CD	2.74	0.51
1:C:526:SER:N	1:C:529:TYR:HB2	2.24	0.51
1:C:163:PRO:HB3	1:C:748:ASP:OD2	2.11	0.50
1:C:7:LEU:HD13	1:C:57:ALA:HB2	1.92	0.50
1:A:650:PHE:CE2	1:A:673:LEU:HD21	2.43	0.50
1:C:443:ALA:H	1:C:446:ASP:HA	1.75	0.50
1:C:443:ALA:H	1:C:446:ASP:CA	2.24	0.50
1:C:474:PHE:CD2	1:C:475:SER:N	2.79	0.50
1:C:785:PRO:O	1:C:786:ASP:HB2	2.12	0.50
1:A:368:LEU:HD21	1:A:405:LEU:HD13	1.93	0.50
1:C:226:THR:O	1:C:234:ARG:HD3	2.11	0.50
1:C:445:ASN:CG	1:C:446:ASP:O	2.49	0.50
1:A:394:LEU:CD1	1:A:435:ILE:HG12	2.42	0.50
1:C:540:ALA:O	1:C:543:CYS:HB2	2.10	0.50
1:C:583:LEU:HB2	2:D:43:ARG:NH2	2.26	0.50
1:A:287:CYS:O	1:A:291:MET:HG3	2.12	0.50
1:C:337:ASP:OD1	1:C:337:ASP:C	2.49	0.50
1:C:343:ASN:HD21	1:C:346:LYS:CD	2.25	0.50
1:C:403:LYS:HZ2	1:C:441:GLU:HB2	1.77	0.50
1:C:65:LEU:HD13	1:C:116:ILE:HG13	1.94	0.50
1:A:431:THR:O	1:A:435:ILE:HG13	2.12	0.50
1:A:739:LEU:HB3	1:A:765:CYS:SG	2.51	0.50
1:C:549:LYS:HG2	1:C:549:LYS:O	2.12	0.50
1:A:722:LEU:HD11	2:B:58:TYR:CE1	2.43	0.50
1:A:523:ASN:ND2	1:A:523:ASN:C	2.65	0.50
2:B:48:LEU:O	2:B:48:LEU:HD23	2.12	0.50
1:C:126:TRP:N	1:C:127:PRO:HD3	2.26	0.50
1:C:547:VAL:HG13	1:C:550:THR:HB	1.93	0.50
1:C:547:VAL:O	1:C:550:THR:HB	2.12	0.50
1:C:588:LEU:CD2	1:C:611:LEU:HD11	2.41	0.50
1:C:784:HIS:CB	1:C:785:PRO:CA	2.89	0.50
2:D:48:LEU:HD22	2:D:52:LYS:HD2	1.94	0.50
1:A:90:GLU:HG3	1:A:94:TYR:HE2	1.75	0.50
1:C:297:ALA:HA	1:C:300:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PHE:CZ	1:C:40:LEU:HD11	2.46	0.50
1:C:496:THR:OG1	1:C:496:THR:O	2.30	0.50
1:C:749:LYS:H	1:C:749:LYS:CD	2.24	0.50
1:C:856:ASN:O	1:C:857:LYS:HB2	2.12	0.50
1:A:639:LEU:HB3	1:A:642:GLU:HB2	1.93	0.49
2:B:60:ASN:HA	2:B:63:ARG:HB2	1.94	0.49
1:C:491:GLN:HE21	1:C:491:GLN:HA	1.77	0.49
1:C:72:ILE:HB	1:C:703:GLU:OE1	2.10	0.49
1:A:403:LYS:O	1:A:407:ILE:HG12	2.12	0.49
1:C:166:LEU:HD13	1:C:166:LEU:O	2.12	0.49
1:C:487:VAL:HG23	1:C:487:VAL:O	2.11	0.49
1:C:697:LEU:HD23	1:C:700:LEU:HD11	1.92	0.49
1:A:615:PHE:HA	1:A:618:THR:HG22	1.94	0.49
1:C:323:VAL:HB	1:C:324:PRO:HD3	1.94	0.49
1:C:460:LEU:HB3	1:C:506:ILE:HG21	1.94	0.49
1:A:740:GLN:HB2	1:A:793:ARG:HH22	1.78	0.49
1:A:821:LEU:O	1:A:825:LEU:HB2	2.12	0.49
1:C:496:THR:HB	1:C:542:ASP:CB	2.42	0.49
1:C:543:CYS:O	1:C:545:PRO:O	2.31	0.49
1:C:632:VAL:O	1:C:636:VAL:HG23	2.13	0.49
1:C:686:ILE:HB	1:C:687:PRO:HD3	1.94	0.49
1:A:117:ALA:O	1:A:121:ILE:HG12	2.13	0.49
1:A:488:ALA:HB3	1:A:490:ASP:N	2.26	0.49
1:A:531:SER:O	1:A:535:ILE:HB	2.12	0.49
1:A:93:ASN:OD1	1:A:93:ASN:O	2.29	0.49
1:C:565:GLU:HG3	1:C:618:THR:HB	1.95	0.49
1:C:178:ILE:HG21	1:C:217:PHE:CE2	2.48	0.49
1:A:105:ARG:HB3	1:A:106:PRO:CD	2.32	0.49
1:A:686:ILE:N	1:A:687:PRO:HD2	2.27	0.49
1:A:678:CYS:SG	1:A:720:ILE:HD13	2.52	0.49
1:A:789:LEU:HD22	1:C:18:LEU:HD11	1.94	0.49
1:C:497:TYR:HD1	1:C:498:CYS:H	1.56	0.49
1:A:122:PRO:HA	1:A:165:GLN:NE2	2.28	0.49
1:A:234:ARG:NH2	1:A:275:VAL:HG11	2.28	0.49
1:A:497:TYR:HE1	1:A:539:SER:HA	1.77	0.49
1:A:93:ASN:OD1	1:A:97:GLN:OE1	2.30	0.49
1:C:482:TYR:CG	1:C:538:ASN:HB3	2.48	0.49
1:C:503:PHE:CE1	1:C:536:VAL:HG12	2.46	0.49
1:C:744:GLN:O	1:C:745:ALA:C	2.50	0.49
1:A:497:TYR:CE1	1:A:539:SER:HA	2.48	0.49
1:A:445:ASN:HB3	1:A:448:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PRO:HA	1:C:204:PHE:CE2	2.43	0.49
1:C:421:SER:HB3	1:C:424:VAL:HG23	1.95	0.49
1:A:649:ALA:O	1:A:653:PHE:CD2	2.61	0.48
1:A:800:PHE:O	1:A:804:ILE:HG13	2.12	0.48
1:C:6:ILE:HG13	1:C:24:PHE:CD1	2.48	0.48
1:C:558:LEU:HD21	1:C:607:VAL:CG1	2.44	0.48
1:C:447:VAL:HG12	1:C:448:TYR:N	2.26	0.48
1:A:36:PHE:CE2	1:A:40:LEU:HD11	2.48	0.48
1:C:504:GLU:C	1:C:506:ILE:H	2.17	0.48
1:A:679:ARG:HH21	2:B:55:ARG:CG	2.25	0.48
1:A:791:GLN:HB3	1:A:792:PRO:HD3	1.96	0.48
1:A:800:PHE:HA	1:A:803:HIS:HB3	1.94	0.48
2:B:39:GLU:O	2:B:43:ARG:HG3	2.13	0.48
1:C:558:LEU:HD21	1:C:607:VAL:HG13	1.94	0.48
1:A:109:ALA:O	1:A:113:VAL:HG23	2.13	0.48
1:A:742:ALA:HB2	1:A:761:LEU:HD23	1.94	0.48
1:C:157:ILE:O	1:C:161:ILE:HB	2.13	0.48
1:C:503:PHE:CE2	1:C:547:VAL:HG21	2.41	0.48
1:A:256:MET:HG2	1:A:314:TYR:CD1	2.48	0.48
1:A:696:LEU:CD2	1:A:713:ILE:HD12	2.43	0.48
1:A:723:ALA:O	1:A:725:GLY:N	2.46	0.48
1:A:342:TRP:HE3	2:B:28:LEU:HD13	1.78	0.48
1:A:377:ASN:ND2	1:A:379:ASP:HB2	2.29	0.48
1:C:161:ILE:HG12	1:C:166:LEU:HB2	1.94	0.48
1:C:588:LEU:HD23	1:C:631:ALA:HB1	1.93	0.48
1:A:619:ALA:HA	1:A:620:GLY:HA2	1.51	0.48
1:C:507:VAL:HG12	1:C:535:ILE:HG23	1.96	0.48
1:C:62:LYS:NZ	1:C:62:LYS:HB3	2.28	0.48
1:C:608:MET:HB2	1:C:635:LEU:HD23	1.94	0.48
1:A:447:VAL:O	1:A:447:VAL:HG22	2.14	0.48
1:A:628:ALA:O	1:A:632:VAL:HG23	2.14	0.48
1:C:38:VAL:O	1:C:42:ARG:HG3	2.13	0.48
1:A:359:CYS:HB3	1:A:362:ASP:HB2	1.95	0.47
1:A:90:GLU:HG2	1:A:94:TYR:CE2	2.44	0.47
1:C:823:GLY:HA3	1:C:864:TRP:CZ3	2.49	0.47
1:C:449:LEU:HA	1:C:453:LEU:HB2	1.96	0.47
1:C:579:ASP:HA	1:C:582:SER:HB2	1.95	0.47
1:C:89:ARG:O	1:C:93:ASN:HB2	2.14	0.47
1:A:568:ILE:HD13	1:A:574:ARG:CZ	2.43	0.47
1:A:833:VAL:O	1:A:837:VAL:HG23	2.14	0.47
1:C:544:TYR:HA	1:C:547:VAL:CB	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:HB2	1:A:314:TYR:CE2	2.49	0.47
1:A:540:ALA:HB3	1:A:543:CYS:SG	2.54	0.47
1:A:831:LYS:N	1:A:833:VAL:HG23	2.29	0.47
1:C:549:LYS:HA	1:C:552:LEU:HD12	1.96	0.47
1:A:783:VAL:HG12	1:A:785:PRO:HB3	1.96	0.47
1:A:495:ALA:CA	1:A:541:LYS:HG3	2.31	0.47
1:A:428:ALA:O	1:A:432:VAL:HG23	2.14	0.47
1:A:497:TYR:HD1	1:A:540:ALA:HB2	1.77	0.47
1:C:46:ASN:ND2	1:C:48:GLY:H	2.13	0.47
1:A:783:VAL:HG12	1:A:785:PRO:HG3	1.95	0.47
1:A:796:PHE:HA	1:A:799:SER:HB2	1.95	0.47
2:D:55:ARG:O	2:D:59:VAL:HG23	2.14	0.47
1:A:44:LEU:HG	1:A:98:THR:HG21	1.96	0.47
1:A:495:ALA:O	1:A:542:ASP:CG	2.53	0.47
1:A:596:GLN:HG3	1:A:597:HIS:N	2.30	0.47
1:C:447:VAL:HB	1:C:448:TYR:CD2	2.50	0.47
1:C:586:ALA:C	1:C:588:LEU:N	2.68	0.47
1:C:782:ASN:O	1:C:783:VAL:C	2.53	0.47
1:C:591:VAL:HG23	1:C:592:LEU:N	2.28	0.47
1:C:801:ILE:HG21	1:C:822:ILE:HD11	1.96	0.47
1:A:397:PRO:HB2	1:A:402:LEU:HD13	1.97	0.47
1:A:448:TYR:C	1:A:451:PRO:HD2	2.35	0.47
1:C:336:ASN:HD21	1:C:338:ASP:CB	2.28	0.47
1:C:438:LEU:C	1:C:440:PRO:HD3	2.34	0.47
1:A:651:LYS:CB	1:A:652:PRO:HD3	2.45	0.46
1:C:33:LEU:HB3	1:C:34:PRO:HD3	1.97	0.46
1:C:431:THR:O	1:C:435:ILE:HG13	2.15	0.46
1:C:495:ALA:CB	1:C:541:LYS:HG3	2.45	0.46
1:A:238:LEU:O	1:A:242:VAL:HG23	2.15	0.46
1:A:3:LEU:HD22	1:A:7:LEU:HG	1.96	0.46
1:A:701:GLY:HA2	1:A:702:ASN:HA	1.64	0.46
1:A:161:ILE:HG21	1:A:166:LEU:HD12	1.98	0.46
1:C:62:LYS:HG3	1:C:111:GLN:HB3	1.96	0.46
1:C:80:TRP:NE1	1:C:116:ILE:HG23	2.31	0.46
1:C:142:SER:HB3	1:C:146:MET:HG2	1.97	0.46
1:C:256:MET:HG2	1:C:314:TYR:CD1	2.50	0.46
1:C:334:ASP:C	1:C:334:ASP:OD1	2.53	0.46
1:C:499:LEU:O	1:C:503:PHE:N	2.48	0.46
1:A:762:ARG:NH1	1:A:804:ILE:HA	2.30	0.46
1:C:148:GLU:O	1:C:152:GLU:HG3	2.16	0.46
1:C:853:SER:HB2	1:C:855:THR:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PHE:O	1:A:40:LEU:HG	2.15	0.46
1:A:629:LEU:HD22	1:A:673:LEU:HD12	1.98	0.46
1:C:449:LEU:C	1:C:453:LEU:HB2	2.36	0.46
1:C:33:LEU:CD2	1:C:79:ARG:HD2	2.45	0.46
1:A:795:GLU:O	1:A:799:SER:N	2.48	0.46
1:A:214:GLU:O	1:A:218:ILE:HG13	2.16	0.46
1:C:179:GLN:HE21	1:C:179:GLN:HA	1.79	0.46
1:C:442:ALA:CB	1:C:443:ALA:CB	2.90	0.46
1:A:284:SER:HB2	1:A:354:LEU:HD12	1.97	0.46
1:A:377:ASN:ND2	1:A:379:ASP:H	2.13	0.46
1:C:343:ASN:C	1:C:343:ASN:HD22	2.19	0.46
1:A:864:TRP:HE1	1:A:867:LYS:HZ2	1.64	0.46
1:C:231:THR:O	1:C:234:ARG:HB2	2.16	0.46
1:C:510:LEU:C	1:C:512:GLU:H	2.19	0.46
1:C:68:LYS:N	1:C:68:LYS:HD3	2.31	0.46
1:C:747:VAL:HB	1:C:758:LEU:HD22	1.97	0.46
1:C:797:ILE:O	1:C:801:ILE:HG12	2.16	0.46
1:A:242:VAL:HG22	1:A:282:PHE:HD1	1.82	0.45
1:A:399:PRO:C	1:A:401:GLN:H	2.20	0.45
1:A:39:GLU:O	1:A:43:VAL:HG23	2.16	0.45
1:A:696:LEU:HD22	1:A:713:ILE:HD12	1.98	0.45
1:A:739:LEU:HD23	1:A:740:GLN:N	2.31	0.45
1:C:589:GLN:HG3	1:C:590:ASN:N	2.28	0.45
1:C:673:LEU:HD22	1:C:677:LEU:HG	1.97	0.45
1:A:717:PHE:HB3	1:A:731:TYR:CZ	2.51	0.45
1:C:447:VAL:O	1:C:449:LEU:HD13	2.16	0.45
1:A:121:ILE:HB	1:A:122:PRO:HD3	1.97	0.45
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.98	0.45
1:A:574:ARG:CA	1:A:574:ARG:NE	2.79	0.45
1:A:711:PRO:HG2	1:A:760:GLU:CD	2.37	0.45
1:C:525:ARG:HG2	1:C:529:TYR:CD2	2.50	0.45
1:A:170:SER:O	1:A:174:LEU:HB2	2.17	0.45
1:A:489:ASP:CG	1:A:489:ASP:O	2.54	0.45
1:A:632:VAL:HA	1:A:635:LEU:HD23	1.99	0.45
2:D:40:GLN:CD	2:D:40:GLN:H	2.19	0.45
1:A:632:VAL:O	1:A:636:VAL:HG23	2.16	0.45
1:A:685:ILE:O	1:A:685:ILE:HG22	2.17	0.45
1:C:181:MET:HB2	1:C:181:MET:HE3	1.83	0.45
1:C:202:LEU:HD11	1:C:240:ASN:HD22	1.81	0.45
1:C:472:TRP:CZ3	1:C:473:ALA:HB2	2.51	0.45
1:C:502:SER:HB2	1:C:505:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:THR:HG22	1:C:587:THR:O	2.17	0.45
1:A:757:TYR:O	1:A:758:LEU:C	2.55	0.45
1:C:300:ALA:HB1	1:C:305:ARG:O	2.16	0.45
1:C:514:THR:HG21	1:C:532:LEU:HD12	1.97	0.45
1:C:596:GLN:O	1:C:596:GLN:HG2	2.16	0.45
1:A:479:GLU:HA	1:A:538:ASN:OD1	2.16	0.45
1:A:824:ASP:CG	2:B:63:ARG:HH11	2.20	0.45
1:C:343:ASN:HD21	1:C:346:LYS:HD2	1.80	0.45
1:C:503:PHE:O	1:C:506:ILE:HG12	2.17	0.45
1:C:91:VAL:O	1:C:95:VAL:HG23	2.17	0.45
1:A:562:LEU:HB3	1:A:614:MET:HB2	1.98	0.45
1:A:678:CYS:SG	1:A:720:ILE:HA	2.56	0.45
1:C:360:GLU:HB3	1:C:396:GLY:C	2.37	0.45
1:A:318:ALA:O	1:A:322:LEU:HG	2.17	0.45
1:A:591:VAL:O	1:A:595:VAL:CG2	2.64	0.45
1:A:626:GLU:CD	1:A:666:VAL:HA	2.37	0.45
1:C:331:THR:HG21	1:C:382:TYR:CE1	2.52	0.45
1:C:602:GLN:O	1:C:606:VAL:HG23	2.17	0.45
1:C:702:ASN:C	1:C:704:ASN:H	2.19	0.45
1:C:706:HIS:CG	1:C:707:ARG:H	2.35	0.45
1:A:32:ASN:ND2	1:A:34:PRO:HD2	2.32	0.45
1:A:380:TRP:CE2	1:A:381:ARG:HG3	2.52	0.45
1:A:568:ILE:HD13	1:A:574:ARG:NE	2.32	0.45
1:A:728:PHE:CD1	1:A:731:TYR:HE1	2.32	0.45
1:C:489:ASP:OD2	1:C:489:ASP:N	2.49	0.45
1:A:218:ILE:O	1:A:222:VAL:HG23	2.17	0.44
1:A:356:ALA:HA	1:A:363:ILE:HG21	1.99	0.44
1:A:856:ASN:O	1:A:857:LYS:CB	2.62	0.44
1:C:519:GLY:HA3	1:C:524:LEU:HD12	1.98	0.44
1:A:234:ARG:HH22	1:A:275:VAL:HG11	1.82	0.44
1:A:522:ASN:O	1:A:523:ASN:ND2	2.30	0.44
1:C:343:ASN:ND2	1:C:346:LYS:H	2.15	0.44
1:C:84:ASP:O	1:C:88:ARG:HG3	2.18	0.44
1:C:428:ALA:O	1:C:432:VAL:HG23	2.17	0.44
1:C:444:ILE:CG2	1:C:445:ASN:N	2.80	0.44
1:C:693:MET:HE1	1:C:696:LEU:HD12	2.00	0.44
1:A:126:TRP:N	1:A:127:PRO:HD3	2.33	0.44
1:A:376:LYS:O	1:A:376:LYS:HG3	2.17	0.44
1:C:243:LYS:HD3	1:C:752:TYR:OH	2.18	0.44
1:C:374:HIS:O	1:C:383:ARG:HA	2.18	0.44
1:C:475:SER:C	1:C:477:LEU:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LEU:C	1:C:524:LEU:HD13	2.38	0.44
1:C:395:GLU:HB3	1:C:434:ARG:NH2	2.33	0.44
1:C:444:ILE:HG23	1:C:445:ASN:N	2.32	0.44
1:C:499:LEU:HG	1:C:503:PHE:CB	2.46	0.44
1:A:235:VAL:O	1:A:239:GLN:HG3	2.18	0.44
1:A:397:PRO:HB2	1:A:402:LEU:CD1	2.48	0.44
1:A:561:VAL:HG11	1:A:581:GLN:HB2	2.00	0.44
1:C:368:LEU:HB3	1:C:369:PRO:HD3	1.99	0.44
1:C:422:VAL:HG22	1:C:466:VAL:HA	1.99	0.44
1:C:706:HIS:HB3	1:C:709:VAL:HG23	1.99	0.44
1:A:739:LEU:HD12	1:A:800:PHE:CE2	2.52	0.44
1:C:482:TYR:C	1:C:482:TYR:CD2	2.91	0.44
1:C:531:SER:C	1:C:533:MET:N	2.71	0.44
1:C:633:SER:OG	1:C:673:LEU:HG	2.17	0.44
1:C:802:ASP:OD1	1:C:840:ARG:HG2	2.18	0.44
1:C:833:VAL:O	1:C:837:VAL:HG23	2.17	0.44
1:A:291:MET:HE2	1:A:358:CYS:N	2.33	0.44
1:C:238:LEU:O	1:C:242:VAL:HG23	2.17	0.44
1:C:24:PHE:O	1:C:27:ARG:HG2	2.18	0.44
1:C:343:ASN:HB2	1:C:344:PRO:CD	2.46	0.44
1:C:460:LEU:HD11	1:C:535:ILE:HD11	2.00	0.44
1:C:46:ASN:HD22	1:C:46:ASN:C	2.21	0.44
1:C:471:CYS:HA	1:C:474:PHE:CZ	2.49	0.44
1:C:493:GLU:HA	1:C:494:PRO:HD3	1.83	0.44
1:C:511:LEU:O	1:C:515:ASP:HB2	2.18	0.44
1:C:516:ARG:HA	1:C:517:PRO:HD3	1.82	0.44
1:C:632:VAL:HG21	1:C:650:PHE:CE1	2.53	0.44
1:A:168:ASP:HB2	1:A:169:LYS:HE2	2.00	0.43
1:A:406:VAL:HG21	1:A:439:LEU:HD12	1.99	0.43
1:C:449:LEU:HD12	1:C:453:LEU:CD2	2.47	0.43
1:C:486:ASP:HB3	1:C:494:PRO:CG	2.36	0.43
1:A:571:THR:O	1:A:576:GLN:HB2	2.18	0.43
1:A:766:LEU:HD22	1:A:821:LEU:HD12	2.00	0.43
1:A:849:GLU:HA	1:A:852:ARG:NE	2.24	0.43
1:A:679:ARG:NH2	2:B:55:ARG:HG2	2.31	0.43
1:C:130:ILE:HB	1:C:131:PRO:HD3	2.00	0.43
1:C:387:VAL:HG11	1:C:428:ALA:HA	2.00	0.43
1:A:453:LEU:HD11	1:A:499:LEU:HD23	2.00	0.43
1:A:864:TRP:HE1	1:A:867:LYS:NZ	2.16	0.43
1:C:105:ARG:CB	1:C:106:PRO:HD3	2.44	0.43
1:C:403:LYS:NZ	1:C:441:GLU:HG3	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:LEU:CD1	1:C:601:LEU:H	2.31	0.43
1:A:343:ASN:HD22	1:A:343:ASN:C	2.22	0.43
1:A:591:VAL:O	1:A:595:VAL:CG1	2.67	0.43
1:A:648:GLU:OE1	1:A:648:GLU:HA	2.17	0.43
1:C:560:GLN:HB3	1:C:560:GLN:HE21	1.54	0.43
1:C:614:MET:SD	1:C:618:THR:HG21	2.58	0.43
1:C:749:LYS:N	1:C:749:LYS:HD3	2.31	0.43
1:A:467:ALA:O	1:A:470:VAL:HB	2.19	0.43
1:A:557:ARG:O	1:A:561:VAL:HG23	2.18	0.43
1:A:625:GLN:CD	1:A:625:GLN:H	2.21	0.43
1:C:22:GLN:O	1:C:26:GLU:HB2	2.18	0.43
1:C:39:GLU:O	1:C:43:VAL:HG23	2.19	0.43
1:C:790:VAL:HG12	1:C:790:VAL:O	2.19	0.43
1:A:417:MET:HB2	1:A:455:CYS:SG	2.59	0.43
1:A:444:ILE:HA	1:A:449:LEU:HD22	2.00	0.43
1:A:542:ASP:OD1	1:A:542:ASP:C	2.56	0.43
1:A:839:ALA:HB1	1:C:105:ARG:CG	2.40	0.43
1:C:745:ALA:HB1	1:C:758:LEU:HD11	2.00	0.43
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.91	0.43
1:A:453:LEU:HD23	1:A:474:PHE:HE1	1.84	0.43
1:A:593:ARG:HE	2:B:50:LEU:CD2	2.31	0.43
1:A:757:TYR:O	1:A:760:GLU:HB2	2.18	0.43
1:A:796:PHE:O	1:A:800:PHE:HD2	2.01	0.43
1:C:443:ALA:H	1:C:446:ASP:H	1.66	0.43
1:A:449:LEU:HD13	1:A:449:LEU:HA	1.78	0.43
1:A:549:LYS:O	1:A:553:VAL:HG23	2.19	0.43
1:A:710:LYS:CB	1:A:711:PRO:HD3	2.49	0.43
1:A:714:LEU:N	1:A:714:LEU:HD12	2.34	0.43
1:C:65:LEU:O	1:C:76:TYR:HB3	2.18	0.43
1:A:104:TYR:CD2	1:A:106:PRO:HD2	2.53	0.43
1:C:449:LEU:O	1:C:453:LEU:CB	2.62	0.43
1:A:174:LEU:HD22	1:A:178:ILE:HG13	2.00	0.43
1:C:853:SER:CA	1:C:854:LYS:C	2.78	0.43
1:A:240:ASN:O	1:A:244:ILE:HG13	2.19	0.42
1:A:548:GLN:O	1:A:552:LEU:HD12	2.18	0.42
1:C:659:LYS:HG2	1:C:695:LEU:HD22	2.01	0.42
1:A:736:LEU:HD22	1:A:793:ARG:CG	2.49	0.42
1:A:815:VAL:HG22	1:A:846:LEU:HD11	2.00	0.42
1:A:92:LYS:HD3	1:A:120:GLU:OE1	2.19	0.42
1:C:387:VAL:HG22	1:C:416:LEU:HD13	2.00	0.42
1:C:482:TYR:CE1	1:C:493:GLU:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:GLU:O	1:A:487:VAL:HG13	2.19	0.42
1:C:343:ASN:ND2	1:C:346:LYS:HD3	2.35	0.42
1:C:547:VAL:HG13	1:C:550:THR:CB	2.48	0.42
1:A:104:TYR:O	1:A:105:ARG:C	2.58	0.42
1:A:410:MET:HB2	1:A:411:PRO:HD3	2.01	0.42
1:C:414:ILE:HG12	1:C:452:LEU:CG	2.50	0.42
1:C:414:ILE:HG21	1:C:451:PRO:O	2.19	0.42
1:C:429:ALA:CA	1:C:477:LEU:HD11	2.48	0.42
1:A:584:LEU:C	1:A:586:ALA:H	2.23	0.42
1:A:739:LEU:HD12	1:A:800:PHE:CZ	2.54	0.42
1:C:295:ILE:HG22	1:C:295:ILE:O	2.20	0.42
1:C:512:GLU:HA	1:C:515:ASP:HB2	2.01	0.42
1:C:812:ASP:OD1	1:C:855:THR:HG23	2.19	0.42
1:C:868:GLU:HA	1:C:871:LYS:HE2	2.01	0.42
1:A:206:LYS:HG2	1:A:206:LYS:H	1.46	0.42
1:A:403:LYS:HE2	1:A:439:LEU:HD22	2.01	0.42
1:C:92:LYS:HD3	1:C:120:GLU:OE1	2.20	0.42
1:C:343:ASN:HD21	1:C:346:LYS:H	1.66	0.42
1:C:434:ARG:CZ	1:C:438:LEU:HD11	2.50	0.42
1:A:192:LEU:HD13	1:A:232:ARG:HB3	2.01	0.42
1:A:46:ASN:HA	1:A:47:PRO:HD3	1.85	0.42
1:A:495:ALA:HB2	1:A:541:LYS:HE2	2.01	0.42
1:A:720:ILE:HG22	1:A:728:PHE:CE1	2.54	0.42
1:A:802:ASP:OD1	1:A:840:ARG:HB3	2.20	0.42
1:C:700:LEU:HD13	1:C:738:THR:HG21	2.01	0.42
1:A:661:TYR:HD1	1:A:699:ASN:HD22	1.65	0.42
1:A:98:THR:HG22	1:A:102:GLU:HG3	2.02	0.42
1:C:264:THR:HG21	1:C:282:PHE:CD2	2.55	0.42
1:C:40:LEU:CB	1:C:61:ILE:HD11	2.49	0.42
1:A:403:LYS:HB2	1:A:404:PRO:HD3	2.01	0.42
1:A:383:ARG:HH11	1:A:424:VAL:HG21	1.83	0.42
1:A:599:ASP:C	1:A:601:LEU:H	2.24	0.42
1:A:781:GLU:HA	1:A:781:GLU:OE2	2.20	0.42
1:C:377:ASN:HD22	1:C:378:PRO:N	2.18	0.42
1:C:360:GLU:HB3	1:C:397:PRO:N	2.35	0.42
1:C:429:ALA:CB	1:C:477:LEU:CD1	2.83	0.42
1:C:537:LYS:HD3	1:C:538:ASN:N	2.34	0.42
1:C:174:LEU:HA	1:C:174:LEU:HD23	1.80	0.42
1:C:226:THR:HG22	1:C:237:ALA:HB1	2.01	0.42
1:A:104:TYR:CE2	1:A:106:PRO:HD2	2.55	0.41
1:A:291:MET:O	1:A:295:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:HG23	1:A:9:LYS:NZ	2.35	0.41
1:C:585:CYS:HB2	1:C:627:ASP:OD1	2.20	0.41
1:C:824:ASP:OD1	2:D:63:ARG:HD3	2.19	0.41
1:A:488:ALA:HB1	1:A:490:ASP:H	1.84	0.41
1:A:580:LEU:O	1:A:584:LEU:HG	2.20	0.41
1:C:336:ASN:HD21	1:C:338:ASP:HB3	1.84	0.41
1:C:368:LEU:HA	1:C:371:ILE:HD12	2.02	0.41
1:A:471:CYS:HB3	1:A:531:SER:HB2	2.02	0.41
1:A:544:TYR:O	1:A:547:VAL:HG12	2.20	0.41
1:A:663:GLU:OE2	1:A:666:VAL:HG21	2.20	0.41
1:C:443:ALA:H	1:C:446:ASP:N	2.18	0.41
1:C:504:GLU:C	1:C:506:ILE:N	2.74	0.41
1:C:722:LEU:O	1:C:722:LEU:HD23	2.20	0.41
1:A:181:MET:HB2	1:A:181:MET:HE3	1.89	0.41
1:A:192:LEU:HD22	1:A:232:ARG:HD2	2.02	0.41
1:A:3:LEU:HD12	1:A:39:GLU:CD	2.41	0.41
1:A:787:VAL:HB	1:A:828:ALA:HB1	2.02	0.41
1:C:312:LYS:HB3	1:C:312:LYS:NZ	2.36	0.41
1:C:583:LEU:HD12	1:C:583:LEU:C	2.40	0.41
1:C:857:LYS:HD3	1:C:857:LYS:HA	1.78	0.41
1:C:722:LEU:HD22	2:D:58:TYR:HE2	1.85	0.41
1:A:543:CYS:C	1:A:545:PRO:HD2	2.39	0.41
1:A:581:GLN:HA	1:A:584:LEU:HD12	2.03	0.41
1:A:12:SER:HA	1:A:13:PRO:HD3	1.89	0.41
1:A:25:LEU:HD13	1:A:60:GLN:NE2	2.36	0.41
1:A:736:LEU:HD22	1:A:793:ARG:CD	2.49	0.41
1:C:121:ILE:HD11	1:C:129:LEU:HD23	2.02	0.41
1:C:253:GLU:OE1	1:C:312:LYS:HE3	2.21	0.41
1:C:316:LYS:NZ	1:C:316:LYS:HB3	2.36	0.41
1:C:39:GLU:HA	1:C:42:ARG:HD3	2.01	0.41
1:C:591:VAL:CG2	1:C:592:LEU:N	2.83	0.41
1:A:238:LEU:HD23	1:A:241:LEU:HD12	2.02	0.41
1:A:261:PHE:HE1	1:A:318:ALA:HB2	1.85	0.41
1:A:374:HIS:CA	1:A:377:ASN:HB2	2.39	0.41
1:A:503:PHE:O	1:A:507:VAL:HG23	2.20	0.41
1:A:464:PRO:CB	1:A:522:ASN:HB2	2.51	0.41
1:C:250:GLN:H	1:C:250:GLN:HG2	1.56	0.41
1:C:784:HIS:H	1:C:784:HIS:CD2	2.36	0.41
1:A:439:LEU:N	1:A:440:PRO:HD3	2.35	0.41
1:C:482:TYR:CD1	1:C:538:ASN:HB3	2.56	0.41
1:C:654:LEU:O	1:C:654:LEU:HD13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:PHE:CE1	1:A:507:VAL:HG21	2.56	0.41
1:C:27:ARG:O	1:C:31:GLU:HB2	2.21	0.41
1:C:46:ASN:HA	1:C:47:PRO:HD3	1.92	0.41
1:C:526:SER:HA	1:C:583:LEU:HD21	2.03	0.41
1:C:821:LEU:HD13	1:C:821:LEU:O	2.21	0.41
1:A:157:ILE:HG22	1:A:166:LEU:HD11	2.03	0.41
1:A:503:PHE:CE2	1:A:546:ALA:HB3	2.55	0.41
1:A:646:TYR:HB2	1:A:647:MET:H	1.47	0.41
1:A:660:ASN:OD1	1:A:663:GLU:HB2	2.21	0.41
1:A:752:TYR:HA	1:A:755:VAL:HG12	2.03	0.41
1:A:90:GLU:O	1:A:94:TYR:CE2	2.72	0.41
1:C:548:GLN:HG3	1:C:549:LYS:N	2.36	0.41
1:A:596:GLN:HB2	1:A:596:GLN:HE21	1.55	0.41
1:C:496:THR:HA	1:C:500:SER:CB	2.51	0.41
1:C:793:ARG:O	1:C:797:ILE:HG13	2.21	0.41
1:A:338:ASP:C	1:A:340:ASP:H	2.25	0.40
1:A:596:GLN:HG2	1:A:598:GLN:H	1.86	0.40
1:C:612:LEU:HD12	1:C:646:TYR:HD2	1.86	0.40
1:A:569:GLN:HB2	1:A:573:ASP:CB	2.52	0.40
1:C:474:PHE:CD2	1:C:474:PHE:C	2.94	0.40
1:C:524:LEU:HD13	1:C:524:LEU:O	2.21	0.40
1:A:130:ILE:O	1:A:134:VAL:HG23	2.21	0.40
1:A:267:ALA:O	1:A:276:ALA:HA	2.21	0.40
1:A:453:LEU:HD11	1:A:499:LEU:CD2	2.51	0.40
1:A:578:ASN:ND2	1:A:581:GLN:HB3	2.35	0.40
1:A:692:VAL:HG13	1:A:696:LEU:HD12	2.03	0.40
1:C:168:ASP:HB3	1:C:169:LYS:HE2	2.03	0.40
1:C:406:VAL:O	1:C:410:MET:HG2	2.21	0.40
1:C:523:ASN:O	1:C:524:LEU:C	2.60	0.40
1:C:667:CYS:O	1:C:671:VAL:HG23	2.22	0.40
1:C:788:MET:HA	1:C:791:GLN:HB2	2.03	0.40
1:C:80:TRP:HA	1:C:83:ILE:HD12	2.03	0.40
1:A:37:LEU:HD13	1:A:80:TRP:HZ3	1.87	0.40
1:A:853:SER:OG	1:A:854:LYS:HA	2.21	0.40
1:A:89:ARG:HA	1:A:92:LYS:CE	2.51	0.40
2:B:26:PRO:HB2	2:B:27:ARG:H	1.73	0.40
1:C:217:PHE:O	1:C:221:VAL:HG23	2.21	0.40
1:C:686:ILE:HA	1:C:689:CYS:SG	2.61	0.40
1:C:867:LYS:O	1:C:871:LYS:HG3	2.22	0.40
1:A:550:THR:O	1:A:554:ILE:HG13	2.22	0.40
1:A:654:LEU:HD23	1:A:654:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:HIS:N	1:A:784:HIS:CD2	2.89	0.40
1:A:840:ARG:HA	1:A:841:PRO:HD3	1.78	0.40
2:B:35:TYR:O	2:B:35:TYR:HD2	2.05	0.40
1:C:443:ALA:N	1:C:446:ASP:H	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	871/876 (99%)	761 (87%)	104 (12%)	6 (1%)	22	59
1	C	867/876 (99%)	753 (87%)	109 (13%)	5 (1%)	25	62
2	B	37/40 (92%)	27 (73%)	10 (27%)	0	100	100
2	D	24/40 (60%)	24 (100%)	0	0	100	100
All	All	1799/1832 (98%)	1565 (87%)	223 (12%)	11 (1%)	25	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	LYS
1	C	447	VAL
1	C	702	ASN
1	A	724	ILE
1	A	129	LEU
1	C	747	VAL
1	A	256	MET
1	A	693	MET
1	C	256	MET
1	C	783	VAL
1	A	339	ASP

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	749/751 (100%)	677 (90%)	72 (10%)	8	29
1	C	747/751 (100%)	680 (91%)	67 (9%)	9	32
2	B	38/39 (97%)	35 (92%)	3 (8%)	12	40
2	D	25/39 (64%)	22 (88%)	3 (12%)	5	21
All	All	1559/1580 (99%)	1414 (91%)	145 (9%)	9	31

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	68	LYS
1	A	96	LEU
1	A	97	GLN
1	A	169	LYS
1	A	174	LEU
1	A	204	PHE
1	A	206	LYS
1	A	209	PHE
1	A	210	ASP
1	A	234	ARG
1	A	286	VAL
1	A	292	ASP
1	A	338	ASP
1	A	340	ASP
1	A	343	ASN
1	A	379	ASP
1	A	382	TYR
1	A	394	LEU
1	A	398	GLU
1	A	449	LEU
1	A	474	PHE
1	A	487	VAL
1	A	490	ASP

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	492	GLU
1	A	493	GLU
1	A	496	THR
1	A	498	CYS
1	A	502	SER
1	A	503	PHE
1	A	523	ASN
1	A	535	ILE
1	A	541	LYS
1	A	563	GLN
1	A	564	MET
1	A	573	ASP
1	A	574	ARG
1	A	577	PHE
1	A	578	ASN
1	A	580	LEU
1	A	581	GLN
1	A	587	THR
1	A	596	GLN
1	A	599	ASP
1	A	602	GLN
1	A	615	PHE
1	A	616	GLN
1	A	635	LEU
1	A	644	LEU
1	A	646	TYR
1	A	650	PHE
1	A	694	GLN
1	A	696	LEU
1	A	699	ASN
1	A	710	LYS
1	A	724	ILE
1	A	734	VAL
1	A	735	VAL
1	A	739	LEU
1	A	744	GLN
1	A	780	GLN
1	A	786	ASP
1	A	788	MET
1	A	791	GLN
1	A	793	ARG

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Mol	Chain	Res	Type
1	A	800	PHE
1	A	801	ILE
1	A	825	LEU
1	A	855	THR
1	A	856	ASN
1	A	863	THR
2	B	38	LEU
2	B	54	LYS
2	B	63	ARG
1	C	1	MET
1	C	3	LEU
1	C	23	LYS
1	C	27	ARG
1	C	46	ASN
1	C	49	ASN
1	C	62	LYS
1	C	68	LYS
1	C	72	ILE
1	C	111	GLN
1	C	169	LYS
1	C	179	GLN
1	C	204	PHE
1	C	208	ASN
1	C	234	ARG
1	C	243	LYS
1	C	247	LEU
1	C	250	GLN
1	C	288	ASP
1	C	309	HIS
1	C	336	ASN
1	C	343	ASN
1	C	377	ASN
1	C	402	LEU
1	C	417	MET
1	C	423	VAL
1	C	445	ASN
1	C	446	ASP
1	C	449	LEU
1	C	452	LEU
1	C	453	LEU
1	C	456	LEU
1	C	458	GLU

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Mol	Chain	Res	Type
1	C	460	LEU
1	C	472	TRP
1	C	491	GLN
1	C	493	GLU
1	C	497	TYR
1	C	503	PHE
1	C	505	LEU
1	C	506	ILE
1	C	515	ASP
1	C	529	TYR
1	C	541	LYS
1	C	544	TYR
1	C	554	ILE
1	C	560	GLN
1	C	564	MET
1	C	576	GLN
1	C	596	GLN
1	C	612	LEU
1	C	621	SER
1	C	656	ILE
1	C	673	LEU
1	C	685	ILE
1	C	731	TYR
1	C	746	GLN
1	C	749	LYS
1	C	751	ASP
1	C	753	ASP
1	C	759	ASN
1	C	779	ASP
1	C	784	HIS
1	C	787	VAL
1	C	804	ILE
1	C	815	VAL
1	C	831	LYS
2	D	40	GLN
2	D	48	LEU
2	D	56	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	51	GLN
1	A	97	GLN
1	A	111	GLN
1	A	124	ASN
1	A	125	GLN
1	A	132	GLN
1	A	141	ASN
1	A	159	GLN
1	A	165	GLN
1	A	179	GLN
1	A	200	ASN
1	A	227	GLN
1	A	240	ASN
1	A	278	GLN
1	A	303	GLN
1	A	343	ASN
1	A	377	ASN
1	A	401	GLN
1	A	408	GLN
1	A	523	ASN
1	A	563	GLN
1	A	578	ASN
1	A	581	GLN
1	A	590	ASN
1	A	596	GLN
1	A	602	GLN
1	A	694	GLN
1	A	699	ASN
1	A	741	GLN
1	A	774	GLN
1	A	780	GLN
1	A	784	HIS
1	A	856	ASN
2	B	40	GLN
2	B	60	ASN
1	C	22	GLN
1	C	46	ASN
1	C	49	ASN
1	C	111	GLN
1	C	165	GLN
1	C	179	GLN
1	C	220	GLN

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Mol	Chain	Res	Type
1	C	240	ASN
1	C	278	GLN
1	C	320	GLN
1	C	336	ASN
1	C	343	ASN
1	C	377	ASN
1	C	401	GLN
1	C	408	GLN
1	C	491	GLN
1	C	560	GLN
1	C	563	GLN
1	C	578	ASN
1	C	596	GLN
1	C	597	HIS
1	C	602	GLN
1	C	682	GLN
1	C	684	ASN
1	C	694	GLN
1	C	704	ASN
1	C	740	GLN
1	C	780	GLN
1	C	784	HIS
1	C	810	HIS

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, 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	873/876 (99%)	-0.02	34 (3%) 39 24	44, 93, 158, 220	0
1	C	871/876 (99%)	-0.15	27 (3%) 49 32	43, 74, 118, 165	0
2	B	39/40 (97%)	0.17	2 (5%) 28 15	59, 110, 142, 153	0
2	D	26/40 (65%)	-0.42	0 100 100	50, 62, 100, 109	0
All	All	1809/1832 (98%)	-0.09	63 (3%) 44 27	43, 81, 142, 220	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	792	PRO	10.2
1	A	853	SER	7.8
1	C	535	ILE	7.6
1	A	873	LYS	7.2
1	A	623	GLY	6.6
1	C	569	GLN	6.0
1	A	686	ILE	5.5
1	A	752	TYR	5.1
1	C	521	GLN	5.1
1	A	489	ASP	5.1
1	A	749	LYS	5.0
1	C	519	GLY	4.9
1	A	620	GLY	4.6
1	A	750	SER	4.4
1	C	498	CYS	4.3
1	A	703	GLU	4.2
1	C	520	HIS	4.0
1	C	495	ALA	3.8
1	C	783	VAL	3.7
1	C	782	ASN	3.7
1	A	755	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	708	SER	3.6
1	C	465	ARG	3.5
1	A	624	VAL	3.4
1	C	518	ASP	3.4
1	A	789	LEU	3.3
1	A	566	SER	3.3
1	A	700	LEU	3.2
1	C	597	HIS	3.2
1	C	540	ALA	3.2
1	A	662	ALA	3.2
1	C	599	ASP	3.2
1	A	782	ASN	3.1
1	C	539	SER	3.1
1	A	780	GLN	3.1
1	C	307	PRO	3.1
1	A	856	ASN	3.0
1	C	489	ASP	3.0
1	C	542	ASP	3.0
1	C	566	SER	3.0
1	C	570	SER	2.9
1	A	571	THR	2.9
1	A	872	LEU	2.8
1	C	526	SER	2.8
1	C	577	PHE	2.8
1	A	741	GLN	2.7
1	C	490	ASP	2.7
1	A	845	GLU	2.6
1	A	685	ILE	2.6
1	A	706	HIS	2.5
1	C	1	MET	2.4
1	A	446	ASP	2.4
1	C	337	ASP	2.4
1	A	461	SER	2.4
1	C	596	GLN	2.4
1	C	512	GLU	2.2
1	A	625	GLN	2.2
2	B	58	TYR	2.2
1	A	744	GLN	2.1
2	B	35	TYR	2.1
1	A	705	VAL	2.0
1	A	490	ASP	2.0
1	A	710	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.