



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:56 AM UTC

PDB ID : 3CQF / pdb_00003cqf
Title : Crystal structure of anthrolysin O (ALO)
Authors : Bourdeau, R.W.; Malito, E.; Tang, W.J.
Deposited on : 2008-04-02
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

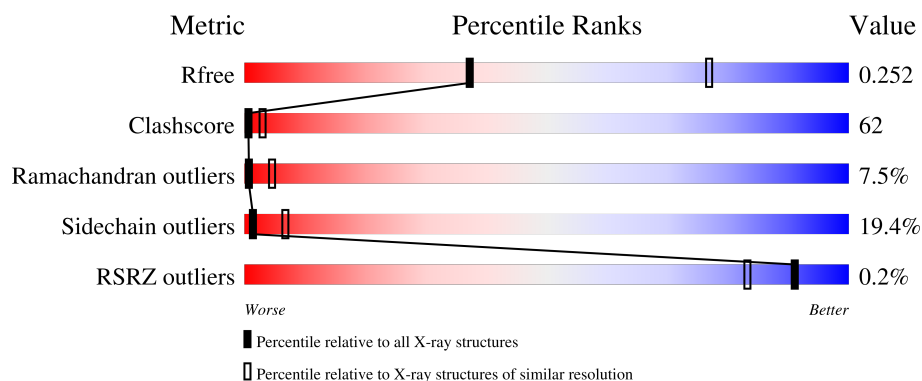
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

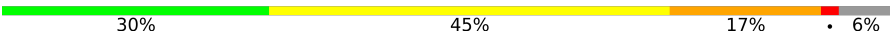
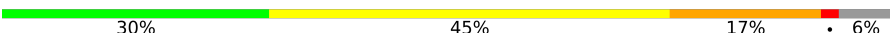
The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	489	 30% 45% 17% • 6%
1	B	489	 30% 45% 17% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7101 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 Thiol-activated cytolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3537	2229	588	714	6			
1	B	462	Total	C	N	O	S	0	0	0
			3537	2229	588	714	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP Q81N62
A	25	HIS	-	expression tag	UNP Q81N62
A	26	HIS	-	expression tag	UNP Q81N62
A	27	HIS	-	expression tag	UNP Q81N62
A	28	HIS	-	expression tag	UNP Q81N62
A	29	HIS	-	expression tag	UNP Q81N62
A	30	HIS	-	expression tag	UNP Q81N62
A	31	ALA	-	expression tag	UNP Q81N62
A	32	ALA	-	expression tag	UNP Q81N62
A	33	ALA	-	expression tag	UNP Q81N62
A	34	MET	-	expression tag	UNP Q81N62
B	24	MET	-	expression tag	UNP Q81N62
B	25	HIS	-	expression tag	UNP Q81N62
B	26	HIS	-	expression tag	UNP Q81N62
B	27	HIS	-	expression tag	UNP Q81N62
B	28	HIS	-	expression tag	UNP Q81N62
B	29	HIS	-	expression tag	UNP Q81N62
B	30	HIS	-	expression tag	UNP Q81N62
B	31	ALA	-	expression tag	UNP Q81N62
B	32	ALA	-	expression tag	UNP Q81N62
B	33	ALA	-	expression tag	UNP Q81N62
B	34	MET	-	expression tag	UNP Q81N62

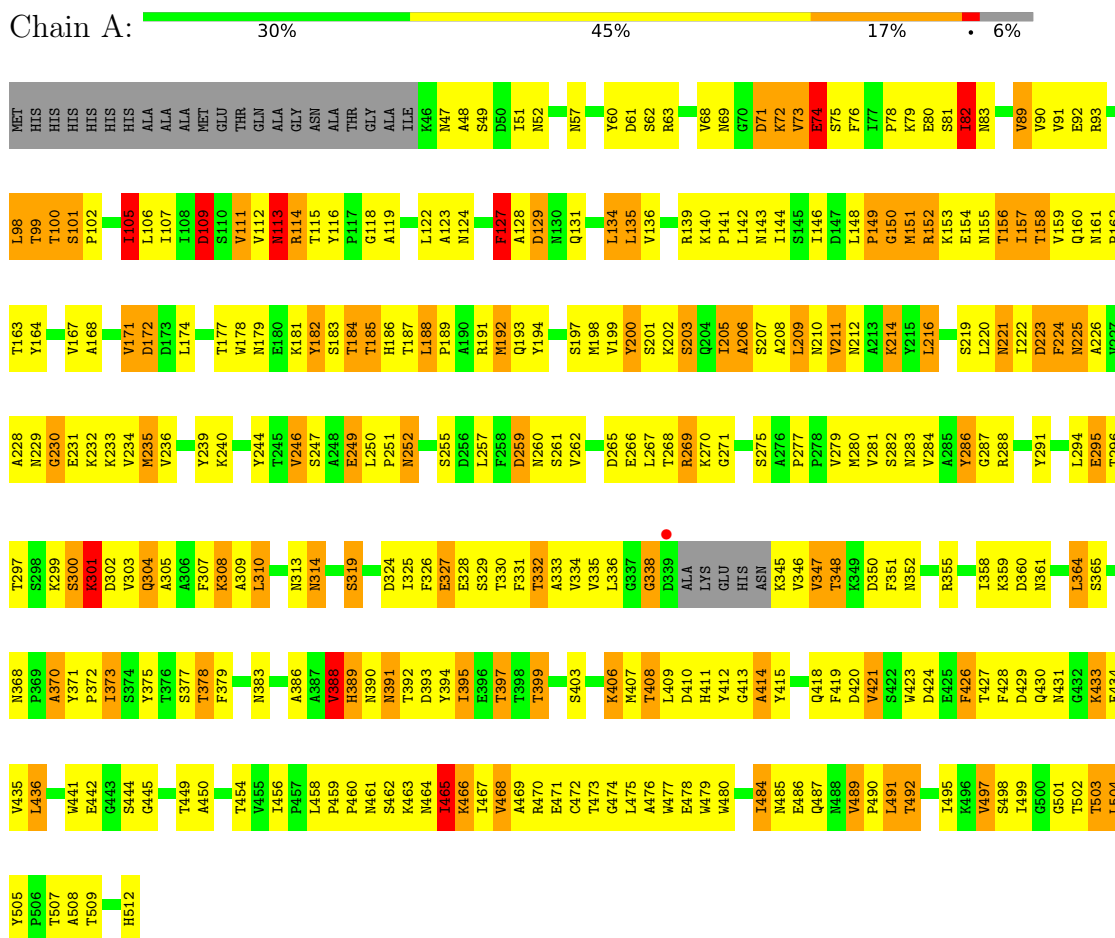
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total 11	O 11	0	0
2	B	16	Total 16	O 16	0	0

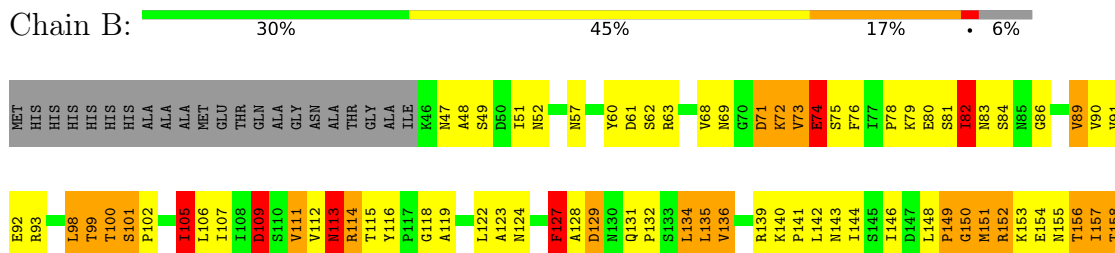
3 Residue-property plots

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: Thiol-activated cytolysin



- Molecule 1: Thiol-activated cytolysin





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.74Å 141.75Å 294.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.10) 98.4 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.268 , 0.294 (Not available) , 0.252	Depositor DCC
R_{free} test set	2675 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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	0.87	3/3606 (0.1%)	1.21	23/4922 (0.5%)
1	B	0.87	3/3606 (0.1%)	1.21	22/4922 (0.4%)
All	All	0.87	6/7212 (0.1%)	1.21	45/9844 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	TYR	CA-C	5.96	1.57	1.52
1	A	200	TYR	CA-C	5.75	1.56	1.52
1	A	484	ILE	CA-CB	5.58	1.61	1.54
1	B	246	VAL	CA-CB	-5.33	1.48	1.54
1	B	484	ILE	CA-CB	5.16	1.61	1.54
1	A	246	VAL	CA-CB	-5.13	1.47	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	VAL	N-CA-C	10.55	117.50	106.21
1	B	388	VAL	N-CA-C	10.24	117.17	106.21
1	A	140	LYS	CA-C-N	-8.12	112.35	120.31
1	A	140	LYS	C-N-CA	-8.12	112.35	120.31
1	B	153	LYS	N-CA-C	-7.71	103.70	113.72
1	B	140	LYS	CA-C-N	-7.50	112.96	120.31
1	B	140	LYS	C-N-CA	-7.50	112.96	120.31
1	A	153	LYS	N-CA-C	-7.44	104.04	113.72
1	A	489	VAL	CA-C-N	6.81	128.35	119.84
1	A	489	VAL	C-N-CA	6.81	128.35	119.84
1	B	489	VAL	CA-C-N	6.69	128.21	119.84
1	B	489	VAL	C-N-CA	6.69	128.21	119.84
1	A	476	ALA	CB-CA-C	-6.69	108.85	116.54
1	B	48	ALA	N-CA-C	-6.64	104.28	112.38
1	A	136	VAL	N-CA-C	6.57	117.80	108.93
1	B	476	ALA	CB-CA-C	-6.51	109.05	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASN	N-CA-C	6.39	120.00	111.30
1	A	48	ALA	N-CA-C	-6.24	104.77	112.38
1	B	149	PRO	N-CA-CB	6.16	109.71	103.25
1	A	99	THR	N-CA-C	6.01	117.78	109.54
1	A	149	PRO	N-CA-CB	5.99	109.54	103.25
1	B	136	VAL	N-CA-C	5.88	116.87	108.93
1	B	99	THR	N-CA-C	5.74	117.40	109.54
1	A	246	VAL	CB-CA-C	-5.73	103.21	111.34
1	B	246	VAL	CB-CA-C	-5.60	103.90	111.63
1	A	188	LEU	N-CA-C	5.53	116.92	109.24
1	A	161	ASN	CA-C-N	5.47	126.68	119.84
1	A	161	ASN	C-N-CA	5.47	126.68	119.84
1	A	127	PHE	N-CA-C	-5.45	104.98	111.03
1	B	161	ASN	CA-C-N	5.43	126.63	119.84
1	B	161	ASN	C-N-CA	5.43	126.63	119.84
1	A	131	GLN	CA-C-N	-5.39	114.40	119.85
1	A	131	GLN	C-N-CA	-5.39	114.40	119.85
1	A	89	VAL	CB-CA-C	-5.26	104.15	110.99
1	B	388	VAL	CB-CA-C	-5.25	107.34	113.22
1	B	234	VAL	N-CA-C	5.24	115.82	108.17
1	A	105	ILE	CB-CA-C	-5.20	102.76	111.29
1	A	388	VAL	CB-CA-C	-5.17	107.43	113.22
1	B	197	SER	N-CA-C	5.16	116.68	108.79
1	A	313	ASN	N-CA-C	5.15	114.83	108.19
1	B	89	VAL	CB-CA-C	-5.12	104.33	110.99
1	A	389	HIS	N-CA-C	5.03	117.84	110.30
1	B	131	GLN	CA-C-N	-5.02	114.78	119.85
1	B	131	GLN	C-N-CA	-5.02	114.78	119.85
1	B	127	PHE	N-CA-C	-5.02	105.50	110.97

There are no chirality outliers.

There are no planarity outliers.

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	3537	0	3406	435	0
1	B	3537	0	3406	432	0
2	A	11	0	0	1	0
2	B	16	0	0	1	0
All	All	7101	0	6812	864	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 62.

All (864) 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:B:504:LEU:HD23	1:B:504:LEU:C	1.54	1.31
1:A:152:ARG:NH2	1:A:178:TRP:HB2	1.46	1.30
1:B:152:ARG:NH2	1:B:178:TRP:HB2	1.47	1.26
1:A:504:LEU:C	1:A:504:LEU:HD23	1.56	1.22
1:A:433:LYS:HA	1:A:433:LYS:CE	1.71	1.17
1:B:181:LYS:O	1:B:182:TYR:CD2	1.98	1.17
1:A:181:LYS:O	1:A:182:TYR:CD2	1.98	1.16
1:B:433:LYS:HA	1:B:433:LYS:CE	1.73	1.15
1:B:234:VAL:HG22	1:B:295:GLU:HB2	1.25	1.15
1:A:433:LYS:HE2	1:A:433:LYS:CA	1.77	1.14
1:B:152:ARG:HH21	1:B:178:TRP:CB	1.61	1.14
1:B:433:LYS:HE2	1:B:433:LYS:CA	1.78	1.13
1:A:152:ARG:HH21	1:A:178:TRP:CB	1.61	1.12
1:A:135:LEU:O	1:A:135:LEU:CD2	1.98	1.11
1:A:332:THR:CG2	1:A:347:VAL:HG23	1.82	1.10
1:B:465:ILE:HG22	1:B:466:LYS:H	1.12	1.10
1:B:332:THR:CG2	1:B:347:VAL:HG23	1.82	1.10
1:A:239:TYR:CE1	1:A:358:ILE:HD13	1.88	1.09
1:A:251:PRO:HD3	1:A:280:MET:HE1	1.33	1.08
1:A:406:LYS:HA	1:A:406:LYS:HZ2	1.16	1.08
1:A:334:VAL:HG12	1:A:345:LYS:HG3	1.35	1.08
1:A:234:VAL:HG22	1:A:295:GLU:HB2	1.24	1.08
1:B:239:TYR:CE1	1:B:358:ILE:HD13	1.88	1.08
1:B:251:PRO:HD3	1:B:280:MET:HE1	1.32	1.08
1:B:388:VAL:O	1:B:388:VAL:CG1	2.01	1.07
1:A:200:TYR:HD1	1:A:394:TYR:CE1	1.73	1.07
1:A:135:LEU:C	1:A:135:LEU:HD23	1.79	1.07
1:A:332:THR:HG23	1:A:347:VAL:CG2	1.85	1.07
1:B:200:TYR:HD1	1:B:394:TYR:CE1	1.72	1.06
1:A:465:ILE:HG22	1:A:466:LYS:H	1.15	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:HG23	1:B:347:VAL:CG2	1.86	1.06
1:B:334:VAL:HG12	1:B:345:LYS:HG3	1.35	1.05
1:B:465:ILE:HG21	1:B:489:VAL:HB	1.33	1.05
1:B:135:LEU:CD2	1:B:135:LEU:O	2.04	1.04
1:B:135:LEU:HD23	1:B:135:LEU:C	1.81	1.04
1:A:388:VAL:CG1	1:A:388:VAL:O	2.01	1.04
1:A:465:ILE:HG21	1:A:489:VAL:HB	1.35	1.04
1:A:406:LYS:HZ3	1:A:406:LYS:HB2	1.15	1.03
1:B:200:TYR:CD1	1:B:394:TYR:HE1	1.77	1.03
1:A:200:TYR:CD1	1:A:394:TYR:HE1	1.77	1.03
1:A:230:GLY:O	1:A:299:LYS:HE2	1.58	1.02
1:A:504:LEU:HD23	1:A:504:LEU:O	1.58	1.02
1:B:406:LYS:HB2	1:B:406:LYS:HZ3	1.18	1.02
1:B:406:LYS:HZ2	1:B:406:LYS:HA	1.21	1.02
1:A:465:ILE:HG22	1:A:466:LYS:N	1.69	1.01
1:B:504:LEU:HD23	1:B:504:LEU:O	1.57	1.01
1:B:230:GLY:O	1:B:299:LYS:HE2	1.60	1.01
1:A:135:LEU:O	1:A:135:LEU:HD23	1.57	1.00
1:B:203:SER:HB2	1:B:392:THR:HG23	1.41	1.00
1:B:388:VAL:O	1:B:388:VAL:HG12	1.59	1.00
1:A:294:LEU:HD23	1:A:331:PHE:HD1	1.26	0.99
1:A:433:LYS:NZ	1:A:434:GLU:H	1.58	0.99
1:A:388:VAL:O	1:A:388:VAL:HG12	1.61	0.99
1:B:327:GLU:OE2	1:B:327:GLU:HA	1.62	0.99
1:B:465:ILE:HG22	1:B:466:LYS:N	1.67	0.99
1:A:209:LEU:HD11	1:A:236:VAL:HG12	1.42	0.99
1:B:71:ASP:O	1:B:72:LYS:O	1.79	0.98
1:A:327:GLU:OE2	1:A:327:GLU:HA	1.58	0.98
1:B:209:LEU:HD11	1:B:236:VAL:HG12	1.40	0.98
1:B:433:LYS:NZ	1:B:434:GLU:H	1.60	0.98
1:A:203:SER:HB2	1:A:392:THR:HG23	1.42	0.98
1:A:310:LEU:HD23	1:A:310:LEU:O	1.64	0.98
1:B:294:LEU:HD23	1:B:331:PHE:HD1	1.26	0.97
1:A:504:LEU:C	1:A:504:LEU:CD2	2.37	0.97
1:B:428:PHE:HA	1:B:433:LYS:O	1.63	0.97
1:B:233:LYS:HE3	1:B:399:THR:HB	1.47	0.97
1:B:294:LEU:HD23	1:B:331:PHE:CD1	2.00	0.97
1:A:252:ASN:N	1:A:252:ASN:HD22	1.61	0.97
1:B:411:HIS:CD2	1:B:413:GLY:H	1.81	0.96
1:A:71:ASP:O	1:A:72:LYS:O	1.81	0.96
1:B:504:LEU:C	1:B:504:LEU:CD2	2.35	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ILE:CG2	1:B:466:LYS:N	2.29	0.96
1:B:203:SER:HB2	1:B:392:THR:CG2	1.95	0.95
1:B:310:LEU:O	1:B:310:LEU:HD23	1.65	0.95
1:A:294:LEU:HD23	1:A:331:PHE:CD1	1.99	0.95
1:A:411:HIS:CD2	1:A:413:GLY:H	1.82	0.95
1:B:135:LEU:O	1:B:135:LEU:HD23	1.65	0.95
1:B:411:HIS:HD2	1:B:413:GLY:H	1.08	0.94
1:A:411:HIS:HD2	1:A:413:GLY:H	1.08	0.94
1:B:209:LEU:HD11	1:B:236:VAL:CG1	1.97	0.94
1:A:200:TYR:HD1	1:A:394:TYR:HE1	0.98	0.94
1:B:502:THR:HG22	1:B:504:LEU:N	1.83	0.93
1:B:109:ASP:OD1	1:B:338:GLY:HA2	1.69	0.93
1:B:252:ASN:N	1:B:252:ASN:HD22	1.61	0.93
1:B:473:THR:HG22	1:B:479:TRP:C	1.93	0.93
1:A:203:SER:HB2	1:A:392:THR:CG2	1.98	0.92
1:A:209:LEU:HD11	1:A:236:VAL:CG1	1.98	0.92
1:A:233:LYS:HE3	1:A:399:THR:HB	1.50	0.92
1:A:473:THR:HG22	1:A:479:TRP:C	1.93	0.92
1:B:200:TYR:HD1	1:B:394:TYR:HE1	0.98	0.92
1:A:465:ILE:CG2	1:A:466:LYS:N	2.31	0.91
1:B:332:THR:HG23	1:B:347:VAL:HG23	0.95	0.91
1:A:428:PHE:HA	1:A:433:LYS:O	1.69	0.91
1:A:109:ASP:OD1	1:A:338:GLY:HA2	1.70	0.91
1:B:111:VAL:HG13	1:B:114:ARG:HD3	1.51	0.91
1:A:502:THR:HG22	1:A:504:LEU:N	1.85	0.90
1:A:149:PRO:O	1:A:151:MET:N	2.05	0.90
1:A:406:LYS:HZ3	1:A:406:LYS:CB	1.84	0.90
1:A:111:VAL:O	1:A:111:VAL:HG12	1.73	0.89
1:A:334:VAL:HG12	1:A:345:LYS:CG	2.03	0.88
1:A:111:VAL:HG13	1:A:114:ARG:HD3	1.55	0.88
1:B:73:VAL:O	1:B:74:GLU:HB3	1.72	0.88
1:B:149:PRO:O	1:B:151:MET:N	2.05	0.88
1:B:406:LYS:HZ3	1:B:406:LYS:CB	1.85	0.88
1:A:234:VAL:CG2	1:A:295:GLU:HB2	2.04	0.88
1:A:406:LYS:CB	1:A:406:LYS:NZ	2.37	0.87
1:A:234:VAL:HG22	1:A:295:GLU:CB	2.03	0.87
1:B:234:VAL:HG22	1:B:295:GLU:CB	2.03	0.87
1:B:100:THR:HG22	1:B:101:SER:H	1.39	0.87
1:B:234:VAL:CG2	1:B:295:GLU:HB2	2.05	0.87
1:B:150:GLY:H	1:B:178:TRP:HE1	1.22	0.87
1:A:191:ARG:HD3	2:A:514:HOH:O	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HA	1:A:406:LYS:NZ	1.90	0.86
1:B:139:ARG:NH1	1:B:257:LEU:HD22	1.90	0.86
1:B:252:ASN:N	1:B:252:ASN:ND2	2.19	0.86
1:A:100:THR:HG22	1:A:101:SER:H	1.40	0.86
1:A:332:THR:HG23	1:A:347:VAL:HG23	0.93	0.86
1:A:99:THR:HG22	1:A:99:THR:O	1.74	0.86
1:B:99:THR:O	1:B:99:THR:HG22	1.74	0.86
1:B:334:VAL:HG12	1:B:345:LYS:CG	2.06	0.86
1:A:135:LEU:O	1:A:135:LEU:HD22	1.73	0.85
1:A:73:VAL:O	1:A:74:GLU:HB3	1.76	0.85
1:A:150:GLY:H	1:A:178:TRP:HE1	1.21	0.85
1:A:406:LYS:HB2	1:A:406:LYS:NZ	1.89	0.85
1:A:201:SER:C	1:A:224:PHE:HE1	1.85	0.84
1:B:135:LEU:O	1:B:135:LEU:HD22	1.76	0.84
1:B:406:LYS:HB2	1:B:406:LYS:NZ	1.93	0.84
1:A:406:LYS:NZ	1:A:406:LYS:CA	2.41	0.83
1:B:201:SER:C	1:B:224:PHE:HE1	1.86	0.83
1:B:252:ASN:ND2	1:B:252:ASN:H	1.75	0.83
1:B:406:LYS:HA	1:B:406:LYS:NZ	1.92	0.83
1:B:502:THR:HG22	1:B:504:LEU:H	1.43	0.83
1:A:252:ASN:N	1:A:252:ASN:ND2	2.20	0.83
1:B:228:ALA:O	1:B:397:THR:HG21	1.78	0.83
1:A:202:LYS:N	1:A:224:PHE:CE1	2.47	0.82
1:B:111:VAL:HG12	1:B:111:VAL:O	1.78	0.82
1:A:406:LYS:HZ2	1:A:406:LYS:CA	1.91	0.82
1:A:135:LEU:CD2	1:A:135:LEU:C	2.49	0.82
1:B:202:LYS:N	1:B:224:PHE:CE1	2.48	0.82
1:A:228:ALA:O	1:A:397:THR:HG21	1.80	0.81
1:B:406:LYS:NZ	1:B:406:LYS:CA	2.43	0.81
1:B:406:LYS:CB	1:B:406:LYS:NZ	2.41	0.81
1:B:442:GLU:OE2	1:B:442:GLU:HA	1.80	0.81
1:A:139:ARG:NH1	1:A:257:LEU:HD22	1.95	0.80
1:A:442:GLU:OE2	1:A:442:GLU:HA	1.81	0.80
1:B:157:ILE:CG2	1:B:158:THR:N	2.45	0.80
1:A:200:TYR:CD1	1:A:394:TYR:CE1	2.60	0.79
1:A:93:ARG:HH11	1:A:229:ASN:HA	1.46	0.79
1:A:157:ILE:CG2	1:A:158:THR:N	2.45	0.79
1:B:93:ARG:HH11	1:B:229:ASN:HA	1.45	0.79
1:A:116:TYR:CE2	1:A:119:ALA:HB2	2.18	0.79
1:A:334:VAL:CG1	1:A:345:LYS:HG3	2.12	0.79
1:A:252:ASN:ND2	1:A:252:ASN:H	1.77	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:CG2	1:A:206:ALA:N	2.46	0.78
1:A:232:LYS:HE2	1:A:295:GLU:HG3	1.66	0.78
1:B:89:VAL:HG12	1:B:90:VAL:O	1.84	0.78
1:A:201:SER:C	1:A:224:PHE:CE1	2.61	0.78
1:B:123:ALA:HB3	1:B:277:PRO:HD2	1.65	0.78
1:B:220:LEU:O	1:B:221:ASN:HB2	1.85	0.77
1:B:504:LEU:HD22	1:B:505:TYR:CD1	2.19	0.77
1:B:504:LEU:CD2	1:B:505:TYR:CG	2.67	0.77
1:A:388:VAL:O	1:A:388:VAL:HG13	1.84	0.77
1:B:201:SER:C	1:B:224:PHE:CE1	2.62	0.77
1:A:288:ARG:HE	1:A:368:ASN:HB3	1.51	0.76
1:B:334:VAL:CG1	1:B:345:LYS:HG3	2.14	0.76
1:B:433:LYS:HA	1:B:433:LYS:HE2	0.84	0.76
1:B:465:ILE:CG2	1:B:489:VAL:HB	2.14	0.76
1:A:205:ILE:HG22	1:A:206:ALA:H	1.51	0.76
1:A:490:PRO:HG2	1:A:512:HIS:CE1	2.21	0.76
1:B:406:LYS:HZ2	1:B:406:LYS:CA	1.97	0.76
1:A:420:ASP:HB2	1:A:468:VAL:HG23	1.66	0.76
1:A:123:ALA:HB3	1:A:277:PRO:HD2	1.66	0.76
1:B:79:LYS:HD2	1:B:92:GLU:HG3	1.68	0.76
1:B:116:TYR:CE2	1:B:119:ALA:HB2	2.21	0.76
1:A:502:THR:HG22	1:A:504:LEU:H	1.47	0.76
1:A:504:LEU:HD22	1:A:505:TYR:CD1	2.21	0.76
1:B:205:ILE:CG2	1:B:206:ALA:N	2.48	0.75
1:B:225:ASN:O	1:B:228:ALA:N	2.19	0.75
1:B:223:ASP:O	1:B:223:ASP:OD1	2.05	0.75
1:A:171:VAL:CG2	1:A:246:VAL:HG21	2.17	0.75
1:B:232:LYS:HE2	1:B:295:GLU:HG3	1.67	0.75
1:A:504:LEU:CD2	1:A:505:TYR:CG	2.70	0.75
1:B:388:VAL:O	1:B:388:VAL:HG13	1.86	0.75
1:B:364:LEU:HD12	1:B:365:SER:H	1.52	0.74
1:A:239:TYR:CE1	1:A:358:ILE:CD1	2.70	0.74
1:A:225:ASN:O	1:A:228:ALA:N	2.19	0.74
1:B:484:ILE:HD11	1:B:508:ALA:HB1	1.68	0.74
1:A:73:VAL:O	1:A:74:GLU:CB	2.35	0.74
1:A:223:ASP:OD1	1:A:223:ASP:O	2.05	0.74
1:A:220:LEU:O	1:A:221:ASN:HB2	1.88	0.74
1:A:89:VAL:HG12	1:A:90:VAL:O	1.87	0.74
1:A:465:ILE:CG2	1:A:489:VAL:HB	2.15	0.74
1:B:107:ILE:HD11	1:B:375:TYR:HD2	1.53	0.74
1:B:222:ILE:HB	1:B:224:PHE:CE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:O	1:B:74:GLU:CB	2.35	0.73
1:A:79:LYS:HD2	1:A:92:GLU:HG3	1.70	0.73
1:A:299:LYS:HB3	1:A:399:THR:HG21	1.70	0.73
1:A:222:ILE:HB	1:A:224:PHE:CE2	2.24	0.73
1:B:200:TYR:CD1	1:B:394:TYR:CE1	2.60	0.73
1:B:378:THR:HG22	1:B:383:ASN:HA	1.70	0.72
1:B:71:ASP:O	1:B:72:LYS:C	2.31	0.72
1:B:484:ILE:CD1	1:B:508:ALA:HB1	2.19	0.72
1:A:71:ASP:O	1:A:72:LYS:C	2.32	0.72
1:A:199:VAL:HG23	1:A:199:VAL:O	1.88	0.71
1:B:299:LYS:HB3	1:B:399:THR:HG21	1.71	0.71
1:B:205:ILE:HG22	1:B:206:ALA:H	1.55	0.71
1:A:433:LYS:HZ1	1:A:434:GLU:H	1.36	0.71
1:B:63:ARG:HA	1:B:389:HIS:CD2	2.25	0.71
1:A:107:ILE:HD11	1:A:375:TYR:HD2	1.56	0.71
1:A:279:VAL:HG12	1:A:379:PHE:CD2	2.25	0.71
1:A:364:LEU:HD12	1:A:365:SER:H	1.54	0.71
1:A:484:ILE:HD11	1:A:508:ALA:HB1	1.71	0.71
1:A:251:PRO:HD3	1:A:280:MET:CE	2.17	0.71
1:B:135:LEU:CD2	1:B:135:LEU:C	2.49	0.71
1:B:279:VAL:HG12	1:B:379:PHE:CD2	2.25	0.71
1:A:100:THR:HG22	1:A:101:SER:N	2.06	0.71
1:A:266:GLU:O	1:A:270:LYS:HB2	1.90	0.71
1:A:378:THR:HG22	1:A:383:ASN:HA	1.72	0.71
1:B:200:TYR:O	1:B:224:PHE:HD1	1.74	0.71
1:A:63:ARG:HA	1:A:389:HIS:CD2	2.27	0.70
1:A:171:VAL:HG22	1:A:246:VAL:HG21	1.73	0.70
1:A:395:ILE:O	1:A:395:ILE:HG22	1.91	0.70
1:B:100:THR:HG22	1:B:101:SER:N	2.05	0.70
1:B:171:VAL:CG2	1:B:246:VAL:HG21	2.21	0.70
1:B:395:ILE:HG22	1:B:395:ILE:O	1.91	0.70
1:B:433:LYS:HZ3	1:B:434:GLU:H	1.38	0.70
1:A:192:MET:HE3	1:A:194:TYR:HB2	1.72	0.70
1:A:200:TYR:O	1:A:224:PHE:HD1	1.74	0.70
1:A:484:ILE:CD1	1:A:508:ALA:HB1	2.21	0.70
1:B:433:LYS:HZ1	1:B:434:GLU:H	1.38	0.70
1:B:139:ARG:HD2	1:B:257:LEU:O	1.92	0.70
1:A:214:LYS:NZ	1:A:214:LYS:HB3	2.07	0.70
1:B:420:ASP:HB2	1:B:468:VAL:HG23	1.72	0.70
1:B:473:THR:HG22	1:B:479:TRP:O	1.91	0.70
1:B:502:THR:CG2	1:B:504:LEU:H	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LYS:HA	1:A:433:LYS:HE2	0.83	0.69
1:B:288:ARG:HE	1:B:368:ASN:HB3	1.57	0.69
1:B:291:TYR:HB2	1:B:334:VAL:HG22	1.72	0.69
1:B:181:LYS:C	1:B:182:TYR:CD2	2.70	0.69
1:A:171:VAL:HG12	1:A:172:ASP:N	2.08	0.69
1:A:310:LEU:O	1:A:310:LEU:CD2	2.39	0.69
1:B:239:TYR:CE1	1:B:358:ILE:CD1	2.70	0.69
1:B:310:LEU:HD23	1:B:310:LEU:C	2.17	0.69
1:A:139:ARG:HD2	1:A:257:LEU:O	1.93	0.69
1:A:150:GLY:H	1:A:178:TRP:NE1	1.90	0.69
1:A:181:LYS:C	1:A:182:TYR:CD2	2.71	0.69
1:A:410:ASP:HB3	1:A:412:TYR:HE2	1.58	0.69
1:A:420:ASP:OD2	1:A:470:ARG:NH2	2.24	0.69
1:B:157:ILE:HG22	1:B:158:THR:N	2.06	0.69
1:A:433:LYS:HZ3	1:A:434:GLU:H	1.37	0.69
1:A:473:THR:HG22	1:A:479:TRP:O	1.91	0.69
1:A:157:ILE:HG22	1:A:158:THR:N	2.08	0.68
1:B:143:ASN:OD1	1:B:158:THR:HB	1.92	0.68
1:B:199:VAL:HG23	1:B:199:VAL:O	1.92	0.68
1:B:490:PRO:HG2	1:B:512:HIS:CE1	2.28	0.68
1:B:266:GLU:O	1:B:270:LYS:HB2	1.94	0.68
1:B:251:PRO:HD3	1:B:280:MET:CE	2.17	0.67
1:B:504:LEU:HD22	1:B:505:TYR:CG	2.28	0.67
1:A:107:ILE:HD11	1:A:375:TYR:CD2	2.30	0.67
1:B:107:ILE:HD11	1:B:375:TYR:CD2	2.28	0.67
1:A:310:LEU:HD23	1:A:310:LEU:C	2.17	0.67
1:B:492:THR:HG21	1:B:512:HIS:CD2	2.30	0.67
1:B:310:LEU:O	1:B:310:LEU:CD2	2.40	0.67
1:A:291:TYR:HB2	1:A:334:VAL:HG22	1.76	0.67
1:A:429:ASP:OD1	1:A:433:LYS:N	2.23	0.67
1:B:150:GLY:H	1:B:178:TRP:NE1	1.91	0.67
1:B:222:ILE:O	1:B:224:PHE:HD2	1.78	0.67
1:B:225:ASN:O	1:B:226:ALA:C	2.38	0.67
1:B:429:ASP:OD1	1:B:433:LYS:N	2.22	0.67
1:A:222:ILE:O	1:A:224:PHE:HD2	1.78	0.66
1:A:409:LEU:HD11	1:A:456:ILE:HD11	1.76	0.66
1:B:364:LEU:HD12	1:B:365:SER:N	2.09	0.66
1:B:411:HIS:CD2	1:B:413:GLY:N	2.62	0.66
1:B:420:ASP:OD2	1:B:470:ARG:NH2	2.25	0.66
1:A:205:ILE:CG2	1:A:206:ALA:H	2.08	0.66
1:B:82:ILE:HD13	1:B:83:ASN:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HE3	1:A:234:VAL:O	1.96	0.66
1:B:203:SER:C	1:B:392:THR:HG21	2.21	0.66
1:A:82:ILE:HD13	1:A:83:ASN:N	2.10	0.66
1:A:143:ASN:OD1	1:A:158:THR:HB	1.95	0.66
1:A:223:ASP:O	1:A:225:ASN:N	2.28	0.66
1:A:127:PHE:C	1:A:129:ASP:H	2.03	0.66
1:B:459:PRO:O	1:B:462:SER:OG	2.12	0.66
1:B:223:ASP:O	1:B:225:ASN:N	2.28	0.66
1:A:100:THR:HG22	1:A:102:PRO:HD3	1.78	0.66
1:A:364:LEU:HD12	1:A:365:SER:N	2.11	0.66
1:B:192:MET:HE3	1:B:194:TYR:HB2	1.77	0.65
1:B:214:LYS:NZ	1:B:214:LYS:HB3	2.11	0.65
1:A:459:PRO:O	1:A:462:SER:OG	2.14	0.65
1:B:410:ASP:HB3	1:B:412:TYR:HE2	1.59	0.65
1:B:100:THR:HG22	1:B:102:PRO:HD3	1.78	0.65
1:A:225:ASN:O	1:A:226:ALA:C	2.39	0.65
1:A:299:LYS:HB3	1:A:399:THR:CG2	2.27	0.65
1:B:352:ASN:HA	1:B:355:ARG:HG3	1.78	0.65
1:A:411:HIS:CD2	1:A:413:GLY:N	2.62	0.65
1:B:171:VAL:HG22	1:B:246:VAL:HG21	1.78	0.65
1:B:502:THR:HG22	1:B:503:THR:N	2.12	0.65
1:B:409:LEU:HD12	1:B:454:THR:CG2	2.27	0.64
1:A:504:LEU:HD22	1:A:505:TYR:CG	2.32	0.64
1:B:307:PHE:C	1:B:309:ALA:N	2.53	0.64
1:B:310:LEU:C	1:B:310:LEU:CD2	2.71	0.64
1:A:441:TRP:O	1:A:444:SER:HB2	1.97	0.64
1:A:478:GLU:O	1:A:479:TRP:CD1	2.49	0.64
1:B:171:VAL:HG12	1:B:172:ASP:N	2.12	0.64
1:B:407:MET:HE2	1:B:467:ILE:HD11	1.80	0.64
1:B:299:LYS:HB3	1:B:399:THR:CG2	2.26	0.64
1:B:409:LEU:HD11	1:B:456:ILE:HD11	1.78	0.64
1:B:502:THR:CG2	1:B:503:THR:N	2.61	0.64
1:A:99:THR:O	1:A:99:THR:CG2	2.46	0.64
1:A:352:ASN:HA	1:A:355:ARG:HG3	1.78	0.64
1:B:427:THR:O	1:B:435:VAL:N	2.21	0.64
1:A:239:TYR:HE1	1:A:358:ILE:HD13	1.58	0.64
1:B:109:ASP:CG	1:B:338:GLY:HA2	2.23	0.64
1:A:492:THR:HG21	1:A:512:HIS:CD2	2.34	0.63
1:B:127:PHE:C	1:B:129:ASP:H	2.05	0.63
1:B:198:MET:HE3	1:B:234:VAL:O	1.98	0.63
1:A:214:LYS:NZ	1:A:214:LYS:CB	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ARG:NH1	1:B:229:ASN:HA	2.14	0.63
1:B:233:LYS:CE	1:B:399:THR:HB	2.26	0.63
1:B:478:GLU:O	1:B:479:TRP:CD1	2.51	0.63
1:A:208:ALA:C	1:A:210:ASN:H	2.06	0.63
1:B:504:LEU:CD2	1:B:505:TYR:CD1	2.83	0.62
1:A:469:ALA:HB3	1:A:484:ILE:HB	1.81	0.62
1:A:300:SER:O	1:A:302:ASP:N	2.32	0.62
1:A:109:ASP:CG	1:A:338:GLY:HA2	2.24	0.62
1:A:205:ILE:HG23	1:A:206:ALA:N	2.15	0.62
1:A:310:LEU:CD2	1:A:310:LEU:C	2.71	0.62
1:A:427:THR:O	1:A:435:VAL:N	2.22	0.62
1:A:502:THR:CG2	1:A:504:LEU:H	2.10	0.62
1:B:307:PHE:O	1:B:309:ALA:N	2.32	0.62
1:B:466:LYS:HG3	1:B:487:GLN:HB3	1.81	0.62
1:A:233:LYS:CE	1:A:399:THR:HB	2.29	0.61
1:A:411:HIS:HD2	1:A:413:GLY:N	1.90	0.61
1:B:239:TYR:HE1	1:B:358:ILE:HD13	1.57	0.61
1:B:307:PHE:C	1:B:309:ALA:H	2.08	0.61
1:A:111:VAL:O	1:A:111:VAL:CG1	2.48	0.61
1:A:203:SER:C	1:A:392:THR:HG21	2.24	0.61
1:B:296:THR:HA	1:B:328:GLU:O	2.00	0.61
1:B:423:TRP:CD2	1:B:458:LEU:HD21	2.35	0.61
1:A:127:PHE:O	1:A:129:ASP:N	2.34	0.61
1:A:423:TRP:CD2	1:A:458:LEU:HD21	2.35	0.61
1:A:283:ASN:C	1:A:283:ASN:OD1	2.43	0.61
1:A:296:THR:HA	1:A:328:GLU:O	2.00	0.61
1:A:281:VAL:HG12	1:A:281:VAL:O	2.01	0.61
1:B:200:TYR:HB2	1:B:394:TYR:HD1	1.66	0.61
1:B:469:ALA:HB3	1:B:484:ILE:HB	1.83	0.61
1:A:181:LYS:O	1:A:182:TYR:HD2	1.76	0.61
1:B:100:THR:HB	1:B:390:ASN:HB3	1.83	0.61
1:A:200:TYR:HB2	1:A:394:TYR:HD1	1.65	0.61
1:A:423:TRP:CE3	1:A:458:LEU:HD21	2.36	0.61
1:B:259:ASP:OD1	1:B:260:ASN:N	2.34	0.61
1:B:283:ASN:OD1	1:B:283:ASN:C	2.43	0.61
1:B:359:LYS:C	1:B:361:ASN:H	2.09	0.60
1:A:297:THR:OG1	1:A:328:GLU:HB3	2.02	0.60
1:B:107:ILE:HD11	1:B:115:THR:HG21	1.83	0.60
1:B:187:THR:HB	2:B:515:HOH:O	2.00	0.60
1:B:211:VAL:HG23	1:B:212:ASN:N	2.15	0.60
1:B:411:HIS:CD2	1:B:411:HIS:C	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG12	1:B:91:VAL:O	2.01	0.60
1:B:205:ILE:CG2	1:B:206:ALA:H	2.13	0.60
1:A:73:VAL:HG22	1:A:393:ASP:HB3	1.82	0.60
1:A:409:LEU:HD12	1:A:454:THR:CG2	2.31	0.60
1:B:73:VAL:HG22	1:B:393:ASP:HB3	1.83	0.60
1:B:107:ILE:CD1	1:B:375:TYR:HD2	2.15	0.60
1:A:504:LEU:CD2	1:A:505:TYR:CD1	2.84	0.60
1:A:411:HIS:CD2	1:A:411:HIS:C	2.80	0.59
1:A:420:ASP:HA	1:A:444:SER:OG	2.03	0.59
1:B:233:LYS:HE3	1:B:399:THR:CB	2.29	0.59
1:B:423:TRP:CE3	1:B:458:LEU:HD21	2.36	0.59
1:A:206:ALA:O	1:A:207:SER:C	2.41	0.59
1:A:291:TYR:CE2	1:A:336:LEU:HD21	2.37	0.59
1:A:307:PHE:C	1:A:309:ALA:N	2.55	0.59
1:B:205:ILE:HG23	1:B:206:ALA:N	2.17	0.59
1:B:441:TRP:O	1:B:444:SER:HB2	2.03	0.59
1:A:107:ILE:HD11	1:A:115:THR:HG21	1.84	0.59
1:B:223:ASP:C	1:B:225:ASN:H	2.11	0.59
1:B:281:VAL:HG12	1:B:281:VAL:O	2.02	0.59
1:A:472:CYS:HB2	1:A:477:TRP:CZ2	2.37	0.59
1:B:152:ARG:NH2	1:B:178:TRP:CB	2.38	0.59
1:A:307:PHE:O	1:A:309:ALA:N	2.36	0.59
1:A:407:MET:HE2	1:A:467:ILE:HD11	1.84	0.59
1:A:466:LYS:HG3	1:A:487:GLN:HB3	1.85	0.59
1:A:491:LEU:C	1:A:492:THR:HG22	2.26	0.59
1:B:106:LEU:HD11	1:B:212:ASN:HB2	1.85	0.59
1:B:113:ASN:N	1:B:113:ASN:HD22	2.01	0.59
1:A:152:ARG:HH21	1:A:178:TRP:HB2	0.65	0.59
1:B:206:ALA:O	1:B:207:SER:C	2.45	0.58
1:B:208:ALA:C	1:B:210:ASN:H	2.11	0.58
1:A:106:LEU:HD11	1:A:212:ASN:HB2	1.85	0.58
1:A:223:ASP:C	1:A:225:ASN:H	2.11	0.58
1:B:127:PHE:O	1:B:129:ASP:N	2.36	0.58
1:A:91:VAL:HG12	1:A:91:VAL:O	2.02	0.58
1:A:359:LYS:C	1:A:361:ASN:H	2.10	0.58
1:B:291:TYR:CE2	1:B:336:LEU:HD21	2.38	0.58
1:A:211:VAL:HG23	1:A:212:ASN:N	2.18	0.58
1:A:229:ASN:O	1:A:231:GLU:N	2.36	0.58
1:B:420:ASP:HA	1:B:444:SER:OG	2.03	0.58
1:A:294:LEU:HD22	1:A:307:PHE:CD1	2.39	0.58
1:A:477:TRP:HE3	1:A:480:TRP:CD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:THR:OG1	1:B:328:GLU:HB3	2.03	0.58
1:A:152:ARG:NH2	1:A:178:TRP:CB	2.38	0.58
1:A:307:PHE:C	1:A:309:ALA:H	2.11	0.58
1:A:150:GLY:O	1:A:152:ARG:HG3	2.04	0.58
1:B:423:TRP:CD2	1:B:458:LEU:CD2	2.87	0.58
1:A:100:THR:HB	1:A:390:ASN:HB3	1.84	0.58
1:B:122:LEU:HD11	1:B:271:GLY:HA3	1.86	0.58
1:B:197:SER:O	1:B:235:MET:HB2	2.03	0.58
1:B:492:THR:CG2	1:B:512:HIS:CD2	2.87	0.58
1:B:472:CYS:HB2	1:B:477:TRP:CZ2	2.38	0.57
1:A:279:VAL:HG12	1:A:379:PHE:HD2	1.69	0.57
1:A:502:THR:HG22	1:A:503:THR:N	2.20	0.57
1:B:229:ASN:O	1:B:231:GLU:N	2.34	0.57
1:B:411:HIS:HD2	1:B:413:GLY:N	1.91	0.57
1:B:107:ILE:CG1	1:B:375:TYR:HD2	2.18	0.57
1:A:107:ILE:CD1	1:A:375:TYR:HD2	2.17	0.57
1:A:181:LYS:C	1:A:182:TYR:HD2	2.12	0.57
1:B:181:LYS:C	1:B:182:TYR:HD2	2.11	0.57
1:A:423:TRP:CD2	1:A:458:LEU:CD2	2.87	0.57
1:A:199:VAL:O	1:A:199:VAL:CG2	2.52	0.57
1:B:279:VAL:HG12	1:B:379:PHE:HD2	1.68	0.57
1:A:93:ARG:NH1	1:A:229:ASN:HA	2.17	0.57
1:A:113:ASN:N	1:A:113:ASN:HD22	2.03	0.57
1:B:300:SER:O	1:B:302:ASP:N	2.37	0.56
1:B:214:LYS:NZ	1:B:214:LYS:CB	2.67	0.56
1:A:122:LEU:HD11	1:A:271:GLY:HA3	1.87	0.56
1:A:163:THR:O	1:A:164:TYR:C	2.47	0.56
1:A:288:ARG:NE	1:A:368:ASN:HB3	2.18	0.56
1:B:157:ILE:HG23	1:B:158:THR:N	2.21	0.56
1:B:403:SER:HA	1:B:460:PRO:HB3	1.87	0.56
1:A:492:THR:CG2	1:A:512:HIS:CD2	2.89	0.56
1:A:347:VAL:O	1:A:347:VAL:CG1	2.54	0.56
1:B:52:ASN:OD1	1:B:255:SER:HB3	2.05	0.56
1:A:502:THR:CG2	1:A:503:THR:N	2.68	0.56
1:B:127:PHE:C	1:B:127:PHE:HD1	2.14	0.56
1:B:491:LEU:C	1:B:492:THR:HG22	2.30	0.56
1:A:107:ILE:CG1	1:A:375:TYR:HD2	2.17	0.56
1:A:127:PHE:C	1:A:127:PHE:HD1	2.14	0.56
1:B:118:GLY:O	1:B:139:ARG:NH2	2.35	0.56
1:B:99:THR:O	1:B:99:THR:CG2	2.46	0.56
1:B:203:SER:HB2	1:B:392:THR:HG21	1.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LYS:HZ3	1:B:406:LYS:CA	2.14	0.56
1:A:209:LEU:HD11	1:A:236:VAL:HG11	1.87	0.55
1:A:149:PRO:C	1:A:151:MET:H	2.09	0.55
1:A:239:TYR:HE1	1:A:358:ILE:CD1	2.16	0.55
1:B:209:LEU:HD11	1:B:236:VAL:HG11	1.87	0.55
1:B:477:TRP:HE3	1:B:480:TRP:CD1	2.24	0.55
1:B:63:ARG:HA	1:B:389:HIS:HD2	1.71	0.55
1:B:139:ARG:HH12	1:B:257:LEU:HD22	1.70	0.55
1:B:150:GLY:O	1:B:152:ARG:HG3	2.05	0.55
1:B:288:ARG:HD3	1:B:361:ASN:OD1	2.06	0.55
1:A:472:CYS:HB2	1:A:477:TRP:CE2	2.41	0.55
1:A:504:LEU:HD23	1:A:505:TYR:N	2.19	0.55
1:A:148:LEU:HD13	1:A:178:TRP:CD2	2.41	0.55
1:A:470:ARG:NH1	1:A:470:ARG:HB2	2.22	0.55
1:B:127:PHE:C	1:B:127:PHE:CD1	2.83	0.55
1:A:359:LYS:C	1:A:361:ASN:N	2.65	0.55
1:B:148:LEU:HD13	1:B:178:TRP:CD2	2.42	0.55
1:B:472:CYS:HB2	1:B:477:TRP:CE2	2.41	0.55
1:B:347:VAL:CG1	1:B:347:VAL:O	2.54	0.55
1:B:76:PHE:O	1:B:78:PRO:HD3	2.07	0.55
1:A:127:PHE:C	1:A:127:PHE:CD1	2.83	0.55
1:A:288:ARG:HD3	1:A:361:ASN:OD1	2.07	0.55
1:A:466:LYS:HA	1:A:486:GLU:O	2.06	0.55
1:A:76:PHE:O	1:A:78:PRO:HD3	2.07	0.54
1:B:152:ARG:HH21	1:B:178:TRP:HB2	0.65	0.54
1:B:223:ASP:OD1	1:B:223:ASP:C	2.49	0.54
1:B:260:ASN:C	1:B:262:VAL:H	2.14	0.54
1:A:157:ILE:HG23	1:A:158:THR:N	2.21	0.54
1:A:197:SER:O	1:A:235:MET:HB2	2.07	0.54
1:B:359:LYS:C	1:B:361:ASN:N	2.64	0.54
1:B:359:LYS:O	1:B:361:ASN:N	2.41	0.54
1:A:491:LEU:C	1:A:492:THR:CG2	2.81	0.54
1:B:335:VAL:O	1:B:336:LEU:C	2.50	0.54
1:A:52:ASN:OD1	1:A:255:SER:HB3	2.07	0.54
1:A:409:LEU:HD23	1:A:497:VAL:CG2	2.37	0.54
1:B:100:THR:CG2	1:B:101:SER:H	2.17	0.54
1:B:504:LEU:HD23	1:B:505:TYR:N	2.17	0.54
1:B:163:THR:O	1:B:164:TYR:C	2.48	0.54
1:A:127:PHE:C	1:A:129:ASP:N	2.65	0.53
1:B:222:ILE:O	1:B:224:PHE:CD2	2.60	0.53
1:B:504:LEU:CD2	1:B:505:TYR:CD2	2.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:O	1:A:224:PHE:CD2	2.60	0.53
1:B:307:PHE:O	1:B:308:LYS:C	2.50	0.53
1:B:216:LEU:CD2	1:B:220:LEU:HD12	2.39	0.53
1:A:101:SER:N	1:A:102:PRO:HD3	2.23	0.53
1:A:63:ARG:HA	1:A:389:HIS:HD2	1.71	0.53
1:A:203:SER:HB2	1:A:392:THR:HG21	1.85	0.53
1:A:113:ASN:HD22	1:A:113:ASN:H	1.57	0.53
1:A:223:ASP:OD1	1:A:223:ASP:C	2.50	0.53
1:A:504:LEU:CD2	1:A:505:TYR:CD2	2.92	0.53
1:B:504:LEU:HD21	1:B:505:TYR:CD2	2.43	0.53
1:A:177:THR:HG22	1:A:178:TRP:N	2.23	0.53
1:A:259:ASP:OD1	1:A:260:ASN:N	2.39	0.53
1:A:206:ALA:O	1:A:208:ALA:N	2.42	0.53
1:A:334:VAL:HG12	1:A:345:LYS:CB	2.39	0.53
1:B:101:SER:N	1:B:102:PRO:HD3	2.23	0.53
1:B:504:LEU:HD21	1:B:505:TYR:CE2	2.44	0.53
1:B:155:ASN:O	1:B:174:LEU:HD11	2.09	0.53
1:B:283:ASN:OD1	1:B:284:VAL:N	2.41	0.53
1:B:466:LYS:HA	1:B:486:GLU:O	2.08	0.53
1:A:299:LYS:CB	1:A:399:THR:HG21	2.30	0.52
1:B:111:VAL:O	1:B:111:VAL:CG1	2.53	0.52
1:A:504:LEU:HD21	1:A:505:TYR:CD2	2.44	0.52
1:B:149:PRO:C	1:B:151:MET:H	2.09	0.52
1:A:222:ILE:O	1:A:224:PHE:N	2.42	0.52
1:A:371:TYR:HE1	1:A:373:ILE:HD11	1.74	0.52
1:B:155:ASN:O	1:B:174:LEU:CD1	2.58	0.52
1:B:279:VAL:CG1	1:B:379:PHE:CD2	2.92	0.52
1:A:279:VAL:CG1	1:A:379:PHE:CD2	2.92	0.52
1:A:283:ASN:OD1	1:A:284:VAL:N	2.42	0.52
1:A:359:LYS:O	1:A:361:ASN:N	2.42	0.52
1:A:116:TYR:CE1	1:A:164:TYR:HB2	2.45	0.52
1:A:152:ARG:HB3	1:A:154:GLU:HG2	1.92	0.52
1:B:199:VAL:O	1:B:199:VAL:CG2	2.57	0.52
1:B:214:LYS:HB3	1:B:214:LYS:HZ1	1.75	0.52
1:A:181:LYS:O	1:A:182:TYR:CG	2.59	0.52
1:B:116:TYR:CE1	1:B:164:TYR:HB2	2.44	0.52
1:A:403:SER:HA	1:A:460:PRO:HB3	1.91	0.52
1:B:113:ASN:HD22	1:B:113:ASN:H	1.58	0.52
1:B:216:LEU:HD21	1:B:220:LEU:HD12	1.91	0.52
1:B:239:TYR:HE1	1:B:358:ILE:CD1	2.15	0.52
1:A:214:LYS:HB3	1:A:214:LYS:HZ1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LEU:C	1:B:492:THR:CG2	2.84	0.51
1:A:409:LEU:HD12	1:A:454:THR:HG21	1.93	0.51
1:A:490:PRO:O	1:A:492:THR:HG23	2.10	0.51
1:A:105:ILE:HD13	1:A:105:ILE:N	2.24	0.51
1:A:504:LEU:HD21	1:A:505:TYR:CE2	2.45	0.51
1:B:409:LEU:HD23	1:B:497:VAL:CG2	2.41	0.51
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.45	0.51
1:A:208:ALA:C	1:A:210:ASN:N	2.69	0.51
1:A:307:PHE:O	1:A:308:LYS:C	2.52	0.51
1:B:177:THR:HG22	1:B:178:TRP:N	2.25	0.51
1:A:184:THR:C	1:A:186:HIS:N	2.66	0.51
1:B:249:GLU:O	1:B:250:LEU:C	2.51	0.51
1:B:294:LEU:HD22	1:B:307:PHE:CD1	2.45	0.51
1:B:371:TYR:HE1	1:B:373:ILE:HD11	1.74	0.51
1:A:139:ARG:CB	1:A:162:PRO:HD2	2.41	0.51
1:A:335:VAL:O	1:A:336:LEU:C	2.52	0.51
1:A:406:LYS:HZ3	1:A:406:LYS:CA	2.17	0.51
1:A:477:TRP:O	1:A:478:GLU:C	2.53	0.51
1:B:105:ILE:HD13	1:B:105:ILE:N	2.24	0.51
1:B:226:ALA:HB1	1:B:232:LYS:HB2	1.93	0.51
1:B:463:LYS:O	1:B:464:ASN:HB2	2.11	0.51
1:B:433:LYS:CE	1:B:433:LYS:CA	2.59	0.51
1:B:492:THR:CG2	1:B:512:HIS:HD2	2.24	0.51
1:B:124:ASN:O	1:B:127:PHE:HB3	2.11	0.51
1:B:291:TYR:HB2	1:B:334:VAL:CG2	2.40	0.50
1:B:409:LEU:HD12	1:B:454:THR:HG21	1.92	0.50
1:A:260:ASN:C	1:A:262:VAL:H	2.19	0.50
1:B:477:TRP:O	1:B:478:GLU:C	2.54	0.50
1:A:216:LEU:CD2	1:A:220:LEU:HD12	2.41	0.50
1:A:472:CYS:HB2	1:A:477:TRP:CH2	2.46	0.50
1:A:118:GLY:O	1:A:139:ARG:NH2	2.38	0.50
1:A:155:ASN:O	1:A:174:LEU:HD11	2.11	0.50
1:A:226:ALA:HB1	1:A:232:LYS:HB2	1.94	0.50
1:B:466:LYS:HA	1:B:487:GLN:HA	1.94	0.50
1:B:490:PRO:O	1:B:492:THR:HG23	2.10	0.50
1:A:100:THR:CG2	1:A:101:SER:H	2.18	0.50
1:B:472:CYS:HB2	1:B:477:TRP:CH2	2.47	0.50
1:A:216:LEU:HD21	1:A:220:LEU:HD12	1.93	0.50
1:A:246:VAL:HG12	1:A:247:SER:N	2.25	0.50
1:B:98:LEU:HD11	1:B:208:ALA:HB2	1.93	0.50
1:A:171:VAL:HG21	1:A:246:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:CB	1:B:162:PRO:HD2	2.42	0.50
1:A:294:LEU:CD2	1:A:331:PHE:CD1	2.85	0.49
1:A:98:LEU:HD11	1:A:208:ALA:HB2	1.94	0.49
1:A:141:PRO:HB3	1:A:160:GLN:HA	1.94	0.49
1:A:326:PHE:HA	1:A:329:SER:HB2	1.94	0.49
1:A:116:TYR:CD2	1:A:119:ALA:HB2	2.47	0.49
1:A:199:VAL:HG12	1:A:205:ILE:HG12	1.95	0.49
1:A:200:TYR:O	1:A:224:PHE:CD1	2.59	0.49
1:A:466:LYS:HA	1:A:487:GLN:HA	1.94	0.49
1:B:222:ILE:O	1:B:224:PHE:N	2.41	0.49
1:B:326:PHE:HA	1:B:329:SER:HB2	1.95	0.49
1:A:184:THR:O	1:A:185:THR:C	2.55	0.49
1:B:112:VAL:HG13	1:B:113:ASN:N	2.28	0.49
1:A:327:GLU:OE2	1:A:327:GLU:CA	2.37	0.49
1:B:394:TYR:CD2	1:B:394:TYR:N	2.80	0.49
1:A:415:TYR:CD1	1:A:415:TYR:O	2.65	0.49
1:B:409:LEU:HD12	1:B:454:THR:HG22	1.93	0.49
1:B:470:ARG:HB2	1:B:470:ARG:NH1	2.27	0.49
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.47	0.49
1:B:184:THR:C	1:B:186:HIS:N	2.70	0.49
1:B:327:GLU:OE2	1:B:327:GLU:CA	2.40	0.49
1:B:465:ILE:HG21	1:B:489:VAL:CB	2.24	0.49
1:A:463:LYS:O	1:A:464:ASN:HB2	2.12	0.49
1:B:100:THR:CG2	1:B:101:SER:N	2.75	0.49
1:B:181:LYS:O	1:B:182:TYR:CG	2.60	0.49
1:A:210:ASN:CG	1:A:210:ASN:O	2.55	0.49
1:A:233:LYS:HE3	1:A:399:THR:CB	2.32	0.48
1:B:200:TYR:O	1:B:224:PHE:CD1	2.60	0.48
1:B:223:ASP:C	1:B:225:ASN:N	2.69	0.48
1:B:294:LEU:CD2	1:B:331:PHE:CD1	2.86	0.48
1:A:134:LEU:HD23	1:A:135:LEU:H	1.78	0.48
1:B:79:LYS:HD2	1:B:92:GLU:CG	2.42	0.48
1:B:288:ARG:NE	1:B:368:ASN:HB3	2.25	0.48
1:A:300:SER:O	1:A:301:LYS:C	2.56	0.48
1:B:198:MET:HE3	1:B:198:MET:HA	1.95	0.48
1:B:411:HIS:HD2	1:B:412:TYR:N	2.11	0.48
1:A:300:SER:C	1:A:302:ASP:N	2.70	0.48
1:A:345:LYS:HG2	1:A:346:VAL:N	2.28	0.48
1:B:116:TYR:CD2	1:B:119:ALA:HB2	2.49	0.48
1:A:124:ASN:O	1:A:127:PHE:HB3	2.13	0.48
1:A:152:ARG:HD3	1:A:155:ASN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:C	1:A:302:ASP:H	2.21	0.48
1:A:499:ILE:HA	1:A:507:THR:O	2.13	0.48
1:B:265:ASP:O	1:B:266:GLU:C	2.57	0.48
1:A:473:THR:HG22	1:A:480:TRP:N	2.25	0.48
1:B:152:ARG:HB3	1:B:154:GLU:HG2	1.95	0.48
1:B:296:THR:HB	1:B:329:SER:OG	2.14	0.48
1:B:421:VAL:HG22	1:B:467:ILE:HG12	1.95	0.48
1:A:60:TYR:CE1	1:A:277:PRO:HG2	2.49	0.48
1:A:155:ASN:O	1:A:174:LEU:CD1	2.61	0.48
1:A:179:ASN:O	1:A:183:SER:HB2	2.13	0.48
1:A:394:TYR:N	1:A:394:TYR:CD2	2.80	0.48
1:B:473:THR:HG22	1:B:480:TRP:N	2.27	0.48
1:A:267:LEU:O	1:A:270:LYS:N	2.45	0.48
1:A:105:ILE:HD13	1:A:105:ILE:H	1.79	0.48
1:A:473:THR:HG22	1:A:480:TRP:HA	1.96	0.48
1:B:407:MET:CE	1:B:467:ILE:HD11	2.42	0.48
1:B:423:TRP:CE2	1:B:458:LEU:CD2	2.96	0.48
1:A:304:GLN:HG3	1:A:305:ALA:N	2.29	0.48
1:B:74:GLU:HG3	1:B:75:SER:N	2.28	0.48
1:A:208:ALA:O	1:A:210:ASN:N	2.46	0.47
1:A:294:LEU:HD23	1:A:331:PHE:CE1	2.48	0.47
1:A:409:LEU:HD23	1:A:497:VAL:HG21	1.94	0.47
1:B:93:ARG:NH1	1:B:229:ASN:HB3	2.29	0.47
1:A:334:VAL:HG12	1:A:345:LYS:HB2	1.96	0.47
1:A:408:THR:O	1:A:408:THR:HG22	2.13	0.47
1:A:324:ASP:O	1:A:327:GLU:HB2	2.14	0.47
1:A:414:ALA:HB2	1:B:270:LYS:HE3	1.95	0.47
1:A:423:TRP:CE2	1:A:458:LEU:CD2	2.97	0.47
1:B:419:PHE:CZ	1:B:499:ILE:HD13	2.47	0.47
1:B:90:VAL:HG12	1:B:91:VAL:N	2.29	0.47
1:B:246:VAL:HG12	1:B:247:SER:N	2.28	0.47
1:B:415:TYR:O	1:B:415:TYR:CD1	2.68	0.47
1:A:421:VAL:HG22	1:A:467:ILE:HG12	1.96	0.47
1:B:141:PRO:HB3	1:B:160:GLN:HA	1.95	0.47
1:A:115:THR:HG21	1:A:375:TYR:CD2	2.49	0.47
1:A:171:VAL:CG1	1:A:172:ASP:N	2.78	0.47
1:B:105:ILE:HD13	1:B:105:ILE:H	1.78	0.47
1:A:111:VAL:HG13	1:A:114:ARG:CD	2.38	0.47
1:A:411:HIS:HD2	1:A:412:TYR:N	2.12	0.47
1:A:420:ASP:HB2	1:A:468:VAL:CG2	2.41	0.47
1:B:68:VAL:CG1	1:B:69:ASN:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:HA3	1:B:182:TYR:CD1	2.50	0.47
1:B:304:GLN:HG3	1:B:305:ALA:N	2.30	0.47
1:B:426:PHE:CE1	1:B:461:ASN:HB2	2.49	0.47
1:A:93:ARG:NH1	1:A:229:ASN:HB3	2.29	0.47
1:A:79:LYS:HD2	1:A:92:GLU:CG	2.43	0.47
1:A:375:TYR:HE1	1:A:377:SER:OG	1.97	0.47
1:B:156:THR:O	1:B:156:THR:HG22	2.13	0.47
1:B:199:VAL:HG12	1:B:205:ILE:HG12	1.97	0.47
1:B:345:LYS:HG2	1:B:346:VAL:N	2.30	0.47
1:B:484:ILE:CG1	1:B:508:ALA:HB1	2.44	0.47
1:A:484:ILE:CG1	1:A:508:ALA:HB1	2.45	0.47
1:B:179:ASN:O	1:B:183:SER:HB2	2.15	0.47
1:A:139:ARG:HH12	1:A:257:LEU:HD22	1.78	0.46
1:A:489:VAL:HA	1:A:490:PRO:HD2	1.64	0.46
1:B:334:VAL:HG12	1:B:345:LYS:CB	2.45	0.46
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.68	0.46
1:A:150:GLY:HA3	1:A:182:TYR:CD1	2.50	0.46
1:A:291:TYR:HB2	1:A:334:VAL:CG2	2.43	0.46
1:A:407:MET:CE	1:A:467:ILE:HD11	2.45	0.46
1:B:152:ARG:HD3	1:B:155:ASN:HB3	1.97	0.46
1:B:260:ASN:C	1:B:262:VAL:N	2.73	0.46
1:B:375:TYR:HE1	1:B:377:SER:OG	1.99	0.46
1:A:157:ILE:HG23	1:A:158:THR:H	1.81	0.46
1:A:469:ALA:CB	1:A:484:ILE:HB	2.44	0.46
1:A:508:ALA:C	1:A:509:THR:HG23	2.41	0.46
1:B:111:VAL:CG1	1:B:114:ARG:HD3	2.36	0.46
1:B:112:VAL:HG13	1:B:113:ASN:H	1.80	0.46
1:B:508:ALA:C	1:B:509:THR:HG23	2.40	0.46
1:A:112:VAL:HG13	1:A:113:ASN:N	2.31	0.46
1:B:408:THR:HG22	1:B:408:THR:O	2.15	0.46
1:B:418:GLN:NE2	1:B:445:GLY:O	2.49	0.46
1:B:267:LEU:O	1:B:270:LYS:N	2.48	0.46
1:A:294:LEU:HD22	1:A:307:PHE:CE1	2.50	0.46
1:B:157:ILE:HG23	1:B:158:THR:H	1.80	0.46
1:B:210:ASN:O	1:B:210:ASN:CG	2.57	0.46
1:B:499:ILE:HA	1:B:507:THR:O	2.16	0.46
1:B:160:GLN:HA	1:B:160:GLN:NE2	2.30	0.46
1:B:202:LYS:O	1:B:203:SER:C	2.59	0.46
1:B:300:SER:C	1:B:302:ASP:N	2.72	0.46
1:B:484:ILE:HD11	1:B:508:ALA:CB	2.41	0.46
1:A:205:ILE:HD12	1:A:205:ILE:HA	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD23	1:B:497:VAL:HG21	1.97	0.45
1:A:68:VAL:CG1	1:A:69:ASN:N	2.79	0.45
1:A:74:GLU:HG3	1:A:75:SER:N	2.30	0.45
1:A:184:THR:O	1:A:186:HIS:N	2.49	0.45
1:A:465:ILE:HG21	1:A:489:VAL:CB	2.26	0.45
1:A:492:THR:CG2	1:A:512:HIS:HD2	2.27	0.45
1:B:325:ILE:C	1:B:327:GLU:H	2.25	0.45
1:B:294:LEU:HD23	1:B:331:PHE:CE1	2.49	0.45
1:A:205:ILE:O	1:A:206:ALA:C	2.59	0.45
1:B:60:TYR:CE1	1:B:277:PRO:HG2	2.52	0.45
1:B:442:GLU:OE2	1:B:442:GLU:CA	2.56	0.45
1:A:426:PHE:CE1	1:A:461:ASN:HB2	2.51	0.45
1:B:184:THR:O	1:B:185:THR:C	2.59	0.45
1:A:155:ASN:OD1	1:A:156:THR:N	2.49	0.45
1:A:442:GLU:OE2	1:A:442:GLU:CA	2.56	0.45
1:B:300:SER:O	1:B:301:LYS:C	2.59	0.45
1:A:265:ASP:O	1:A:266:GLU:C	2.59	0.45
1:B:223:ASP:O	1:B:223:ASP:CG	2.60	0.45
1:B:300:SER:C	1:B:302:ASP:H	2.24	0.45
1:B:324:ASP:O	1:B:327:GLU:HB2	2.16	0.45
1:B:469:ALA:CB	1:B:484:ILE:HB	2.45	0.45
1:A:296:THR:HG21	1:A:303:VAL:HG22	1.99	0.45
1:B:47:ASN:C	1:B:49:SER:N	2.73	0.45
1:B:171:VAL:HG21	1:B:246:VAL:HG21	1.97	0.45
1:B:206:ALA:O	1:B:208:ALA:N	2.50	0.45
1:A:378:THR:CG2	1:A:383:ASN:C	2.90	0.45
1:A:81:SER:O	1:A:82:ILE:HB	2.17	0.44
1:A:144:ILE:O	1:A:144:ILE:CG1	2.65	0.44
1:A:249:GLU:O	1:A:250:LEU:C	2.56	0.44
1:A:474:GLY:C	1:A:475:LEU:HD23	2.42	0.44
1:B:291:TYR:O	1:B:333:ALA:HA	2.16	0.44
1:B:378:THR:CG2	1:B:383:ASN:HA	2.45	0.44
1:B:473:THR:HG22	1:B:480:TRP:HA	1.99	0.44
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.80	0.44
1:A:198:MET:HE3	1:A:198:MET:HA	1.98	0.44
1:A:291:TYR:O	1:A:333:ALA:HA	2.18	0.44
1:A:156:THR:O	1:A:156:THR:HG22	2.13	0.44
1:A:484:ILE:HG12	1:A:508:ALA:HB1	1.98	0.44
1:B:200:TYR:HD1	1:B:394:TYR:CD1	2.30	0.44
1:A:47:ASN:C	1:A:49:SER:N	2.73	0.44
1:A:188:LEU:HA	1:A:189:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ALA:HB1	1:B:136:VAL:HG11	1.99	0.44
1:B:115:THR:HG21	1:B:375:TYR:CD2	2.52	0.44
1:A:149:PRO:C	1:A:151:MET:N	2.71	0.44
1:A:433:LYS:CE	1:A:433:LYS:CA	2.58	0.44
1:B:508:ALA:C	1:B:509:THR:CG2	2.91	0.44
1:A:148:LEU:HB3	1:A:178:TRP:CD1	2.52	0.44
1:A:268:THR:C	1:A:270:LYS:N	2.75	0.44
1:B:81:SER:O	1:B:82:ILE:HB	2.17	0.44
1:B:208:ALA:C	1:B:210:ASN:N	2.73	0.44
1:B:484:ILE:HG12	1:B:508:ALA:HB1	1.98	0.44
1:A:90:VAL:HG12	1:A:91:VAL:N	2.31	0.44
1:A:296:THR:HB	1:A:329:SER:OG	2.17	0.44
1:A:471:GLU:O	1:A:471:GLU:HG2	2.15	0.44
1:A:472:CYS:HA	1:A:480:TRP:HB3	2.00	0.44
1:B:188:LEU:HA	1:B:189:PRO:HD3	1.82	0.44
1:A:310:LEU:HD21	1:A:351:PHE:CD2	2.52	0.44
1:B:146:ILE:HG23	1:B:148:LEU:H	1.83	0.44
1:B:155:ASN:OD1	1:B:156:THR:N	2.51	0.44
1:B:485:ASN:C	1:B:486:GLU:HG2	2.42	0.44
1:A:325:ILE:C	1:A:327:GLU:H	2.25	0.44
1:B:205:ILE:O	1:B:209:LEU:HB2	2.18	0.44
1:B:371:TYR:O	1:B:372:PRO:C	2.61	0.44
1:B:134:LEU:HD23	1:B:135:LEU:H	1.83	0.43
1:A:424:ASP:HB2	1:A:463:LYS:O	2.18	0.43
1:B:205:ILE:O	1:B:206:ALA:C	2.61	0.43
1:B:346:VAL:HG12	1:B:348:THR:HG23	2.01	0.43
1:B:415:TYR:HB3	1:B:503:THR:HG23	2.00	0.43
1:B:489:VAL:HA	1:B:490:PRO:HD2	1.67	0.43
1:B:107:ILE:CD1	1:B:115:THR:HG21	2.46	0.43
1:B:268:THR:C	1:B:270:LYS:N	2.76	0.43
1:A:160:GLN:HA	1:A:160:GLN:NE2	2.33	0.43
1:A:485:ASN:C	1:A:486:GLU:HG2	2.43	0.43
1:B:378:THR:CG2	1:B:383:ASN:C	2.92	0.43
1:A:73:VAL:O	1:A:74:GLU:HG2	2.19	0.43
1:A:223:ASP:O	1:A:223:ASP:CG	2.62	0.43
1:A:484:ILE:HD11	1:A:508:ALA:CB	2.43	0.43
1:A:501:GLY:HA2	1:B:266:GLU:CD	2.43	0.43
1:A:287:GLY:O	1:A:370:ALA:HA	2.19	0.43
1:B:111:VAL:HG13	1:B:114:ARG:CD	2.34	0.43
1:A:80:GLU:HG2	1:A:81:SER:N	2.33	0.42
1:B:325:ILE:C	1:B:327:GLU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HG22	1:A:102:PRO:CD	2.47	0.42
1:B:167:VAL:O	1:B:168:ALA:C	2.60	0.42
1:B:296:THR:HG21	1:B:303:VAL:HG22	2.01	0.42
1:A:214:LYS:HB3	1:A:214:LYS:HZ2	1.83	0.42
1:A:269:ARG:HE	1:A:269:ARG:HB2	1.61	0.42
1:A:352:ASN:O	1:A:352:ASN:ND2	2.53	0.42
1:B:149:PRO:C	1:B:151:MET:N	2.71	0.42
1:A:255:SER:C	1:A:257:LEU:H	2.27	0.42
1:A:314:ASN:ND2	1:A:314:ASN:N	2.67	0.42
1:A:377:SER:HB2	1:A:386:ALA:HB3	2.00	0.42
1:B:196:GLU:O	1:B:196:GLU:HG2	2.20	0.42
1:B:220:LEU:HD23	1:B:220:LEU:HA	1.83	0.42
1:A:294:LEU:HB3	1:A:307:PHE:CE1	2.53	0.42
1:A:325:ILE:C	1:A:327:GLU:N	2.76	0.42
1:A:409:LEU:HD12	1:A:454:THR:HG22	2.01	0.42
1:B:197:SER:OG	1:B:198:MET:N	2.52	0.42
1:B:209:LEU:CD1	1:B:236:VAL:CG1	2.84	0.42
1:B:474:GLY:C	1:B:475:LEU:HD23	2.44	0.42
1:B:279:VAL:HG12	1:B:379:PHE:HA	2.02	0.42
1:B:415:TYR:CD1	1:B:415:TYR:C	2.98	0.42
1:A:244:TYR:CE2	1:A:286:TYR:HB2	2.55	0.42
1:A:346:VAL:HG12	1:A:348:THR:HG23	2.02	0.42
1:A:508:ALA:C	1:A:509:THR:CG2	2.92	0.42
1:B:377:SER:HB2	1:B:386:ALA:HB3	2.01	0.42
1:A:152:ARG:H	1:A:152:ARG:HD2	1.85	0.42
1:B:181:LYS:O	1:B:182:TYR:HD2	1.75	0.42
1:B:200:TYR:HB2	1:B:394:TYR:CD1	2.51	0.42
1:B:408:THR:O	1:B:497:VAL:HG23	2.20	0.42
1:B:430:GLN:CD	1:B:430:GLN:H	2.28	0.42
1:A:112:VAL:HG13	1:A:113:ASN:H	1.84	0.41
1:A:202:LYS:O	1:A:203:SER:C	2.62	0.41
1:B:84:SER:C	1:B:86:GLY:H	2.28	0.41
1:B:399:THR:HG23	1:B:400:THR:N	2.35	0.41
1:A:371:TYR:O	1:A:372:PRO:C	2.60	0.41
1:A:418:GLN:NE2	1:A:445:GLY:O	2.53	0.41
1:B:68:VAL:HG12	1:B:69:ASN:N	2.35	0.41
1:B:82:ILE:HD13	1:B:82:ILE:C	2.45	0.41
1:B:139:ARG:NH1	1:B:257:LEU:CD2	2.74	0.41
1:B:144:ILE:O	1:B:144:ILE:CG1	2.68	0.41
1:B:205:ILE:HD12	1:B:205:ILE:HA	1.63	0.41
1:B:352:ASN:ND2	1:B:352:ASN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:O	1:A:209:LEU:HB2	2.21	0.41
1:A:433:LYS:CE	1:A:434:GLU:H	2.32	0.41
1:B:114:ARG:NH1	1:B:132:PRO:O	2.53	0.41
1:B:468:VAL:HA	1:B:484:ILE:O	2.20	0.41
1:A:139:ARG:HB2	1:A:162:PRO:HD2	2.01	0.41
1:A:167:VAL:O	1:A:168:ALA:C	2.61	0.41
1:B:412:TYR:N	1:B:412:TYR:CD2	2.89	0.41
1:B:420:ASP:HB2	1:B:468:VAL:CG2	2.45	0.41
1:B:471:GLU:O	1:B:471:GLU:HG2	2.13	0.41
1:A:364:LEU:O	1:A:365:SER:HB3	2.20	0.41
1:A:415:TYR:CD1	1:A:415:TYR:C	2.98	0.41
1:B:71:ASP:OD2	1:B:71:ASP:N	2.53	0.41
1:A:73:VAL:O	1:A:74:GLU:CG	2.68	0.41
1:A:134:LEU:HD23	1:A:135:LEU:N	2.36	0.41
1:A:350:ASP:OD1	1:A:350:ASP:C	2.62	0.41
1:A:430:GLN:H	1:A:430:GLN:CD	2.28	0.41
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.58	0.41
1:A:304:GLN:CG	1:A:305:ALA:N	2.81	0.41
1:B:472:CYS:HA	1:B:480:TRP:HB3	2.03	0.41
1:A:116:TYR:CD1	1:A:164:TYR:HB2	2.55	0.41
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.70	0.41
1:A:260:ASN:C	1:A:262:VAL:N	2.76	0.41
1:B:287:GLY:O	1:B:370:ALA:HA	2.21	0.41
1:B:304:GLN:CG	1:B:305:ALA:N	2.82	0.41
1:B:334:VAL:HG12	1:B:345:LYS:HB2	2.02	0.41
1:B:424:ASP:HB2	1:B:463:LYS:O	2.21	0.41
1:A:407:MET:HA	1:A:495:ILE:O	2.20	0.41
1:B:106:LEU:H	1:B:106:LEU:HD23	1.86	0.41
1:B:148:LEU:HB3	1:B:178:TRP:CD1	2.55	0.41
1:A:146:ILE:HG23	1:A:148:LEU:H	1.86	0.41
1:B:116:TYR:CD1	1:B:164:TYR:HB2	2.56	0.41
1:B:364:LEU:O	1:B:365:SER:HB3	2.21	0.41
1:A:408:THR:O	1:A:497:VAL:HG23	2.20	0.40
1:A:429:ASP:OD1	1:A:429:ASP:N	2.50	0.40
1:A:473:THR:HG22	1:A:480:TRP:CA	2.51	0.40
1:B:436:LEU:HA	1:B:436:LEU:HD12	1.60	0.40
1:A:193:GLN:O	1:A:240:LYS:HB2	2.22	0.40
1:A:502:THR:CG2	1:A:504:LEU:N	2.68	0.40
1:B:407:MET:HA	1:B:495:ILE:O	2.20	0.40
1:B:437:THR:O	1:B:437:THR:HG22	2.22	0.40
1:A:419:PHE:CZ	1:A:499:ILE:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LYS:O	1:B:215:TYR:C	2.64	0.40
1:B:429:ASP:OD1	1:B:429:ASP:N	2.53	0.40
1:A:82:ILE:HD13	1:A:82:ILE:C	2.46	0.40
1:A:106:LEU:H	1:A:106:LEU:HD23	1.87	0.40
1:A:210:ASN:OD1	1:A:210:ASN:C	2.65	0.40
1:A:429:ASP:C	1:A:431:ASN:N	2.79	0.40
1:B:106:LEU:CD1	1:B:212:ASN:HB2	2.51	0.40
1:A:378:THR:HG22	1:A:383:ASN:CA	2.47	0.40
1:A:415:TYR:HB3	1:A:503:THR:HG23	2.02	0.40
1:A:433:LYS:HZ3	1:A:434:GLU:N	2.11	0.40
1:B:80:GLU:HG2	1:B:81:SER:N	2.35	0.40
1:B:294:LEU:HD22	1:B:307:PHE:CE1	2.57	0.40
1:B:425:GLU:OE2	1:B:459:PRO:HG3	2.21	0.40
1:B:434:GLU:HG2	1:B:436:LEU:HD13	2.04	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	458/489 (94%)	358 (78%)	66 (14%)	34 (7%)	1	5
1	B	458/489 (94%)	357 (78%)	66 (14%)	35 (8%)	1	4
All	All	916/978 (94%)	715 (78%)	132 (14%)	69 (8%)	1	4

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	73	VAL
1	A	74	GLU
1	A	100	THR

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Mol	Chain	Res	Type
1	A	151	MET
1	A	209	LEU
1	A	230	GLY
1	A	259	ASP
1	A	304	GLN
1	A	319	SER
1	A	465	ILE
1	B	72	LYS
1	B	73	VAL
1	B	74	GLU
1	B	100	THR
1	B	151	MET
1	B	209	LEU
1	B	224	PHE
1	B	230	GLY
1	B	259	ASP
1	B	304	GLN
1	B	319	SER
1	B	465	ILE
1	A	109	ASP
1	A	113	ASN
1	A	128	ALA
1	A	150	GLY
1	A	182	TYR
1	A	185	THR
1	A	206	ALA
1	A	221	ASN
1	A	223	ASP
1	A	224	PHE
1	A	301	LYS
1	A	308	LYS
1	B	113	ASN
1	B	128	ALA
1	B	150	GLY
1	B	182	TYR
1	B	221	ASN
1	B	223	ASP
1	B	301	LYS
1	B	308	LYS
1	B	370	ALA
1	A	101	SER
1	A	370	ALA

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Mol	Chain	Res	Type
1	B	101	SER
1	B	109	ASP
1	B	206	ALA
1	B	338	GLY
1	A	82	ILE
1	A	172	ASP
1	A	338	GLY
1	A	391	ASN
1	A	414	ALA
1	B	172	ASP
1	B	185	THR
1	B	414	ALA
1	A	249	GLU
1	A	466	LYS
1	B	82	ILE
1	B	249	GLU
1	B	360	ASP
1	B	391	ASN
1	B	466	LYS
1	A	360	ASP
1	A	111	VAL
1	B	111	VAL
1	B	105	ILE

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	387/423 (92%)	313 (81%)	74 (19%)	1	7
1	B	387/423 (92%)	311 (80%)	76 (20%)	1	6
All	All	774/846 (92%)	624 (81%)	150 (19%)	1	7

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	57	ASN
1	A	61	ASP
1	A	62	SER
1	A	71	ASP
1	A	74	GLU
1	A	82	ILE
1	A	98	LEU
1	A	105	ILE
1	A	109	ASP
1	A	113	ASN
1	A	114	ARG
1	A	127	PHE
1	A	129	ASP
1	A	134	LEU
1	A	135	LEU
1	A	142	LEU
1	A	152	ARG
1	A	156	THR
1	A	157	ILE
1	A	158	THR
1	A	159	VAL
1	A	171	VAL
1	A	184	THR
1	A	187	THR
1	A	192	MET
1	A	203	SER
1	A	205	ILE
1	A	211	VAL
1	A	214	LYS
1	A	216	LEU
1	A	219	SER
1	A	225	ASN
1	A	235	MET
1	A	252	ASN
1	A	261	SER
1	A	269	ARG
1	A	275	SER
1	A	282	SER
1	A	286	TYR
1	A	295	GLU
1	A	300	SER
1	A	301	LYS

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Mol	Chain	Res	Type
1	A	310	LEU
1	A	314	ASN
1	A	319	SER
1	A	327	GLU
1	A	330	THR
1	A	332	THR
1	A	347	VAL
1	A	348	THR
1	A	364	LEU
1	A	373	ILE
1	A	378	THR
1	A	388	VAL
1	A	391	ASN
1	A	395	ILE
1	A	397	THR
1	A	399	THR
1	A	406	LYS
1	A	408	THR
1	A	421	VAL
1	A	426	PHE
1	A	433	LYS
1	A	436	LEU
1	A	449	THR
1	A	465	ILE
1	A	468	VAL
1	A	491	LEU
1	A	492	THR
1	A	497	VAL
1	A	498	SER
1	A	503	THR
1	A	504	LEU
1	B	51	ILE
1	B	57	ASN
1	B	61	ASP
1	B	62	SER
1	B	71	ASP
1	B	74	GLU
1	B	82	ILE
1	B	98	LEU
1	B	105	ILE
1	B	109	ASP
1	B	113	ASN

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Mol	Chain	Res	Type
1	B	114	ARG
1	B	127	PHE
1	B	129	ASP
1	B	134	LEU
1	B	135	LEU
1	B	142	LEU
1	B	152	ARG
1	B	156	THR
1	B	157	ILE
1	B	158	THR
1	B	159	VAL
1	B	171	VAL
1	B	177	THR
1	B	184	THR
1	B	187	THR
1	B	203	SER
1	B	205	ILE
1	B	211	VAL
1	B	214	LYS
1	B	216	LEU
1	B	219	SER
1	B	225	ASN
1	B	235	MET
1	B	252	ASN
1	B	261	SER
1	B	263	THR
1	B	269	ARG
1	B	275	SER
1	B	282	SER
1	B	286	TYR
1	B	295	GLU
1	B	300	SER
1	B	301	LYS
1	B	310	LEU
1	B	314	ASN
1	B	319	SER
1	B	327	GLU
1	B	330	THR
1	B	332	THR
1	B	347	VAL
1	B	348	THR
1	B	364	LEU

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Mol	Chain	Res	Type
1	B	378	THR
1	B	388	VAL
1	B	391	ASN
1	B	395	ILE
1	B	397	THR
1	B	399	THR
1	B	406	LYS
1	B	408	THR
1	B	410	ASP
1	B	426	PHE
1	B	433	LYS
1	B	436	LEU
1	B	442	GLU
1	B	449	THR
1	B	465	ILE
1	B	468	VAL
1	B	491	LEU
1	B	492	THR
1	B	497	VAL
1	B	498	SER
1	B	499	ILE
1	B	503	THR
1	B	504	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	130	ASN
1	A	160	GLN
1	A	193	GLN
1	A	212	ASN
1	A	225	ASN
1	A	252	ASN
1	A	260	ASN
1	A	314	ASN
1	A	352	ASN
1	A	389	HIS
1	A	391	ASN
1	A	411	HIS
1	A	418	GLN
1	A	431	ASN

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Mol	Chain	Res	Type
1	A	464	ASN
1	A	488	ASN
1	A	512	HIS
1	B	113	ASN
1	B	130	ASN
1	B	160	GLN
1	B	193	GLN
1	B	212	ASN
1	B	225	ASN
1	B	252	ASN
1	B	260	ASN
1	B	314	ASN
1	B	352	ASN
1	B	389	HIS
1	B	391	ASN
1	B	411	HIS
1	B	418	GLN
1	B	431	ASN
1	B	438	HIS
1	B	464	ASN
1	B	488	ASN
1	B	512	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	462/489 (94%)	-1.01	1 (0%) 91 83	51, 76, 99, 105	0
1	B	462/489 (94%)	-1.03	1 (0%) 91 83	51, 76, 99, 105	0
All	All	924/978 (94%)	-1.02	2 (0%) 91 83	51, 76, 99, 105	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	PHE	2.1
1	A	339	ASP	2.1

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.