



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:45 PM UTC

PDB ID : 3DPN / pdb_00003dpn
Title : Crystal Structure of cpaf s499a mutant
Authors : Chai, J.; Huang, Z.
Deposited on : 2008-07-09
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

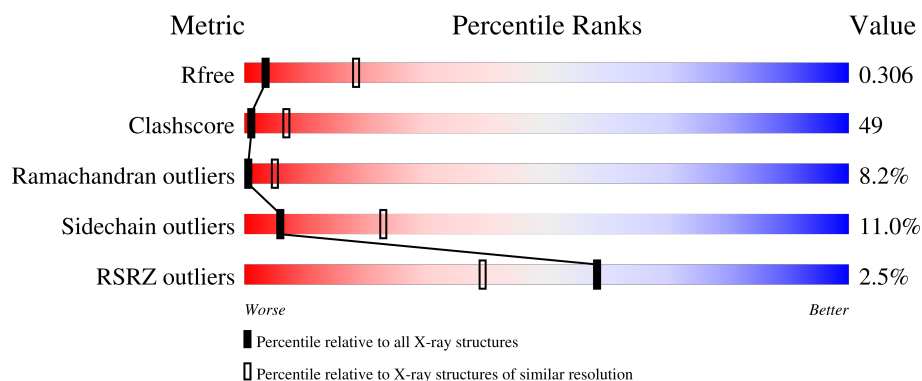
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	583	 3% 31% 48% 11% • 8%
1	B	583	 2% 34% 45% 11% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8476 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 Protein CT_858.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4238	2719	709	796	14			
1	B	537	Total	C	N	O	S	0	0	0
			4238	2719	709	796	14			

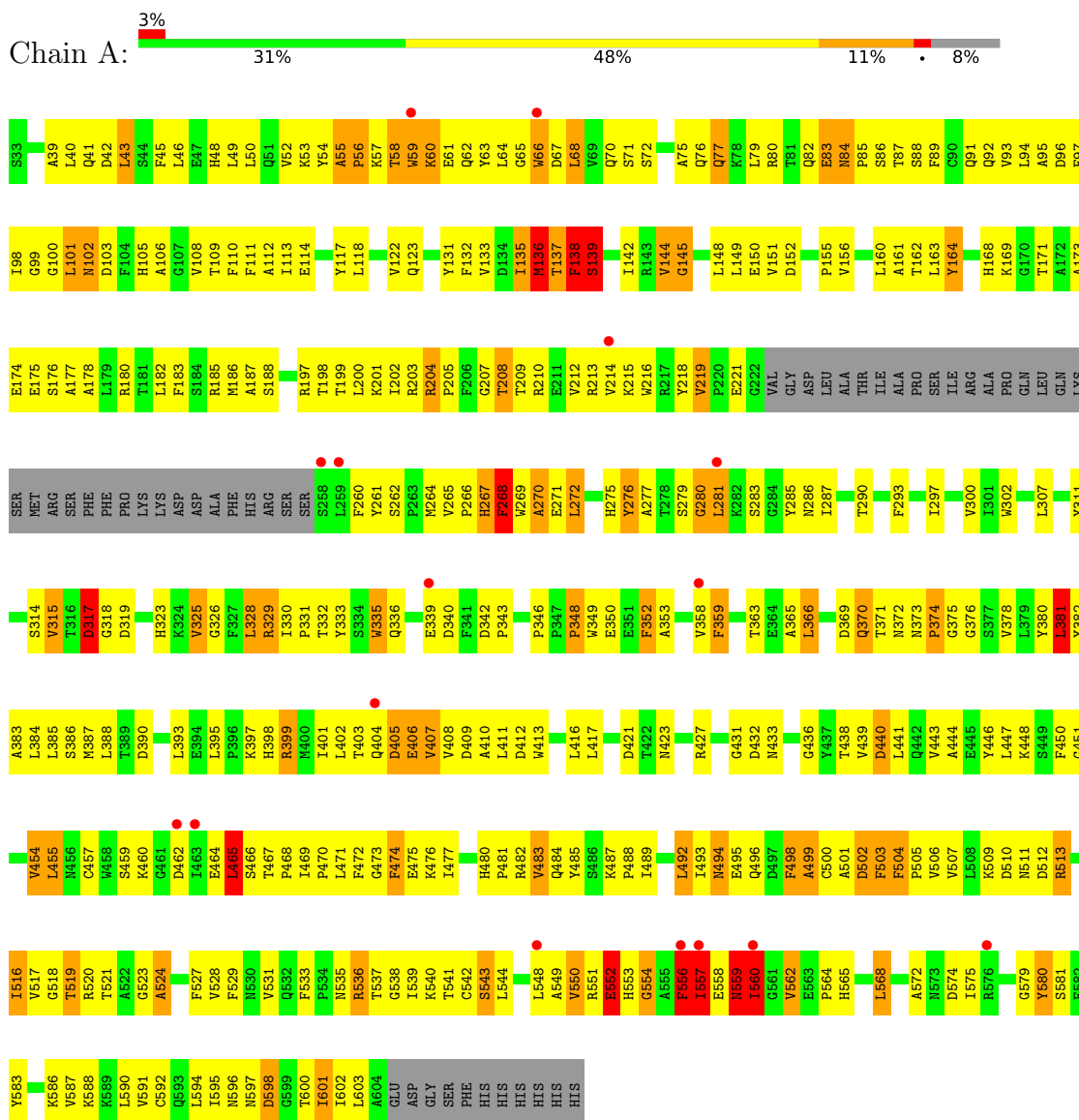
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	ALA	SER	engineered mutation	UNP O84866
A	610	HIS	-	expression tag	UNP O84866
A	611	HIS	-	expression tag	UNP O84866
A	612	HIS	-	expression tag	UNP O84866
A	613	HIS	-	expression tag	UNP O84866
A	614	HIS	-	expression tag	UNP O84866
A	615	HIS	-	expression tag	UNP O84866
B	499	ALA	SER	engineered mutation	UNP O84866
B	610	HIS	-	expression tag	UNP O84866
B	611	HIS	-	expression tag	UNP O84866
B	612	HIS	-	expression tag	UNP O84866
B	613	HIS	-	expression tag	UNP O84866
B	614	HIS	-	expression tag	UNP O84866
B	615	HIS	-	expression tag	UNP O84866

3 Residue-property plots

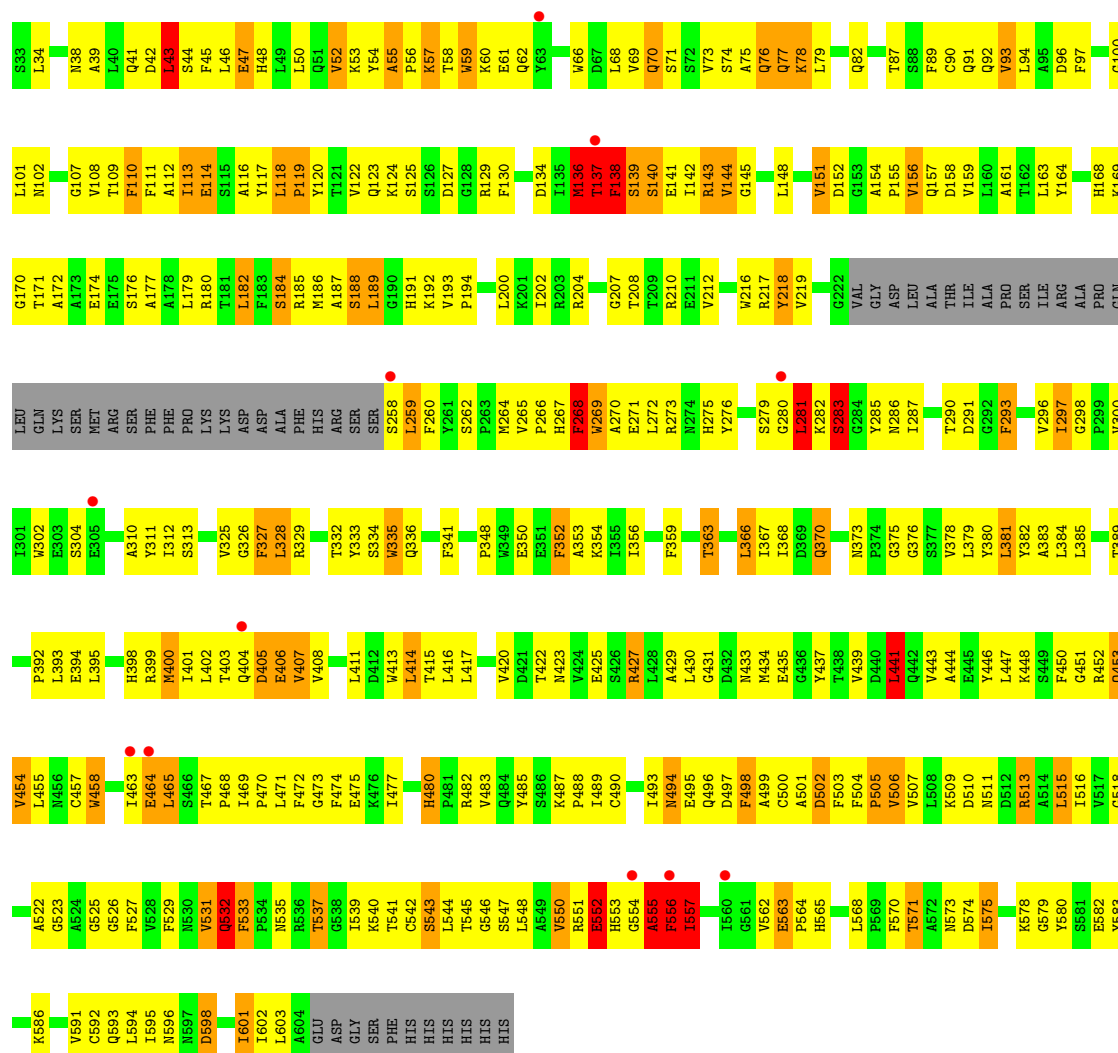
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Protein CT 858



- Molecule 1: Protein CT_858





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.67Å 192.67Å 338.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.30) 99.0 (20.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.305 0.261 , 0.306	Depositor DCC
R_{free} test set	1814 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	100.6	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 119.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8476	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	1/4344 (0.0%)	1.17	36/5905 (0.6%)
1	B	0.59	0/4344	1.20	39/5905 (0.7%)
All	All	0.58	1/8688 (0.0%)	1.18	75/11810 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	THR	CA-CB	6.56	1.62	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	PHE	N-CA-C	15.12	143.00	110.80
1	A	554	GLY	N-CA-C	13.76	129.92	110.38
1	A	406	GLU	N-CA-C	-11.68	97.60	112.90
1	B	556	PHE	N-CA-C	9.97	132.03	110.80
1	B	136	MET	N-CA-C	9.50	125.81	113.18
1	A	330	ILE	N-CA-C	-9.33	100.60	108.63
1	B	413	TRP	N-CA-C	-9.01	101.54	111.36
1	A	407	VAL	N-CA-C	-9.00	101.57	110.30
1	B	575	ILE	N-CA-C	8.74	118.81	110.42
1	B	533	PHE	CA-C-N	8.65	128.67	119.76
1	B	533	PHE	C-N-CA	8.65	128.67	119.76
1	A	137	THR	CA-C-N	-8.46	109.79	122.83
1	A	137	THR	C-N-CA	-8.46	109.79	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	THR	N-CA-C	-8.25	102.93	113.16
1	B	406	GLU	N-CA-C	-8.20	101.61	111.69
1	A	381	LEU	N-CA-C	-8.14	102.10	110.97
1	B	281	LEU	N-CA-C	-7.99	93.78	110.80
1	A	135	ILE	N-CA-C	-7.78	97.28	108.48
1	B	441	LEU	N-CA-C	-7.76	102.15	111.69
1	A	335	TRP	N-CA-C	7.65	119.26	111.07
1	A	557	ILE	N-CA-C	7.54	125.02	109.34
1	B	137	THR	CA-C-N	-7.31	107.58	121.54
1	B	137	THR	C-N-CA	-7.31	107.58	121.54
1	A	267	HIS	N-CA-C	-7.14	102.31	111.02
1	B	293	PHE	N-CA-C	-7.13	103.80	114.64
1	A	359	PHE	N-CA-C	-7.06	105.19	113.88
1	B	352	PHE	N-CA-C	-7.05	103.59	111.28
1	A	562	VAL	N-CA-C	-7.03	98.46	108.58
1	A	399	ARG	N-CA-C	-6.99	98.22	109.96
1	A	575	ILE	N-CA-C	6.92	117.62	110.36
1	B	531	VAL	N-CA-C	6.92	118.09	107.99
1	A	293	PHE	N-CA-C	-6.83	104.05	114.16
1	B	598	ASP	N-CA-C	6.76	125.20	110.80
1	B	71	SER	N-CA-C	-6.56	104.21	111.36
1	A	560	ILE	CB-CA-C	-6.52	100.59	111.29
1	A	187	ALA	N-CA-C	-6.48	104.07	112.23
1	B	76	GLN	N-CA-C	-6.20	103.67	111.11
1	A	553	HIS	N-CA-C	-6.15	103.26	112.54
1	A	329	ARG	N-CA-C	6.12	118.74	108.02
1	B	407	VAL	N-CA-C	-6.12	103.87	110.23
1	B	139	SER	N-CA-C	-6.11	97.80	110.80
1	B	118	LEU	CA-C-N	6.04	127.39	119.84
1	B	118	LEU	C-N-CA	6.04	127.39	119.84
1	A	502	ASP	N-CA-C	-5.93	104.79	112.68
1	B	532	GLN	N-CA-C	-5.89	101.74	110.46
1	A	53	LYS	N-CA-C	5.87	118.39	110.88
1	B	47	GLU	N-CA-C	-5.83	105.27	112.38
1	B	555	ALA	N-CA-C	5.83	123.21	110.80
1	B	557	ILE	N-CA-C	5.78	121.36	109.34
1	B	218	TYR	N-CA-C	5.76	119.35	110.42
1	A	352	PHE	N-CA-C	-5.74	104.94	111.14
1	B	291	ASP	N-CA-C	-5.71	102.02	110.48
1	B	212	VAL	N-CA-C	5.71	116.33	107.99
1	A	556	PHE	N-CA-C	5.64	122.81	110.80
1	A	350	GLU	N-CA-C	-5.43	105.38	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	LEU	N-CA-C	5.42	117.05	111.03
1	B	480	HIS	CA-C-N	5.41	125.08	119.56
1	B	480	HIS	C-N-CA	5.41	125.08	119.56
1	A	342	ASP	CA-C-N	5.37	126.55	119.84
1	A	342	ASP	C-N-CA	5.37	126.55	119.84
1	A	101	LEU	N-CA-C	-5.33	105.88	112.38
1	A	219	VAL	CA-C-N	5.31	125.21	119.85
1	A	219	VAL	C-N-CA	5.31	125.21	119.85
1	A	346	PRO	CA-C-N	5.30	125.84	120.38
1	A	346	PRO	C-N-CA	5.30	125.84	120.38
1	A	565	HIS	N-CA-C	-5.29	105.41	111.07
1	B	262	SER	CA-C-N	5.25	125.50	119.83
1	B	262	SER	C-N-CA	5.25	125.50	119.83
1	A	559	ASN	N-CA-C	5.21	121.90	110.80
1	B	100	GLY	N-CA-C	-5.18	108.65	114.40
1	B	282	LYS	N-CA-C	5.15	119.27	112.89
1	A	207	GLY	N-CA-C	-5.13	107.60	116.01
1	B	502	ASP	N-CA-C	-5.13	105.77	112.23
1	A	71	SER	N-CA-C	-5.07	105.41	112.45
1	B	53	LYS	N-CA-C	5.04	117.41	109.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4238	0	4157	422	0
1	B	4238	0	4157	408	0
All	All	8476	0	8314	828	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 49.

All (828) 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:550:VAL:HG12	1:A:554:GLY:HA2	1.29	1.12
1:B:264:MET:HE3	1:B:526:GLY:H	1.15	1.08
1:B:54:TYR:CZ	1:B:56:PRO:HG2	1.90	1.05
1:A:557:ILE:HG22	1:A:558:GLU:N	1.71	1.04
1:B:47:GLU:HG3	1:B:68:LEU:HD11	1.39	1.04
1:A:398:HIS:HD2	1:A:471:LEU:HD21	1.22	1.01
1:A:54:TYR:CZ	1:A:56:PRO:HG2	1.97	1.00
1:A:408:VAL:HA	1:A:411:LEU:HD12	1.43	0.99
1:A:398:HIS:CD2	1:A:471:LEU:HD21	1.99	0.96
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.48	0.95
1:A:523:GLY:HA2	1:A:560:ILE:HG22	1.47	0.95
1:A:359:PHE:O	1:A:363:THR:HG22	1.65	0.94
1:A:427:ARG:HA	1:A:439:VAL:HG11	1.50	0.92
1:B:516:ILE:H	1:B:565:HIS:CD2	1.90	0.90
1:A:601:ILE:HG22	1:A:602:ILE:HG13	1.54	0.89
1:B:136:MET:HE3	1:B:283:SER:HB3	1.54	0.89
1:A:352:PHE:HD2	1:A:387:MET:HE2	1.38	0.88
1:B:119:PRO:HG3	1:B:137:THR:HB	1.53	0.87
1:B:118:LEU:HG	1:B:216:TRP:CE3	2.10	0.87
1:A:457:CYS:SG	1:A:467:THR:HG22	2.14	0.87
1:A:557:ILE:HG22	1:A:558:GLU:H	1.37	0.87
1:B:264:MET:HE3	1:B:526:GLY:N	1.89	0.86
1:A:427:ARG:HG2	1:A:439:VAL:HB	1.57	0.86
1:A:144:VAL:HG12	1:A:145:GLY:H	1.39	0.86
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.11	0.86
1:A:180:ARG:HD2	1:A:496:GLN:HE21	1.41	0.85
1:B:515:LEU:HD23	1:B:565:HIS:HD2	1.40	0.84
1:B:119:PRO:HB2	1:B:137:THR:H	1.42	0.84
1:A:352:PHE:CD2	1:A:387:MET:HE2	2.12	0.84
1:B:551:ARG:HB3	1:B:555:ALA:HB3	1.58	0.84
1:B:367:ILE:HD11	1:B:591:VAL:HG21	1.61	0.83
1:B:366:LEU:HD13	1:B:368:ILE:HD11	1.61	0.82
1:A:451:GLY:O	1:A:454:VAL:HG23	1.80	0.82
1:A:431:GLY:O	1:A:439:VAL:HG21	1.80	0.81
1:A:523:GLY:CA	1:A:560:ILE:HG22	2.10	0.81
1:B:515:LEU:HD23	1:B:565:HIS:CD2	2.17	0.80
1:B:395:LEU:HD11	1:B:477:ILE:HG13	1.64	0.80
1:B:161:ALA:HA	1:B:164:TYR:CD2	2.17	0.79
1:B:457:CYS:SG	1:B:467:THR:HG22	2.22	0.79
1:B:554:GLY:O	1:B:556:PHE:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ALA:HA	1:A:180:ARG:HD3	1.62	0.79
1:A:468:PRO:HB3	1:A:550:VAL:HG21	1.65	0.79
1:A:556:PHE:O	1:A:557:ILE:HG12	1.83	0.78
1:A:402:LEU:CD2	1:A:454:VAL:HG12	2.14	0.78
1:A:135:ILE:HD11	1:A:142:ILE:HG22	1.65	0.78
1:B:571:THR:HG23	1:B:574:ASP:OD2	1.84	0.78
1:A:176:SER:OG	1:A:495:GLU:HG3	1.83	0.78
1:A:506:VAL:HG13	1:A:507:VAL:N	1.99	0.77
1:B:543:SER:C	1:B:544:LEU:HD23	2.10	0.77
1:A:455:LEU:N	1:A:455:LEU:HD23	1.99	0.76
1:B:592:CYS:HA	1:B:595:ILE:HD12	1.66	0.76
1:B:66:TRP:CH2	1:B:68:LEU:HB2	2.21	0.76
1:B:177:ALA:HA	1:B:180:ARG:HD3	1.67	0.75
1:B:264:MET:CE	1:B:526:GLY:H	1.97	0.75
1:A:43:LEU:HD11	1:A:75:ALA:CB	2.17	0.75
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.66	0.75
1:A:180:ARG:HB2	1:A:180:ARG:HH11	1.52	0.74
1:B:452:ARG:O	1:B:454:VAL:N	2.19	0.74
1:B:112:ALA:O	1:B:188:SER:HB3	1.88	0.73
1:B:326:GLY:O	1:B:366:LEU:HD23	1.88	0.73
1:B:367:ILE:HD11	1:B:591:VAL:CG2	2.18	0.73
1:A:133:VAL:HB	1:A:285:TYR:CE1	2.23	0.73
1:A:556:PHE:C	1:A:557:ILE:HG12	2.13	0.73
1:B:350:GLU:O	1:B:353:ALA:HB3	1.87	0.73
1:B:184:SER:O	1:B:185:ARG:HD3	1.89	0.73
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.23	0.72
1:B:389:THR:HG21	1:B:393:LEU:HD11	1.70	0.72
1:A:43:LEU:HD11	1:A:75:ALA:HB1	1.71	0.72
1:A:144:VAL:HG12	1:A:145:GLY:N	2.04	0.72
1:B:379:LEU:O	1:B:382:TYR:N	2.23	0.72
1:A:550:VAL:CG1	1:A:554:GLY:HA2	2.15	0.71
1:B:55:ALA:HB2	1:B:546:GLY:O	1.90	0.71
1:A:136:MET:HE2	1:A:281:LEU:HA	1.70	0.71
1:B:557:ILE:HG22	1:B:557:ILE:O	1.90	0.71
1:B:144:VAL:HG12	1:B:145:GLY:N	2.06	0.71
1:A:506:VAL:HB	1:A:562:VAL:HG21	1.73	0.70
1:A:267:HIS:CG	1:A:268:PHE:H	2.08	0.70
1:B:119:PRO:CG	1:B:137:THR:HB	2.21	0.70
1:A:529:PHE:O	1:A:543:SER:HA	1.90	0.70
1:B:537:THR:O	1:B:537:THR:HG22	1.90	0.70
1:B:258:SER:O	1:B:260:PHE:N	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ILE:H	1:A:516:ILE:HD12	1.56	0.70
1:A:559:ASN:O	1:A:560:ILE:HB	1.91	0.70
1:B:414:LEU:C	1:B:416:LEU:H	1.99	0.70
1:A:446:TYR:O	1:A:473:GLY:HA3	1.92	0.69
1:B:136:MET:HE3	1:B:283:SER:H	1.57	0.69
1:A:402:LEU:N	1:A:402:LEU:HD12	2.08	0.69
1:B:54:TYR:CZ	1:B:56:PRO:CG	2.74	0.69
1:B:502:ASP:OD2	1:B:562:VAL:HG23	1.93	0.69
1:A:111:PHE:CE1	1:A:540:LYS:HA	2.27	0.69
1:A:352:PHE:HD2	1:A:387:MET:CE	2.06	0.69
1:B:171:THR:OG1	1:B:174:GLU:HG3	1.92	0.68
1:A:54:TYR:CZ	1:A:101:LEU:HD13	2.29	0.68
1:A:401:ILE:C	1:A:402:LEU:HD12	2.18	0.68
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.24	0.68
1:B:433:ASN:HA	1:B:439:VAL:HG23	1.75	0.68
1:A:54:TYR:CE1	1:A:56:PRO:HG2	2.29	0.68
1:A:402:LEU:HD23	1:A:454:VAL:HG12	1.74	0.68
1:A:557:ILE:CG2	1:A:558:GLU:H	1.97	0.68
1:A:352:PHE:CD2	1:A:387:MET:CE	2.76	0.67
1:B:537:THR:O	1:B:537:THR:CG2	2.42	0.67
1:A:180:ARG:NH1	1:A:180:ARG:CB	2.57	0.67
1:A:557:ILE:CG2	1:A:558:GLU:N	2.42	0.67
1:B:398:HIS:HB3	1:B:547:SER:HB2	1.76	0.67
1:A:276:TYR:CE1	1:A:286:ASN:HB3	2.30	0.67
1:A:383:ALA:O	1:A:386:SER:HB3	1.94	0.67
1:B:516:ILE:H	1:B:565:HIS:HD2	1.42	0.67
1:B:552:GLU:OE2	1:B:555:ALA:HB2	1.95	0.67
1:A:587:VAL:O	1:A:591:VAL:HG23	1.95	0.67
1:A:516:ILE:HD12	1:A:516:ILE:N	2.09	0.67
1:B:471:LEU:HD22	1:B:527:PHE:CE1	2.30	0.67
1:A:118:LEU:HD12	1:A:183:PHE:CD2	2.31	0.66
1:B:381:LEU:HD13	1:B:381:LEU:C	2.19	0.66
1:A:559:ASN:O	1:A:560:ILE:CB	2.43	0.66
1:B:467:THR:OG1	1:B:468:PRO:HD2	1.96	0.66
1:A:506:VAL:CG1	1:A:507:VAL:N	2.58	0.66
1:A:518:GLY:O	1:A:564:PRO:HG3	1.95	0.66
1:A:177:ALA:O	1:A:180:ARG:HB2	1.95	0.66
1:B:464:GLU:O	1:B:465:LEU:HB2	1.95	0.66
1:A:536:ARG:HH11	1:A:536:ARG:HB3	1.61	0.66
1:A:535:ASN:ND2	1:A:539:ILE:HB	2.11	0.66
1:B:108:VAL:HG12	1:B:109:THR:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:HIS:CE1	1:B:170:GLY:HA2	2.31	0.65
1:B:543:SER:O	1:B:544:LEU:HD23	1.96	0.65
1:A:446:TYR:C	1:A:473:GLY:HA3	2.20	0.65
1:A:40:LEU:CD2	1:A:76:GLN:HG2	2.27	0.65
1:B:143:ARG:HH21	1:B:204:ARG:NH1	1.95	0.65
1:B:489:ILE:HD12	1:B:513:ARG:HH11	1.62	0.65
1:A:328:LEU:HD11	1:A:352:PHE:HE1	1.62	0.65
1:B:136:MET:CE	1:B:283:SER:HB3	2.27	0.65
1:B:502:ASP:O	1:B:506:VAL:HG12	1.96	0.65
1:B:591:VAL:O	1:B:594:LEU:HB2	1.97	0.65
1:B:359:PHE:O	1:B:363:THR:HB	1.96	0.65
1:B:368:ILE:HD13	1:B:489:ILE:HG23	1.78	0.65
1:B:192:LYS:O	1:B:194:PRO:HD3	1.97	0.65
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.31	0.64
1:A:556:PHE:C	1:A:556:PHE:CD2	2.75	0.64
1:B:143:ARG:NH2	1:B:204:ARG:HD2	2.12	0.64
1:B:601:ILE:HG22	1:B:602:ILE:HG13	1.79	0.64
1:B:161:ALA:HA	1:B:164:TYR:HD2	1.60	0.64
1:A:122:VAL:HG12	1:A:123:GLN:N	2.13	0.64
1:A:602:ILE:HG22	1:A:603:LEU:N	2.11	0.64
1:B:179:LEU:HD23	1:B:182:LEU:HD12	1.79	0.64
1:B:186:MET:H	1:B:191:HIS:CD2	2.16	0.64
1:A:440:ASP:O	1:A:443:VAL:N	2.29	0.64
1:A:494:ASN:N	1:A:494:ASN:HD22	1.93	0.64
1:B:169:LYS:HA	1:B:169:LYS:HE2	1.80	0.64
1:A:180:ARG:CZ	1:A:268:PHE:CZ	2.81	0.64
1:A:369:ASP:HA	1:A:492:LEU:HB2	1.80	0.64
1:B:180:ARG:NH1	1:B:180:ARG:HB2	2.12	0.64
1:A:592:CYS:HA	1:A:595:ILE:HG12	1.80	0.63
1:A:103:ASP:OD1	1:A:105:HIS:HB2	1.99	0.63
1:A:180:ARG:HH11	1:A:180:ARG:CB	2.11	0.63
1:A:393:LEU:HB3	1:A:511:ASN:ND2	2.11	0.63
1:B:136:MET:HE2	1:B:281:LEU:HA	1.79	0.63
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.81	0.63
1:A:114:GLU:HB2	1:A:221:GLU:HB2	1.80	0.63
1:A:182:LEU:HD23	1:A:182:LEU:C	2.24	0.63
1:A:489:ILE:HG13	1:A:513:ARG:NH2	2.14	0.63
1:B:74:SER:O	1:B:77:GLN:HB2	1.98	0.63
1:B:400:MET:HB2	1:B:402:LEU:HD21	1.80	0.63
1:A:297:ILE:HG23	1:A:311:TYR:OH	1.99	0.63
1:A:79:LEU:HD21	1:A:93:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:HD2	1:A:528:VAL:HG12	1.64	0.62
1:B:180:ARG:HD2	1:B:496:GLN:NE2	2.14	0.62
1:A:48:HIS:CE1	1:A:52:VAL:HG21	2.33	0.62
1:B:143:ARG:HE	1:B:204:ARG:NH1	1.96	0.62
1:B:125:SER:HA	1:B:575:ILE:CD1	2.30	0.62
1:A:315:VAL:CG1	1:A:588:LYS:HD2	2.29	0.62
1:A:328:LEU:HD22	1:A:329:ARG:N	2.14	0.62
1:B:108:VAL:HG12	1:B:109:THR:H	1.65	0.62
1:A:59:TRP:CH2	1:A:557:ILE:HB	2.35	0.62
1:A:387:MET:HG2	1:A:480:HIS:HD2	1.64	0.62
1:A:520:ARG:HD3	1:A:559:ASN:OD1	1.99	0.62
1:B:552:GLU:OE2	1:B:555:ALA:CB	2.48	0.62
1:A:204:ARG:HB3	1:A:205:PRO:HD2	1.81	0.62
1:A:326:GLY:O	1:A:366:LEU:HD23	1.99	0.62
1:B:341:PHE:CE1	1:B:348:PRO:HD3	2.35	0.62
1:A:59:TRP:CZ2	1:A:557:ILE:HB	2.35	0.61
1:A:506:VAL:CG1	1:A:507:VAL:H	2.13	0.61
1:B:54:TYR:CE1	1:B:56:PRO:HG2	2.35	0.61
1:B:352:PHE:CE2	1:B:356:ILE:HD11	2.35	0.61
1:B:471:LEU:HD22	1:B:527:PHE:HE1	1.65	0.61
1:B:591:VAL:O	1:B:595:ILE:HG13	2.00	0.61
1:A:592:CYS:HA	1:A:595:ILE:CG1	2.29	0.61
1:B:398:HIS:HA	1:B:548:LEU:O	2.00	0.61
1:B:122:VAL:HG12	1:B:123:GLN:N	2.15	0.61
1:B:38:ASN:O	1:B:39:ALA:C	2.43	0.61
1:A:106:ALA:HA	1:A:543:SER:O	1.99	0.61
1:A:137:THR:HG22	1:A:137:THR:O	2.01	0.61
1:A:409:ASP:HA	1:A:412:ASP:OD2	2.01	0.61
1:B:498:PHE:CD1	1:B:498:PHE:N	2.69	0.61
1:A:583:TYR:O	1:A:587:VAL:HG23	2.00	0.61
1:A:122:VAL:HG13	1:A:131:TYR:O	2.00	0.61
1:A:365:ALA:HB2	1:A:595:ILE:HD13	1.83	0.61
1:B:204:ARG:HB2	1:B:208:THR:HG23	1.82	0.61
1:A:173:ALA:HA	1:A:495:GLU:HB2	1.83	0.61
1:A:332:THR:HA	1:A:374:PRO:HD2	1.83	0.61
1:A:464:GLU:O	1:A:465:LEU:HB2	2.01	0.60
1:B:138:PHE:HD2	1:B:140:SER:HB2	1.65	0.60
1:A:493:ILE:HG13	1:A:519:THR:O	2.01	0.60
1:A:66:TRP:CH2	1:A:68:LEU:HB2	2.37	0.60
1:B:55:ALA:HB3	1:B:56:PRO:CD	2.30	0.60
1:B:56:PRO:O	1:B:57:LYS:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD21	1:A:182:LEU:HD12	1.83	0.60
1:A:365:ALA:HB2	1:A:595:ILE:CD1	2.31	0.60
1:A:432:ASP:C	1:A:439:VAL:HG23	2.26	0.60
1:B:89:PHE:O	1:B:93:VAL:HG23	2.01	0.60
1:A:269:TRP:O	1:A:270:ALA:C	2.45	0.60
1:A:399:ARG:HG3	1:A:399:ARG:HH11	1.67	0.60
1:B:116:ALA:HB3	1:B:185:ARG:HB2	1.83	0.60
1:A:180:ARG:NH1	1:A:180:ARG:HB3	2.15	0.59
1:A:591:VAL:HA	1:A:594:LEU:HD12	1.84	0.59
1:B:542:CYS:SG	1:B:544:LEU:HD21	2.42	0.59
1:A:60:LYS:HD2	1:A:64:LEU:HD12	1.82	0.59
1:B:264:MET:HG2	1:B:526:GLY:O	2.02	0.59
1:B:535:ASN:ND2	1:B:539:ILE:HB	2.18	0.59
1:B:158:ASP:O	1:B:161:ALA:HB3	2.03	0.59
1:B:494:ASN:ND2	1:B:496:GLN:H	1.99	0.59
1:B:136:MET:CE	1:B:281:LEU:HD23	2.31	0.59
1:A:59:TRP:CE2	1:A:557:ILE:HG13	2.38	0.59
1:A:590:LEU:HD23	1:A:600:THR:HG21	1.83	0.59
1:B:45:PHE:O	1:B:48:HIS:HB3	2.02	0.59
1:B:497:ASP:O	1:B:522:ALA:HB3	2.03	0.59
1:A:397:LYS:O	1:A:550:VAL:HG23	2.02	0.59
1:A:269:TRP:O	1:A:272:LEU:N	2.35	0.59
1:B:333:TYR:C	1:B:376:GLY:HA3	2.27	0.59
1:B:601:ILE:HD12	1:B:601:ILE:N	2.18	0.59
1:B:136:MET:HE2	1:B:281:LEU:CA	2.33	0.58
1:B:503:PHE:HA	1:B:506:VAL:CG1	2.33	0.58
1:B:111:PHE:CD2	1:B:540:LYS:HB2	2.37	0.58
1:A:297:ILE:HD11	1:A:325:VAL:CG1	2.33	0.58
1:A:551:ARG:HD2	1:A:552:GLU:HG3	1.84	0.58
1:A:506:VAL:HG22	1:A:510:ASP:OD2	2.04	0.58
1:A:556:PHE:O	1:A:557:ILE:CG1	2.50	0.58
1:A:602:ILE:CG2	1:A:603:LEU:N	2.67	0.58
1:B:111:PHE:CE2	1:B:540:LYS:HB2	2.39	0.58
1:B:417:LEU:HD13	1:B:444:ALA:HB1	1.85	0.58
1:B:136:MET:SD	1:B:281:LEU:HD23	2.43	0.58
1:B:452:ARG:C	1:B:454:VAL:N	2.61	0.58
1:B:187:ALA:C	1:B:189:LEU:H	2.12	0.58
1:B:571:THR:O	1:B:575:ILE:HG13	2.03	0.58
1:A:50:LEU:HD12	1:A:68:LEU:HD12	1.85	0.58
1:A:551:ARG:O	1:A:552:GLU:C	2.47	0.58
1:B:502:ASP:O	1:B:505:PRO:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:VAL:HG12	1:A:518:GLY:N	2.19	0.58
1:A:474:PHE:CD1	1:A:474:PHE:N	2.72	0.58
1:B:110:PHE:N	1:B:110:PHE:CD1	2.71	0.58
1:B:151:VAL:O	1:B:152:ASP:HB2	2.03	0.58
1:B:202:ILE:HG12	1:B:210:ARG:O	2.04	0.58
1:A:72:SER:O	1:A:75:ALA:HB3	2.04	0.57
1:A:59:TRP:O	1:A:61:GLU:N	2.37	0.57
1:A:411:LEU:HD13	1:B:411:LEU:HD11	1.85	0.57
1:A:180:ARG:NH1	1:A:268:PHE:CZ	2.72	0.57
1:B:50:LEU:O	1:B:54:TYR:HB3	2.04	0.57
1:A:118:LEU:HD12	1:A:183:PHE:HD2	1.68	0.57
1:B:119:PRO:CB	1:B:137:THR:HB	2.35	0.57
1:A:135:ILE:O	1:A:136:MET:O	2.22	0.57
1:A:474:PHE:N	1:A:474:PHE:HD1	2.02	0.57
1:A:509:LYS:HB2	1:A:516:ILE:CD1	2.34	0.57
1:B:94:LEU:O	1:B:97:PHE:HB3	2.04	0.57
1:B:407:VAL:O	1:B:411:LEU:HG	2.05	0.57
1:A:541:THR:HG22	1:A:542:CYS:N	2.20	0.57
1:B:494:ASN:C	1:B:494:ASN:HD22	2.12	0.57
1:A:405:ASP:HA	1:A:408:VAL:HG23	1.86	0.56
1:A:307:LEU:CD2	1:A:348:PRO:HB3	2.35	0.56
1:A:591:VAL:O	1:A:594:LEU:HB2	2.05	0.56
1:B:327:PHE:HD2	1:B:327:PHE:C	2.13	0.56
1:B:122:VAL:HG11	1:B:130:PHE:HB3	1.87	0.56
1:B:311:TYR:OH	1:B:327:PHE:CD1	2.56	0.56
1:B:180:ARG:HD2	1:B:496:GLN:HE21	1.70	0.56
1:A:469:ILE:HG23	1:A:470:PRO:HD2	1.88	0.56
1:A:474:PHE:HD1	1:A:474:PHE:H	1.53	0.56
1:B:379:LEU:O	1:B:380:TYR:C	2.49	0.56
1:B:427:ARG:HA	1:B:431:GLY:O	2.04	0.56
1:A:118:LEU:HG	1:A:216:TRP:CE3	2.41	0.56
1:B:265:VAL:HG13	1:B:266:PRO:HD2	1.87	0.56
1:B:138:PHE:CD2	1:B:140:SER:HB2	2.41	0.56
1:B:467:THR:O	1:B:469:ILE:HG13	2.06	0.56
1:B:117:TYR:CD2	1:B:217:ARG:HB2	2.41	0.56
1:B:161:ALA:HA	1:B:164:TYR:CE2	2.40	0.56
1:A:471:LEU:HD22	1:A:527:PHE:HE1	1.71	0.55
1:B:144:VAL:HG12	1:B:145:GLY:H	1.71	0.55
1:B:399:ARG:NH2	1:B:465:LEU:HD23	2.20	0.55
1:A:105:HIS:CD2	1:A:528:VAL:HG12	2.42	0.55
1:A:517:VAL:HG12	1:A:518:GLY:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:SER:OG	1:B:495:GLU:HG3	2.05	0.55
1:B:279:SER:O	1:B:280:GLY:C	2.48	0.55
1:A:387:MET:HG2	1:A:480:HIS:CD2	2.41	0.55
1:A:398:HIS:HD2	1:A:471:LEU:CD2	2.08	0.55
1:B:125:SER:HA	1:B:575:ILE:HD11	1.88	0.55
1:B:327:PHE:C	1:B:327:PHE:CD2	2.83	0.55
1:A:509:LYS:HB2	1:A:516:ILE:HD13	1.88	0.55
1:B:54:TYR:HD1	1:B:544:LEU:HB3	1.72	0.55
1:B:427:ARG:HG2	1:B:439:VAL:HB	1.89	0.55
1:B:398:HIS:HD2	1:B:471:LEU:HG	1.72	0.55
1:A:89:PHE:O	1:A:93:VAL:HG23	2.06	0.55
1:A:98:ILE:C	1:A:100:GLY:H	2.15	0.55
1:A:267:HIS:CG	1:A:268:PHE:N	2.69	0.55
1:A:412:ASP:O	1:A:416:LEU:HB2	2.06	0.55
1:B:114:GLU:HA	1:B:219:VAL:O	2.06	0.55
1:B:450:PHE:C	1:B:452:ARG:N	2.64	0.55
1:B:573:ASN:HB2	1:B:582:GLU:OE2	2.07	0.55
1:A:79:LEU:CD2	1:A:93:VAL:HG11	2.36	0.55
1:A:333:TYR:C	1:A:376:GLY:HA3	2.31	0.55
1:A:405:ASP:HA	1:A:408:VAL:CG2	2.37	0.55
1:B:310:ALA:HA	1:B:327:PHE:O	2.07	0.55
1:B:411:LEU:CD2	1:B:455:LEU:HD11	2.36	0.55
1:B:550:VAL:HG21	1:B:554:GLY:HA2	1.89	0.55
1:A:113:ILE:O	1:A:114:GLU:C	2.50	0.55
1:A:433:ASN:N	1:A:439:VAL:HG23	2.22	0.54
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.35	0.54
1:B:532:GLN:O	1:B:533:PHE:HB3	2.07	0.54
1:B:161:ALA:C	1:B:163:LEU:H	2.16	0.54
1:B:498:PHE:N	1:B:498:PHE:HD1	2.05	0.54
1:B:499:ALA:O	1:B:502:ASP:N	2.32	0.54
1:B:363:THR:HG21	1:B:485:TYR:CE1	2.43	0.54
1:A:307:LEU:HD21	1:A:348:PRO:HB3	1.90	0.54
1:A:441:LEU:HD13	1:A:441:LEU:C	2.33	0.54
1:A:387:MET:HB3	1:A:483:VAL:HG22	1.90	0.54
1:B:450:PHE:O	1:B:454:VAL:HG23	2.08	0.54
1:B:378:VAL:O	1:B:381:LEU:HB3	2.07	0.54
1:B:116:ALA:HB2	1:B:194:PRO:HD2	1.89	0.54
1:B:107:GLY:HA3	1:B:267:HIS:CD2	2.43	0.54
1:A:317:ASP:OD2	1:A:317:ASP:N	2.40	0.53
1:A:557:ILE:HG22	1:A:559:ASN:H	1.73	0.53
1:B:50:LEU:HD23	1:B:544:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:THR:HG21	1:B:485:TYR:HE1	1.73	0.53
1:B:541:THR:HG22	1:B:542:CYS:N	2.24	0.53
1:A:549:ALA:O	1:A:556:PHE:HB3	2.08	0.53
1:B:297:ILE:CD1	1:B:313:SER:HB2	2.39	0.53
1:A:76:GLN:O	1:A:77:GLN:C	2.52	0.53
1:A:110:PHE:HA	1:A:538:GLY:O	2.09	0.53
1:B:56:PRO:O	1:B:59:TRP:N	2.42	0.53
1:B:77:GLN:O	1:B:79:LEU:N	2.41	0.53
1:B:367:ILE:C	1:B:368:ILE:HD12	2.33	0.53
1:A:150:GLU:HG2	1:A:155:PRO:HA	1.90	0.53
1:A:395:LEU:HD21	1:A:477:ILE:HD11	1.90	0.53
1:A:440:ASP:O	1:A:441:LEU:C	2.52	0.53
1:B:494:ASN:ND2	1:B:494:ASN:C	2.64	0.53
1:A:450:PHE:O	1:A:454:VAL:HG22	2.09	0.53
1:A:537:THR:HG22	1:A:537:THR:O	2.08	0.53
1:B:179:LEU:O	1:B:180:ARG:C	2.51	0.53
1:B:204:ARG:HB2	1:B:208:THR:CG2	2.38	0.53
1:B:311:TYR:C	1:B:311:TYR:CD1	2.85	0.53
1:B:333:TYR:N	1:B:375:GLY:O	2.38	0.53
1:B:389:THR:HG21	1:B:393:LEU:CD1	2.39	0.53
1:B:427:ARG:NH1	1:B:427:ARG:HB2	2.24	0.53
1:B:463:ILE:C	1:B:465:LEU:N	2.67	0.53
1:A:265:VAL:HG13	1:A:266:PRO:HD2	1.90	0.53
1:B:269:TRP:O	1:B:270:ALA:C	2.50	0.53
1:B:434:MET:O	1:B:435:GLU:C	2.52	0.53
1:A:556:PHE:C	1:A:556:PHE:HD2	2.16	0.53
1:B:443:VAL:O	1:B:446:TYR:HB2	2.08	0.53
1:B:463:ILE:O	1:B:465:LEU:N	2.42	0.53
1:B:509:LYS:C	1:B:511:ASN:H	2.16	0.53
1:A:182:LEU:HD22	1:A:183:PHE:CD1	2.44	0.52
1:A:280:GLY:O	1:A:281:LEU:C	2.52	0.52
1:A:416:LEU:O	1:A:416:LEU:HD23	2.09	0.52
1:A:487:LYS:CB	1:A:488:PRO:HD2	2.32	0.52
1:B:120:TYR:CD1	1:B:120:TYR:N	2.77	0.52
1:B:463:ILE:C	1:B:465:LEU:H	2.16	0.52
1:B:179:LEU:O	1:B:182:LEU:N	2.37	0.52
1:B:414:LEU:O	1:B:416:LEU:N	2.43	0.52
1:B:433:ASN:CA	1:B:439:VAL:HG23	2.39	0.52
1:A:480:HIS:HB3	1:A:483:VAL:O	2.09	0.52
1:A:506:VAL:HG13	1:A:507:VAL:H	1.69	0.52
1:B:54:TYR:CD1	1:B:544:LEU:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:CZ	1:A:180:ARG:HB3	2.40	0.52
1:A:541:THR:CG2	1:A:542:CYS:N	2.72	0.52
1:B:119:PRO:CB	1:B:137:THR:H	2.16	0.52
1:A:108:VAL:HG12	1:A:109:THR:N	2.24	0.52
1:A:144:VAL:CG1	1:A:145:GLY:H	2.15	0.52
1:A:161:ALA:HA	1:A:164:TYR:CE2	2.45	0.52
1:A:399:ARG:HG3	1:A:399:ARG:NH1	2.25	0.52
1:B:156:VAL:O	1:B:159:VAL:N	2.43	0.52
1:B:379:LEU:O	1:B:382:TYR:HB2	2.09	0.52
1:B:265:VAL:CG1	1:B:266:PRO:HD2	2.39	0.52
1:B:276:TYR:HE1	1:B:286:ASN:HB3	1.74	0.52
1:B:505:PRO:HG2	1:B:506:VAL:H	1.75	0.52
1:A:50:LEU:HD12	1:A:68:LEU:CD1	2.40	0.52
1:A:381:LEU:C	1:A:381:LEU:HD13	2.35	0.52
1:B:39:ALA:HB1	1:B:79:LEU:HD22	1.92	0.52
1:B:180:ARG:HB2	1:B:180:ARG:HH11	1.72	0.52
1:B:403:THR:O	1:B:405:ASP:N	2.43	0.52
1:A:267:HIS:O	1:A:268:PHE:C	2.53	0.51
1:B:452:ARG:C	1:B:454:VAL:H	2.19	0.51
1:A:297:ILE:CD1	1:A:325:VAL:HG11	2.40	0.51
1:A:509:LYS:HG2	1:A:509:LYS:O	2.10	0.51
1:B:43:LEU:O	1:B:46:LEU:N	2.39	0.51
1:B:56:PRO:CD	1:B:545:THR:HB	2.40	0.51
1:B:148:LEU:HD11	1:B:200:LEU:HD22	1.91	0.51
1:B:272:LEU:O	1:B:275:HIS:N	2.39	0.51
1:B:505:PRO:O	1:B:506:VAL:C	2.53	0.51
1:B:601:ILE:HG22	1:B:602:ILE:N	2.25	0.51
1:A:42:ASP:CG	1:A:535:ASN:HB2	2.35	0.51
1:A:439:VAL:HG12	1:A:440:ASP:N	2.26	0.51
1:A:176:SER:O	1:A:177:ALA:C	2.53	0.51
1:B:502:ASP:OD2	1:B:523:GLY:O	2.29	0.51
1:A:451:GLY:O	1:A:454:VAL:CG2	2.57	0.51
1:B:334:SER:HB3	1:B:376:GLY:HA2	1.93	0.51
1:B:541:THR:CG2	1:B:542:CYS:N	2.72	0.51
1:B:516:ILE:N	1:B:565:HIS:HD2	2.08	0.51
1:A:59:TRP:CZ2	1:A:557:ILE:CB	2.94	0.50
1:A:402:LEU:HD21	1:A:454:VAL:HG12	1.92	0.50
1:A:406:GLU:N	1:A:406:GLU:OE2	2.44	0.50
1:B:50:LEU:HD13	1:B:66:TRP:HH2	1.76	0.50
1:B:381:LEU:HD13	1:B:385:LEU:HD12	1.92	0.50
1:A:94:LEU:O	1:A:95:ALA:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:TYR:O	1:A:277:ALA:C	2.51	0.50
1:B:311:TYR:OH	1:B:327:PHE:HD1	1.92	0.50
1:B:470:PRO:HG2	1:B:473:GLY:HA2	1.93	0.50
1:B:503:PHE:O	1:B:504:PHE:C	2.53	0.50
1:A:132:PHE:HE1	1:A:148:LEU:HB2	1.76	0.50
1:A:297:ILE:HD11	1:A:325:VAL:HG12	1.92	0.50
1:A:494:ASN:HD22	1:A:494:ASN:H	1.57	0.50
1:B:56:PRO:HB2	1:B:60:LYS:HG2	1.94	0.50
1:B:441:LEU:HD23	1:B:441:LEU:C	2.35	0.50
1:B:398:HIS:HE2	1:B:503:PHE:HZ	1.59	0.50
1:A:54:TYR:O	1:A:55:ALA:C	2.54	0.50
1:A:398:HIS:CE1	1:A:549:ALA:HB2	2.47	0.50
1:A:597:ASN:O	1:A:598:ASP:HB2	2.10	0.50
1:B:328:LEU:HD22	1:B:329:ARG:N	2.27	0.50
1:A:100:GLY:C	1:A:102:ASN:N	2.69	0.50
1:A:417:LEU:HD12	1:A:417:LEU:O	2.12	0.50
1:A:516:ILE:H	1:A:516:ILE:CD1	2.23	0.50
1:B:143:ARG:NE	1:B:204:ARG:HH11	2.10	0.50
1:A:83:GLU:O	1:A:84:ASN:C	2.54	0.50
1:B:76:GLN:O	1:B:77:GLN:C	2.54	0.50
1:B:176:SER:O	1:B:179:LEU:HB2	2.12	0.50
1:B:59:TRP:C	1:B:61:GLU:N	2.69	0.50
1:A:427:ARG:O	1:A:431:GLY:O	2.29	0.49
1:B:144:VAL:CG1	1:B:145:GLY:N	2.74	0.49
1:B:186:MET:H	1:B:191:HIS:HD2	1.58	0.49
1:A:40:LEU:HD21	1:A:76:GLN:HG2	1.94	0.49
1:A:218:TYR:CG	1:A:219:VAL:N	2.80	0.49
1:A:366:LEU:HB2	1:A:485:TYR:CZ	2.47	0.49
1:A:444:ALA:O	1:A:448:LYS:HG3	2.13	0.49
1:A:265:VAL:CG1	1:A:266:PRO:HD2	2.42	0.49
1:A:390:ASP:HA	1:A:484:GLN:OE1	2.13	0.49
1:B:333:TYR:OH	1:B:504:PHE:CG	2.65	0.49
1:B:450:PHE:O	1:B:452:ARG:N	2.45	0.49
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.78	0.49
1:A:185:ARG:HG3	1:A:185:ARG:NH1	2.27	0.49
1:A:504:PHE:HB3	1:A:505:PRO:HD3	1.94	0.49
1:A:264:MET:HE2	1:A:500:CYS:SG	2.52	0.49
1:A:339:GLU:O	1:A:340:ASP:HB2	2.12	0.49
1:B:551:ARG:CB	1:B:555:ALA:HB3	2.37	0.49
1:B:42:ASP:O	1:B:43:LEU:O	2.30	0.49
1:B:50:LEU:HD13	1:B:66:TRP:CH2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD21	1:B:216:TRP:HA	1.95	0.49
1:B:82:GLN:HG3	1:B:89:PHE:HE2	1.71	0.49
1:B:293:PHE:HZ	1:B:570:PHE:CE1	2.30	0.49
1:B:366:LEU:HD22	1:B:368:ILE:HD12	1.94	0.49
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.95	0.49
1:A:470:PRO:O	1:A:472:PHE:O	2.31	0.48
1:A:498:PHE:CD1	1:A:498:PHE:N	2.81	0.48
1:B:463:ILE:HG13	1:B:464:GLU:N	2.27	0.48
1:B:571:THR:O	1:B:574:ASP:HB2	2.13	0.48
1:A:43:LEU:HD11	1:A:75:ALA:HB3	1.96	0.48
1:A:118:LEU:HG	1:A:216:TRP:CZ3	2.48	0.48
1:A:373:ASN:OD1	1:A:374:PRO:HD2	2.13	0.48
1:A:533:PHE:CD1	1:A:533:PHE:C	2.91	0.48
1:B:76:GLN:O	1:B:77:GLN:O	2.32	0.48
1:B:267:HIS:O	1:B:268:PHE:C	2.56	0.48
1:B:403:THR:O	1:B:407:VAL:HG23	2.12	0.48
1:A:503:PHE:C	1:A:506:VAL:HG12	2.39	0.48
1:B:42:ASP:O	1:B:43:LEU:C	2.55	0.48
1:B:77:GLN:O	1:B:78:LYS:C	2.57	0.48
1:B:328:LEU:O	1:B:368:ILE:HA	2.13	0.48
1:B:568:LEU:HD22	1:B:583:TYR:HD1	1.77	0.48
1:A:439:VAL:O	1:A:440:ASP:HB2	2.12	0.48
1:B:114:GLU:O	1:B:193:VAL:HG21	2.13	0.48
1:B:352:PHE:CG	1:B:384:LEU:HD22	2.48	0.48
1:B:276:TYR:CE1	1:B:286:ASN:HB3	2.48	0.48
1:A:416:LEU:HD23	1:A:416:LEU:C	2.39	0.48
1:B:113:ILE:O	1:B:114:GLU:C	2.56	0.48
1:B:143:ARG:NH2	1:B:204:ARG:NH1	2.62	0.48
1:B:579:GLY:O	1:B:580:TYR:C	2.57	0.48
1:A:279:SER:O	1:A:280:GLY:C	2.57	0.48
1:B:422:THR:O	1:B:423:ASN:C	2.57	0.48
1:B:430:LEU:HB2	1:B:439:VAL:HG11	1.96	0.48
1:B:499:ALA:HA	1:B:525:GLY:HA2	1.95	0.48
1:A:155:PRO:O	1:A:156:VAL:C	2.57	0.47
1:B:89:PHE:O	1:B:92:GLN:HB2	2.14	0.47
1:B:171:THR:HG1	1:B:174:GLU:HG3	1.78	0.47
1:B:327:PHE:HD2	1:B:328:LEU:N	2.11	0.47
1:A:387:MET:SD	1:A:480:HIS:HD2	2.37	0.47
1:A:487:LYS:HB3	1:A:488:PRO:CD	2.32	0.47
1:B:164:TYR:CE1	1:B:168:HIS:NE2	2.82	0.47
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:MET:SD	1:B:378:VAL:HG22	2.54	0.47
1:B:535:ASN:HD21	1:B:539:ILE:HB	1.78	0.47
1:A:87:THR:O	1:A:88:SER:C	2.57	0.47
1:A:372:ASN:H	1:A:494:ASN:HD21	1.62	0.47
1:A:328:LEU:HD22	1:A:328:LEU:C	2.38	0.47
1:A:457:CYS:SG	1:A:466:SER:HB2	2.54	0.47
1:A:493:ILE:HD13	1:A:516:ILE:CG2	2.45	0.47
1:B:122:VAL:HG12	1:B:123:GLN:H	1.79	0.47
1:B:368:ILE:CD1	1:B:489:ILE:HG23	2.44	0.47
1:A:82:GLN:C	1:A:83:GLU:O	2.55	0.47
1:A:586:LYS:O	1:A:590:LEU:HD12	2.14	0.47
1:A:601:ILE:HG22	1:A:602:ILE:N	2.29	0.47
1:B:114:GLU:HG2	1:B:193:VAL:CB	2.44	0.47
1:B:259:LEU:O	1:B:527:PHE:CD2	2.68	0.47
1:B:332:THR:HA	1:B:373:ASN:OD1	2.13	0.47
1:A:122:VAL:HG12	1:A:123:GLN:H	1.79	0.47
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.49	0.47
1:A:202:ILE:HG13	1:A:202:ILE:O	2.15	0.47
1:B:114:GLU:HG2	1:B:193:VAL:HG21	1.97	0.47
1:B:164:TYR:CD1	1:B:168:HIS:CD2	3.03	0.47
1:B:503:PHE:O	1:B:506:VAL:HG13	2.14	0.47
1:A:65:GLY:O	1:A:66:TRP:C	2.58	0.47
1:B:155:PRO:O	1:B:156:VAL:C	2.58	0.47
1:A:441:LEU:HD13	1:A:441:LEU:O	2.15	0.47
1:A:558:GLU:O	1:A:559:ASN:HB2	2.14	0.47
1:B:140:SER:OG	1:B:141:GLU:N	2.47	0.47
1:B:312:ILE:HG23	1:B:325:VAL:O	2.15	0.47
1:A:136:MET:SD	1:A:136:MET:N	2.88	0.47
1:A:144:VAL:CG1	1:A:145:GLY:N	2.74	0.47
1:A:381:LEU:HD13	1:A:382:TYR:N	2.30	0.47
1:A:433:ASN:HD22	1:A:436:GLY:H	1.61	0.47
1:A:466:SER:O	1:A:467:THR:C	2.58	0.47
1:A:503:PHE:O	1:A:507:VAL:HG23	2.15	0.47
1:B:143:ARG:HE	1:B:204:ARG:HH11	1.62	0.47
1:B:437:TYR:CE2	1:B:474:PHE:HE2	2.33	0.47
1:B:503:PHE:O	1:B:506:VAL:CG1	2.62	0.47
1:B:136:MET:HE2	1:B:281:LEU:C	2.40	0.46
1:A:214:VAL:HG12	1:A:215:LYS:N	2.31	0.46
1:B:302:TRP:O	1:B:311:TYR:HB2	2.15	0.46
1:B:446:TYR:CE2	1:B:475:GLU:N	2.78	0.46
1:A:182:LEU:HD22	1:A:183:PHE:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:HA	1:A:527:PHE:CD2	2.50	0.46
1:A:302:TRP:CZ2	1:A:358:VAL:HG11	2.50	0.46
1:B:401:ILE:HG22	1:B:401:ILE:O	2.15	0.46
1:B:444:ALA:O	1:B:448:LYS:HG3	2.15	0.46
1:A:138:PHE:O	1:A:139:SER:C	2.58	0.46
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.46
1:B:483:VAL:HG23	1:B:483:VAL:O	2.15	0.46
1:A:373:ASN:HB3	1:A:501:ALA:HB2	1.96	0.46
1:A:550:VAL:HG12	1:A:554:GLY:CA	2.22	0.46
1:B:60:LYS:HG3	1:B:101:LEU:HD22	1.98	0.46
1:B:382:TYR:O	1:B:383:ALA:C	2.59	0.46
1:A:457:CYS:CB	1:A:466:SER:HB2	2.45	0.46
1:A:602:ILE:CG2	1:A:603:LEU:H	2.29	0.46
1:B:452:ARG:O	1:B:453:GLN:C	2.57	0.46
1:B:499:ALA:O	1:B:500:CYS:C	2.59	0.46
1:B:570:PHE:HE2	1:B:583:TYR:CD2	2.33	0.46
1:A:403:THR:C	1:A:405:ASP:H	2.24	0.46
1:B:73:VAL:O	1:B:74:SER:C	2.59	0.46
1:B:368:ILE:HD12	1:B:368:ILE:N	2.30	0.46
1:B:382:TYR:O	1:B:385:LEU:HB2	2.16	0.46
1:A:317:ASP:HB2	1:A:318:GLY:H	1.58	0.46
1:A:402:LEU:N	1:A:402:LEU:CD1	2.79	0.46
1:A:427:ARG:HA	1:A:439:VAL:CG1	2.35	0.46
1:B:45:PHE:C	1:B:45:PHE:CD2	2.94	0.46
1:B:55:ALA:CB	1:B:56:PRO:CD	2.94	0.46
1:B:152:ASP:C	1:B:154:ALA:N	2.73	0.46
1:A:498:PHE:O	1:A:499:ALA:C	2.59	0.46
1:B:204:ARG:CG	1:B:208:THR:HG23	2.46	0.46
1:B:137:THR:O	1:B:137:THR:CG2	2.64	0.45
1:B:506:VAL:HG13	1:B:507:VAL:H	1.82	0.45
1:B:601:ILE:HD12	1:B:601:ILE:H	1.82	0.45
1:A:177:ALA:O	1:A:178:ALA:C	2.58	0.45
1:A:333:TYR:CE1	1:A:373:ASN:ND2	2.84	0.45
1:A:387:MET:CG	1:A:480:HIS:HD2	2.27	0.45
1:A:467:THR:OG1	1:A:468:PRO:HD2	2.17	0.45
1:B:91:GLN:HA	1:B:110:PHE:CE2	2.51	0.45
1:B:117:TYR:CD2	1:B:217:ARG:CB	2.99	0.45
1:B:271:GLU:O	1:B:272:LEU:C	2.59	0.45
1:A:57:LYS:O	1:A:58:THR:C	2.58	0.45
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.77	0.45
1:B:389:THR:CG2	1:B:393:LEU:HD11	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:PHE:C	1:B:452:ARG:H	2.23	0.45
1:A:54:TYR:O	1:A:54:TYR:CG	2.69	0.45
1:A:423:ASN:HA	1:A:441:LEU:HB2	1.98	0.45
1:A:454:VAL:C	1:A:455:LEU:HD23	2.42	0.45
1:B:118:LEU:HG	1:B:216:TRP:CZ3	2.51	0.45
1:B:143:ARG:NE	1:B:204:ARG:NH1	2.64	0.45
1:B:293:PHE:HZ	1:B:570:PHE:HE1	1.64	0.45
1:B:446:TYR:CD2	1:B:474:PHE:HA	2.52	0.45
1:A:102:ASN:HD22	1:A:102:ASN:HA	1.57	0.45
1:A:407:VAL:HG12	1:A:411:LEU:HD11	1.98	0.45
1:B:70:GLN:C	1:B:70:GLN:CD	2.84	0.45
1:B:82:GLN:CG	1:B:89:PHE:HE2	2.28	0.45
1:B:506:VAL:HG13	1:B:507:VAL:N	2.32	0.45
1:A:118:LEU:CD2	1:A:216:TRP:HA	2.47	0.45
1:A:132:PHE:CE2	1:A:142:ILE:HG21	2.51	0.45
1:A:135:ILE:CD1	1:A:142:ILE:O	2.64	0.45
1:A:403:THR:O	1:A:406:GLU:OE2	2.35	0.45
1:B:55:ALA:HB3	1:B:56:PRO:HD3	1.97	0.45
1:B:180:ARG:NH1	1:B:268:PHE:CZ	2.85	0.45
1:B:414:LEU:C	1:B:416:LEU:N	2.65	0.45
1:B:516:ILE:N	1:B:516:ILE:HD12	2.31	0.45
1:A:197:ARG:HB3	1:A:213:ARG:HE	1.81	0.45
1:A:395:LEU:HB2	1:A:475:GLU:O	2.17	0.45
1:A:443:VAL:O	1:A:446:TYR:HB2	2.17	0.45
1:A:506:VAL:HB	1:A:562:VAL:CG2	2.43	0.45
1:B:157:GLN:H	1:B:157:GLN:CD	2.23	0.45
1:A:45:PHE:O	1:A:46:LEU:C	2.59	0.45
1:A:410:ALA:HB2	1:A:454:VAL:HG21	1.98	0.45
1:B:75:ALA:O	1:B:76:GLN:C	2.60	0.45
1:B:602:ILE:CG2	1:B:603:LEU:N	2.80	0.45
1:A:98:ILE:C	1:A:100:GLY:N	2.75	0.44
1:A:410:ALA:CB	1:A:454:VAL:HG21	2.47	0.44
1:A:413:TRP:CE3	1:A:413:TRP:HA	2.53	0.44
1:A:556:PHE:O	1:A:556:PHE:CD2	2.70	0.44
1:B:134:ASP:OD2	1:B:283:SER:HB2	2.18	0.44
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.32	0.44
1:B:366:LEU:HD22	1:B:368:ILE:CD1	2.47	0.44
1:B:448:LYS:C	1:B:450:PHE:N	2.75	0.44
1:A:135:ILE:HD11	1:A:142:ILE:CG2	2.43	0.44
1:A:427:ARG:CA	1:A:439:VAL:HG11	2.36	0.44
1:B:493:ILE:O	1:B:518:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:SER:O	1:A:91:GLN:HB2	2.17	0.44
1:A:333:TYR:HB2	1:A:375:GLY:O	2.17	0.44
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.63	0.44
1:A:500:CYS:C	1:A:502:ASP:H	2.25	0.44
1:B:143:ARG:NH2	1:B:204:ARG:HH11	2.15	0.44
1:B:152:ASP:C	1:B:154:ALA:H	2.24	0.44
1:A:266:PRO:O	1:A:267:HIS:C	2.59	0.44
1:B:258:SER:C	1:B:260:PHE:H	2.17	0.44
1:A:39:ALA:O	1:A:40:LEU:C	2.60	0.44
1:A:335:TRP:O	1:A:336:GLN:C	2.58	0.44
1:A:539:ILE:H	1:A:539:ILE:HD12	1.82	0.44
1:B:117:TYR:HD2	1:B:217:ARG:CB	2.31	0.44
1:B:152:ASP:O	1:B:154:ALA:N	2.50	0.44
1:B:176:SER:O	1:B:179:LEU:N	2.50	0.44
1:B:186:MET:O	1:B:191:HIS:HB2	2.17	0.44
1:B:302:TRP:CH2	1:B:304:SER:HB2	2.53	0.44
1:A:160:LEU:O	1:A:161:ALA:C	2.61	0.44
1:A:603:LEU:HD23	1:A:603:LEU:O	2.17	0.44
1:B:171:THR:O	1:B:172:ALA:C	2.60	0.44
1:B:568:LEU:HD22	1:B:583:TYR:CD1	2.52	0.44
1:A:151:VAL:HG12	1:A:152:ASP:OD2	2.18	0.44
1:A:297:ILE:HD11	1:A:325:VAL:HG11	1.97	0.44
1:A:318:GLY:C	1:A:319:ASP:OD2	2.61	0.44
1:A:498:PHE:O	1:A:501:ALA:HB3	2.17	0.44
1:B:550:VAL:HG23	1:B:551:ARG:N	2.30	0.44
1:B:551:ARG:O	1:B:552:GLU:C	2.61	0.44
1:A:539:ILE:HD12	1:A:539:ILE:N	2.32	0.44
1:B:108:VAL:CG1	1:B:109:THR:N	2.80	0.44
1:B:127:ASP:OD1	1:B:129:ARG:NH2	2.46	0.44
1:A:49:LEU:HD11	1:A:531:VAL:HG11	2.00	0.44
1:A:133:VAL:HB	1:A:285:TYR:CZ	2.53	0.44
1:A:275:HIS:ND1	1:A:275:HIS:C	2.76	0.44
1:A:276:TYR:CZ	1:A:286:ASN:HB3	2.53	0.44
1:A:358:VAL:O	1:A:358:VAL:CG1	2.66	0.44
1:A:480:HIS:C	1:A:482:ARG:H	2.26	0.44
1:A:574:ASP:HB3	1:A:580:TYR:HA	2.00	0.44
1:B:563:GLU:O	1:B:563:GLU:HG2	2.17	0.44
1:A:373:ASN:HB3	1:A:501:ALA:CB	2.48	0.43
1:B:60:LYS:HA	1:B:60:LYS:HD3	1.82	0.43
1:B:94:LEU:CD1	1:B:537:THR:HG21	2.48	0.43
1:B:107:GLY:HA3	1:B:267:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HA	1:B:119:PRO:HD2	1.76	0.43
1:A:50:LEU:HD21	1:A:98:ILE:CD1	2.48	0.43
1:B:111:PHE:CE2	1:B:540:LYS:CB	3.00	0.43
1:B:168:HIS:NE2	1:B:170:GLY:HA2	2.33	0.43
1:B:531:VAL:O	1:B:531:VAL:HG12	2.18	0.43
1:B:603:LEU:C	1:B:603:LEU:HD23	2.43	0.43
1:A:45:PHE:C	1:A:45:PHE:CD1	2.95	0.43
1:A:122:VAL:CG1	1:A:123:GLN:N	2.78	0.43
1:A:164:TYR:HB3	1:A:168:HIS:CD2	2.54	0.43
1:A:511:ASN:O	1:A:512:ASP:HB2	2.19	0.43
1:A:591:VAL:O	1:A:595:ILE:HG12	2.17	0.43
1:B:138:PHE:HB3	1:B:139:SER:H	1.16	0.43
1:B:392:PRO:HA	1:B:477:ILE:O	2.18	0.43
1:B:411:LEU:HD21	1:B:455:LEU:HD11	2.00	0.43
1:A:138:PHE:O	1:A:139:SER:O	2.36	0.43
1:A:443:VAL:O	1:A:446:TYR:N	2.46	0.43
1:A:498:PHE:O	1:A:501:ALA:N	2.51	0.43
1:B:116:ALA:CB	1:B:194:PRO:HD2	2.48	0.43
1:B:334:SER:O	1:B:336:GLN:N	2.52	0.43
1:A:152:ASP:H	1:A:199:THR:HB	1.83	0.43
1:A:209:THR:O	1:A:210:ARG:HD3	2.17	0.43
1:A:471:LEU:HD22	1:A:527:PHE:CE1	2.53	0.43
1:A:480:HIS:O	1:A:482:ARG:N	2.52	0.43
1:B:420:VAL:HG13	1:B:425:GLU:HB3	2.00	0.43
1:B:592:CYS:O	1:B:593:GLN:C	2.61	0.43
1:A:314:SER:HA	1:A:323:HIS:O	2.19	0.43
1:A:559:ASN:C	1:A:560:ILE:HG13	2.43	0.43
1:B:136:MET:HE1	1:B:281:LEU:HD23	1.98	0.43
1:B:370:GLN:HE21	1:B:370:GLN:HB3	1.52	0.43
1:B:473:GLY:O	1:B:474:PHE:C	2.62	0.43
1:B:504:PHE:HB3	1:B:505:PRO:CD	2.49	0.43
1:B:516:ILE:HG22	1:B:564:PRO:HA	2.00	0.43
1:A:160:LEU:O	1:A:163:LEU:N	2.50	0.43
1:A:352:PHE:CD2	1:A:384:LEU:HD22	2.54	0.43
1:A:568:LEU:C	1:A:568:LEU:CD2	2.92	0.43
1:B:380:TYR:O	1:B:383:ALA:HB3	2.19	0.43
1:B:416:LEU:O	1:B:417:LEU:HD23	2.19	0.43
1:B:556:PHE:O	1:B:557:ILE:C	2.62	0.43
1:A:260:PHE:HA	1:A:527:PHE:CE2	2.54	0.43
1:A:495:GLU:HG2	1:A:496:GLN:HG3	2.00	0.43
1:B:57:LYS:O	1:B:58:THR:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:O	1:B:356:ILE:HG12	2.19	0.43
1:A:94:LEU:O	1:A:97:PHE:HB3	2.18	0.43
1:A:112:ALA:C	1:A:113:ILE:HD13	2.43	0.43
1:A:180:ARG:CD	1:A:496:GLN:HE21	2.23	0.43
1:A:395:LEU:HG	1:A:476:LYS:HA	2.01	0.43
1:A:411:LEU:HD13	1:B:411:LEU:CD1	2.49	0.43
1:A:592:CYS:HA	1:A:595:ILE:HG13	2.00	0.43
1:B:296:VAL:HA	1:B:311:TYR:OH	2.19	0.43
1:A:198:THR:O	1:A:213:ARG:HA	2.19	0.42
1:A:335:TRP:CD1	1:A:335:TRP:H	2.36	0.42
1:A:371:THR:O	1:A:372:ASN:HB2	2.19	0.42
1:B:108:VAL:CG1	1:B:109:THR:H	2.32	0.42
1:A:403:THR:N	1:A:406:GLU:OE2	2.47	0.42
1:A:462:ASP:C	1:A:464:GLU:N	2.73	0.42
1:A:492:LEU:N	1:A:492:LEU:CD2	2.82	0.42
1:A:174:GLU:O	1:A:175:GLU:C	2.62	0.42
1:A:315:VAL:HG11	1:A:588:LYS:HD2	2.01	0.42
1:A:492:LEU:N	1:A:492:LEU:HD23	2.34	0.42
1:A:506:VAL:O	1:A:507:VAL:C	2.62	0.42
1:B:48:HIS:CE1	1:B:52:VAL:HG21	2.55	0.42
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.59	0.42
1:A:398:HIS:ND1	1:A:549:ALA:HA	2.35	0.42
1:A:467:THR:O	1:A:469:ILE:HG13	2.18	0.42
1:A:568:LEU:C	1:A:568:LEU:HD23	2.43	0.42
1:A:171:THR:OG1	1:A:174:GLU:HG3	2.19	0.42
1:A:399:ARG:NH2	1:A:465:LEU:HD23	2.34	0.42
1:B:124:LYS:HG2	1:B:125:SER:O	2.19	0.42
1:A:212:VAL:HG12	1:A:213:ARG:N	2.35	0.42
1:A:500:CYS:C	1:A:502:ASP:N	2.76	0.42
1:A:523:GLY:O	1:A:524:ALA:O	2.37	0.42
1:B:73:VAL:O	1:B:76:GLN:N	2.53	0.42
1:B:458:TRP:O	1:B:458:TRP:CG	2.73	0.42
1:B:551:ARG:HD2	1:B:552:GLU:HG3	2.01	0.42
1:B:564:PRO:O	1:B:565:HIS:C	2.63	0.42
1:A:76:GLN:OE1	1:A:80:ARG:NH1	2.53	0.42
1:A:385:LEU:HD21	1:A:504:PHE:CD1	2.54	0.42
1:A:601:ILE:N	1:A:601:ILE:HD12	2.35	0.42
1:B:601:ILE:H	1:B:601:ILE:CD1	2.32	0.42
1:A:96:ASP:O	1:A:97:PHE:C	2.63	0.41
1:A:136:MET:HG2	1:A:281:LEU:HD23	2.01	0.41
1:A:349:TRP:HB3	1:A:380:TYR:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:THR:O	1:A:407:VAL:HG23	2.19	0.41
1:A:443:VAL:O	1:A:444:ALA:C	2.63	0.41
1:A:493:ILE:HD13	1:A:516:ILE:HG21	2.01	0.41
1:B:90:CYS:O	1:B:91:GLN:C	2.62	0.41
1:B:122:VAL:CG1	1:B:123:GLN:N	2.82	0.41
1:B:186:MET:CE	1:B:275:HIS:HB2	2.50	0.41
1:B:399:ARG:NE	1:B:465:LEU:HG	2.35	0.41
1:B:489:ILE:HG22	1:B:490:CYS:N	2.34	0.41
1:B:601:ILE:N	1:B:601:ILE:CD1	2.81	0.41
1:A:55:ALA:C	1:A:57:LYS:H	2.28	0.41
1:A:353:ALA:HA	1:A:387:MET:HE1	2.01	0.41
1:A:579:GLY:O	1:A:581:SER:N	2.53	0.41
1:B:75:ALA:O	1:B:79:LEU:HD12	2.20	0.41
1:B:427:ARG:HG3	1:B:439:VAL:O	2.20	0.41
1:B:448:LYS:C	1:B:450:PHE:H	2.28	0.41
1:A:533:PHE:CD1	1:A:533:PHE:O	2.74	0.41
1:A:579:GLY:C	1:A:581:SER:N	2.78	0.41
1:A:55:ALA:HB3	1:A:56:PRO:HD3	2.03	0.41
1:A:197:ARG:HD3	1:A:213:ARG:HG2	2.02	0.41
1:A:358:VAL:O	1:A:358:VAL:HG12	2.20	0.41
1:A:446:TYR:HB3	1:A:473:GLY:HA3	2.02	0.41
1:B:416:LEU:HD21	1:B:429:ALA:HB1	2.02	0.41
1:B:515:LEU:HA	1:B:565:HIS:CD2	2.56	0.41
1:A:59:TRP:O	1:A:60:LYS:C	2.62	0.41
1:A:83:GLU:O	1:A:85:PRO:N	2.53	0.41
1:A:464:GLU:O	1:A:465:LEU:CB	2.68	0.41
1:B:48:HIS:ND1	1:B:48:HIS:C	2.79	0.41
1:B:489:ILE:CG2	1:B:490:CYS:N	2.83	0.41
1:B:568:LEU:CD2	1:B:583:TYR:HD1	2.33	0.41
1:A:54:TYR:CE1	1:A:56:PRO:CG	3.03	0.41
1:A:333:TYR:HB2	1:A:375:GLY:C	2.45	0.41
1:A:529:PHE:HB2	1:A:544:LEU:O	2.20	0.41
1:B:272:LEU:O	1:B:273:ARG:C	2.63	0.41
1:B:471:LEU:O	1:B:472:PHE:HB2	2.20	0.41
1:A:67:ASP:O	1:A:68:LEU:C	2.62	0.41
1:A:182:LEU:C	1:A:182:LEU:CD2	2.93	0.41
1:A:204:ARG:HB2	1:A:208:THR:HG23	2.02	0.41
1:A:399:ARG:HB3	1:A:465:LEU:HG	2.01	0.41
1:B:94:LEU:HD12	1:B:537:THR:HG21	2.03	0.41
1:B:516:ILE:N	1:B:565:HIS:CD2	2.72	0.41
1:A:62:GLN:O	1:A:63:TYR:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:O	1:A:92:GLN:C	2.63	0.41
1:A:264:MET:C	1:A:265:VAL:HG23	2.46	0.41
1:A:307:LEU:HD23	1:A:348:PRO:HB3	2.02	0.41
1:A:260:PHE:O	1:A:262:SER:N	2.49	0.41
1:A:311:TYR:CD1	1:A:311:TYR:C	2.99	0.41
1:A:471:LEU:C	1:A:472:PHE:O	2.62	0.41
1:B:59:TRP:CH2	1:B:557:ILE:O	2.73	0.41
1:B:127:ASP:CG	1:B:129:ARG:HH21	2.29	0.41
1:B:139:SER:O	1:B:140:SER:O	2.39	0.41
1:B:163:LEU:HA	1:B:163:LEU:HD23	1.78	0.41
1:B:218:TYR:CG	1:B:219:VAL:N	2.89	0.41
1:B:297:ILE:HD12	1:B:298:GLY:N	2.36	0.41
1:B:450:PHE:O	1:B:451:GLY:C	2.64	0.41
1:B:516:ILE:HG22	1:B:564:PRO:CB	2.50	0.41
1:B:571:THR:HG21	1:B:582:GLU:OE1	2.21	0.41
1:A:149:LEU:HB2	1:A:201:LYS:O	2.21	0.41
1:A:269:TRP:O	1:A:271:GLU:N	2.53	0.41
1:A:395:LEU:HD21	1:A:477:ILE:CD1	2.50	0.41
1:A:447:LEU:O	1:A:450:PHE:HB3	2.21	0.41
1:A:483:VAL:C	1:A:484:GLN:HG3	2.45	0.41
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.88	0.41
1:B:204:ARG:CB	1:B:208:THR:HG23	2.50	0.41
1:A:199:THR:C	1:A:200:LEU:HG	2.46	0.40
1:A:353:ALA:CA	1:A:387:MET:HE1	2.51	0.40
1:A:523:GLY:CA	1:A:560:ILE:CG2	2.92	0.40
1:B:123:GLN:NE2	1:B:285:TYR:HE2	2.19	0.40
1:B:417:LEU:HB3	1:B:448:LYS:HD2	2.02	0.40
1:A:112:ALA:O	1:A:113:ILE:HD13	2.20	0.40
1:A:188:SER:HB3	1:A:271:GLU:OE2	2.21	0.40
1:A:417:LEU:CD1	1:A:448:LYS:HG2	2.52	0.40
1:B:187:ALA:C	1:B:189:LEU:N	2.77	0.40
1:B:353:ALA:O	1:B:354:LYS:C	2.64	0.40
1:A:54:TYR:CE2	1:A:101:LEU:HD13	2.56	0.40
1:A:95:ALA:O	1:A:96:ASP:C	2.65	0.40
1:B:114:GLU:HG2	1:B:193:VAL:HB	2.04	0.40
1:B:136:MET:HE1	1:B:281:LEU:CD2	2.51	0.40
1:A:55:ALA:O	1:A:57:LYS:N	2.55	0.40
1:A:180:ARG:CB	1:A:180:ARG:CZ	2.99	0.40
1:A:265:VAL:HG12	1:A:266:PRO:N	2.37	0.40
1:A:439:VAL:HG12	1:A:440:ASP:H	1.86	0.40
1:B:39:ALA:CB	1:B:79:LEU:HD22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:C	1:B:48:HIS:N	2.77	0.40
1:B:136:MET:CE	1:B:283:SER:H	2.27	0.40
1:B:480:HIS:CE1	1:B:482:ARG:HB2	2.56	0.40
1:B:501:ALA:O	1:B:505:PRO:CD	2.68	0.40
1:A:186:MET:CE	1:A:275:HIS:HB2	2.51	0.40
1:A:203:ARG:C	1:A:204:ARG:O	2.64	0.40
1:A:333:TYR:CD2	1:A:381:LEU:HB2	2.56	0.40
1:A:353:ALA:N	1:A:387:MET:HE1	2.37	0.40
1:B:54:TYR:CE1	1:B:56:PRO:CG	3.02	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	533/583 (91%)	397 (74%)	90 (17%)	46 (9%)	0	4
1	B	533/583 (91%)	404 (76%)	88 (16%)	41 (8%)	1	5
All	All	1066/1166 (91%)	801 (75%)	178 (17%)	87 (8%)	0	5

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	136	MET
1	A	139	SER
1	A	261	TYR
1	A	268	PHE
1	A	283	SER
1	A	317	ASP
1	A	524	ALA
1	A	552	GLU

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Mol	Chain	Res	Type
1	A	559	ASN
1	B	43	LEU
1	B	44	SER
1	B	57	LYS
1	B	77	GLN
1	B	114	GLU
1	B	140	SER
1	B	259	LEU
1	B	268	PHE
1	B	335	TRP
1	B	453	GLN
1	B	465	LEU
1	B	552	GLU
1	B	555	ALA
1	B	556	PHE
1	B	557	ILE
1	B	596	ASN
1	B	598	ASP
1	B	601	ILE
1	A	59	TRP
1	A	66	TRP
1	A	83	GLU
1	A	276	TYR
1	A	280	GLY
1	A	281	LEU
1	A	331	PRO
1	A	404	GLN
1	A	465	LEU
1	A	521	THR
1	A	557	ILE
1	A	580	TYR
1	A	596	ASN
1	A	598	ASP
1	B	62	GLN
1	B	78	LYS
1	B	156	VAL
1	B	281	LEU
1	B	404	GLN
1	B	415	THR
1	B	578	LYS
1	A	144	VAL
1	A	270	ALA

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Mol	Chain	Res	Type
1	A	343	PRO
1	A	405	ASP
1	A	440	ASP
1	A	556	PHE
1	A	560	ILE
1	B	34	LEU
1	B	119	PRO
1	B	188	SER
1	B	283	SER
1	B	464	GLU
1	A	99	GLY
1	A	145	GLY
1	B	207	GLY
1	B	510	ASP
1	A	55	ALA
1	A	204	ARG
1	A	460	LYS
1	A	499	ALA
1	A	572	ALA
1	A	601	ILE
1	B	52	VAL
1	B	55	ALA
1	B	144	VAL
1	B	427	ARG
1	B	505	PRO
1	A	77	GLN
1	A	164	TYR
1	A	504	PHE
1	A	56	PRO
1	A	481	PRO
1	B	69	VAL
1	B	454	VAL
1	B	506	VAL
1	B	408	VAL
1	A	348	PRO
1	A	374	PRO

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	463/505 (92%)	416 (90%)	47 (10%)	7	26
1	B	463/505 (92%)	408 (88%)	55 (12%)	5	20
All	All	926/1010 (92%)	824 (89%)	102 (11%)	6	23

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	43	LEU
1	A	58	THR
1	A	68	LEU
1	A	70	GLN
1	A	84	ASN
1	A	86	SER
1	A	102	ASN
1	A	117	TYR
1	A	136	MET
1	A	138	PHE
1	A	139	SER
1	A	162	THR
1	A	208	THR
1	A	268	PHE
1	A	272	LEU
1	A	290	THR
1	A	300	VAL
1	A	315	VAL
1	A	317	ASP
1	A	325	VAL
1	A	328	LEU
1	A	366	LEU
1	A	370	GLN
1	A	378	VAL
1	A	381	LEU
1	A	421	ASP
1	A	438	THR
1	A	454	VAL
1	A	455	LEU
1	A	459	SER
1	A	465	LEU
1	A	474	PHE

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Mol	Chain	Res	Type
1	A	483	VAL
1	A	492	LEU
1	A	494	ASN
1	A	498	PHE
1	A	503	PHE
1	A	513	ARG
1	A	516	ILE
1	A	519	THR
1	A	536	ARG
1	A	543	SER
1	A	548	LEU
1	A	550	VAL
1	A	552	GLU
1	A	568	LEU
1	B	41	GLN
1	B	43	LEU
1	B	59	TRP
1	B	70	GLN
1	B	87	THR
1	B	93	VAL
1	B	96	ASP
1	B	102	ASN
1	B	110	PHE
1	B	113	ILE
1	B	136	MET
1	B	137	THR
1	B	138	PHE
1	B	142	ILE
1	B	143	ARG
1	B	151	VAL
1	B	182	LEU
1	B	184	SER
1	B	189	LEU
1	B	268	PHE
1	B	269	TRP
1	B	281	LEU
1	B	283	SER
1	B	287	ILE
1	B	290	THR
1	B	297	ILE
1	B	300	VAL
1	B	327	PHE

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Mol	Chain	Res	Type
1	B	328	LEU
1	B	363	THR
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	394	GLU
1	B	400	MET
1	B	405	ASP
1	B	406	GLU
1	B	441	LEU
1	B	447	LEU
1	B	458	TRP
1	B	494	ASN
1	B	498	PHE
1	B	513	ARG
1	B	515	LEU
1	B	529	PHE
1	B	532	GLN
1	B	537	THR
1	B	543	SER
1	B	550	VAL
1	B	552	GLU
1	B	553	HIS
1	B	556	PHE
1	B	563	GLU
1	B	571	THR
1	B	586	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	62	GLN
1	A	84	ASN
1	A	92	GLN
1	A	102	ASN
1	A	105	HIS
1	A	123	GLN
1	A	370	GLN
1	A	423	ASN
1	A	433	ASN
1	A	478	HIS

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Mol	Chain	Res	Type
1	A	480	HIS
1	A	494	ASN
1	A	496	GLN
1	A	532	GLN
1	A	565	HIS
1	A	596	ASN
1	B	84	ASN
1	B	102	ASN
1	B	105	HIS
1	B	123	GLN
1	B	191	HIS
1	B	274	ASN
1	B	275	HIS
1	B	362	ASN
1	B	419	ASN
1	B	423	ASN
1	B	433	ASN
1	B	453	GLN
1	B	456	ASN
1	B	478	HIS
1	B	494	ASN
1	B	496	GLN
1	B	530	ASN
1	B	565	HIS
1	B	596	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	537/583 (92%)	0.05	16 (2%) 52 35	54, 107, 187, 198	0
1	B	537/583 (92%)	-0.17	11 (2%) 65 46	43, 90, 169, 198	0
All	All	1074/1166 (92%)	-0.06	27 (2%) 58 39	43, 98, 181, 198	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	463	ILE	7.0
1	A	463	ILE	6.1
1	B	554	GLY	5.2
1	A	462	ASP	4.1
1	A	259	LEU	3.7
1	B	404	GLN	3.5
1	A	281	LEU	3.4
1	A	560	ILE	3.4
1	B	63	TYR	3.4
1	A	258	SER	3.4
1	A	404	GLN	3.2
1	A	548	LEU	2.9
1	B	280	GLY	2.6
1	B	556	PHE	2.6
1	A	556	PHE	2.5
1	B	305	GLU	2.4
1	B	258	SER	2.4
1	A	66	TRP	2.3
1	B	464	GLU	2.3
1	B	560	ILE	2.2
1	A	557	ILE	2.2
1	A	214	VAL	2.1
1	B	137	THR	2.1
1	A	339	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	TRP	2.0
1	A	358	VAL	2.0
1	A	576	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.