



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:56 PM UTC

PDB ID : 2J04 / pdb_00002j04
Title : The tau60-tau91 subcomplex of yeast transcription factor IIIC
Authors : Mylona, A.; Fernandez-Tornero, C.; Legrand, P.; Muller, C.W.
Deposited on : 2006-07-31
Resolution : 3.20 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

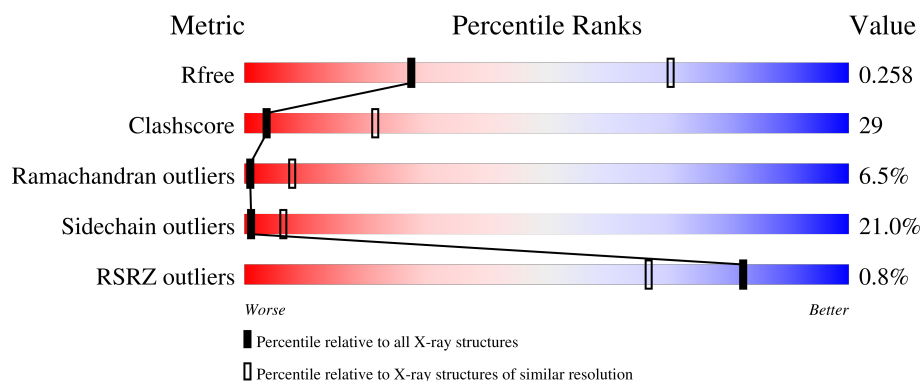
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	588	52% 35% 12% .
1	C	588	45% 39% 13% .
2	B	524	40% 34% 13% . 10%
2	D	524	41% 33% 12% . 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16935 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 HYPOTHETICAL PROTEIN YPL007C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4760	3058	777	902	23			
1	C	586	Total	C	N	O	S	0	0	0
			4751	3052	775	901	23			

- Molecule 2 is a protein called YDR362CP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	472	Total	C	N	O	S	0	0	1
			3715	2384	613	703	15			
2	D	469	Total	C	N	O	S	0	0	1
			3704	2379	609	701	15			

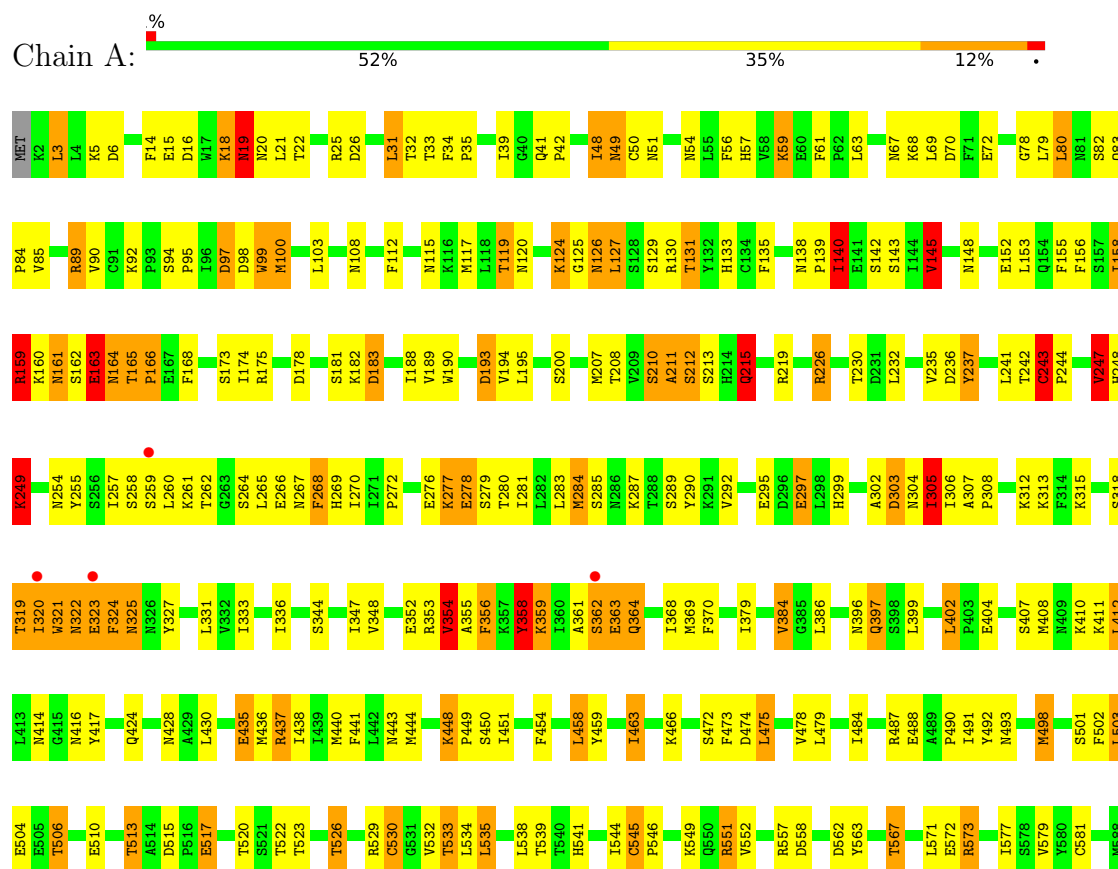
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

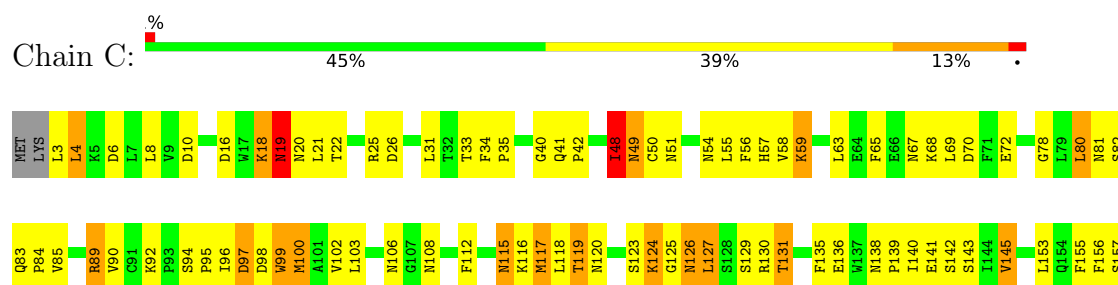
3 Residue-property plots

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: HYPOTHETICAL PROTEIN YPL007C



• Molecule 1: HYPOTHETICAL PROTEIN YPL007C







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.42Å 125.80Å 210.47Å 90.00° 94.49° 90.00°	Depositor
Resolution (Å)	208.51 – 3.20 208.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (208.51-3.20) 98.7 (208.51-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.257 (Not available) , 0.258	Depositor DCC
R_{free} test set	2619 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 128.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16935	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.96	4/4872 (0.1%)	1.17	19/6610 (0.3%)
1	C	0.93	3/4863 (0.1%)	1.15	25/6599 (0.4%)
2	B	0.94	6/3798 (0.2%)	1.21	27/5153 (0.5%)
2	D	0.91	7/3788 (0.2%)	1.17	24/5140 (0.5%)
All	All	0.94	20/17321 (0.1%)	1.17	95/23502 (0.4%)

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	2
1	C	0	3
2	B	0	8
2	D	0	7
All	All	0	20

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	413	LYS	CD-CE	15.06	1.97	1.52
2	B	300	ILE	CA-CB	13.18	1.69	1.53
2	B	413	LYS	CD-CE	11.78	1.87	1.52
1	A	249	LYS	CD-CE	10.98	1.85	1.52
2	D	300	ILE	CA-CB	9.79	1.65	1.53
2	D	413	LYS	CE-NZ	9.13	1.76	1.49
1	C	249	LYS	CD-CE	9.06	1.79	1.52
2	D	320	TYR	C-O	8.95	1.41	1.23
2	B	413	LYS	CE-NZ	8.49	1.74	1.49
2	D	413	LYS	CG-CD	7.26	1.74	1.52
1	A	297	GLU	CD-OE1	6.86	1.38	1.25
2	B	413	LYS	CG-CD	6.21	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	674	GLU	C-N	-6.17	1.24	1.33
1	A	297	GLU	CD-OE2	5.94	1.36	1.25
1	A	320	ILE	CA-CB	5.90	1.62	1.54
1	C	320	ILE	CA-CB	5.83	1.62	1.54
2	B	304	THR	CA-CB	5.57	1.61	1.52
2	D	674	GLU	C-N	-5.46	1.25	1.33
2	D	380	LEU	CA-C	5.31	1.59	1.52
1	C	360	ILE	CA-CB	5.24	1.59	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	599	SER	N-CA-C	12.14	128.04	109.23
2	D	599	SER	N-CA-C	11.12	126.04	109.24
2	D	413	LYS	CG-CD-CE	-9.59	89.24	111.30
2	D	340	CYS	N-CA-C	9.19	120.03	108.45
1	C	532	VAL	N-CA-C	-9.15	103.94	111.81
2	B	294	ASP	N-CA-C	9.14	124.58	110.42
2	B	608	SER	N-CA-C	9.14	121.01	111.14
2	D	585	ARG	N-CA-C	-8.48	103.43	112.93
1	A	268	PHE	N-CA-C	8.45	121.36	108.52
2	B	340	CYS	N-CA-C	8.20	118.78	108.45
2	D	299	ASN	N-CA-C	8.17	121.41	107.93
1	C	268	PHE	N-CA-C	7.89	121.22	108.76
2	B	413	LYS	CG-CD-CE	-7.87	93.21	111.30
2	D	608	SER	N-CA-C	7.83	119.59	111.14
2	B	600	LEU	N-CA-C	7.81	122.08	110.52
2	D	294	ASP	N-CA-C	7.77	122.46	110.42
2	B	585	ARG	N-CA-C	-7.71	104.30	112.93
2	B	619	SER	N-CA-C	7.49	121.53	110.30
2	B	236	HIS	N-CA-C	7.29	119.40	107.23
2	D	236	HIS	N-CA-C	7.17	119.21	107.23
2	B	380	LEU	N-CA-C	7.07	125.85	110.80
2	D	380	LEU	N-CA-C	7.01	125.74	110.80
1	C	493	ASN	N-CA-C	6.99	118.39	108.54
1	A	532	VAL	N-CA-C	-6.97	105.81	111.81
2	D	600	LEU	N-CA-C	6.91	121.14	110.42
1	A	558	ASP	N-CA-C	6.67	118.58	109.11
2	B	648	ASN	N-CA-C	-6.63	100.47	110.28
1	C	161	ASN	N-CA-C	6.43	124.49	110.80
1	C	48	ILE	CB-CA-C	-6.38	101.80	110.42
1	A	161	ASN	N-CA-C	6.29	124.19	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	LYS	N-CA-C	6.28	118.13	110.41
2	B	610	LYS	N-CA-C	6.20	124.01	110.80
2	D	413	LYS	CD-CE-NZ	-6.13	92.29	111.90
2	B	413	LYS	CD-CE-NZ	-6.09	92.42	111.90
2	D	250	ARG	N-CA-C	5.99	123.56	110.80
1	C	164	ASN	N-CA-C	5.95	123.48	110.80
2	D	610	LYS	N-CA-C	5.93	123.44	110.80
2	B	674	GLU	O-C-N	-5.93	113.51	123.00
2	D	403	THR	N-CA-C	-5.89	104.63	112.94
2	D	234	VAL	N-CA-C	5.87	121.54	109.34
1	C	530	CYS	CA-C-N	-5.86	113.54	122.28
1	C	530	CYS	C-N-CA	-5.86	113.54	122.28
1	A	552	VAL	N-CA-C	5.84	117.41	108.71
2	D	562	SER	N-CA-C	5.83	118.05	109.24
2	D	215	PRO	O-C-N	5.83	123.89	121.15
1	A	249	LYS	CG-CD-CE	-5.79	97.99	111.30
2	B	250	ARG	N-CA-C	5.74	123.02	110.80
2	B	234	VAL	N-CA-C	5.73	121.26	109.34
1	A	562	ASP	N-CA-C	5.71	118.18	109.62
2	B	589	GLY	N-CA-C	5.70	126.68	113.18
2	D	583	ALA	N-CA-C	-5.64	98.79	110.80
1	A	145	VAL	CB-CA-C	-5.62	102.25	110.62
1	C	552	VAL	N-CA-C	5.61	116.67	108.53
2	B	403	THR	N-CA-C	-5.58	105.07	112.94
2	B	169	LYS	N-CA-C	-5.58	104.70	112.45
2	B	346	MET	N-CA-C	5.56	117.72	108.99
1	A	319	THR	CA-C-N	5.54	131.95	121.97
1	A	319	THR	C-N-CA	5.54	131.95	121.97
2	D	252	LYS	N-CA-C	5.54	117.22	110.41
1	A	513	THR	N-CA-C	-5.52	106.90	113.97
2	B	232	ARG	N-CA-C	5.50	117.39	110.24
1	A	3	LEU	N-CA-C	5.49	118.34	109.40
2	D	244	GLU	N-CA-C	5.48	118.09	111.40
1	A	164	ASN	N-CA-C	5.48	122.47	110.80
1	A	247	VAL	CB-CA-C	-5.46	102.36	110.33
1	C	40	GLY	N-CA-C	-5.43	100.32	113.18
1	C	145	VAL	CB-CA-C	-5.42	102.16	110.50
2	B	671	LEU	N-CA-C	5.41	118.15	110.10
1	A	140	ILE	CB-CA-C	5.40	116.30	111.71
2	B	244	GLU	N-CA-C	5.39	118.32	111.69
1	C	562	ASP	N-CA-C	5.35	117.83	108.52
1	C	510	GLU	CB-CA-C	-5.32	99.83	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	THR	CA-C-N	5.29	131.49	121.97
1	C	319	THR	C-N-CA	5.29	131.49	121.97
2	B	562	SER	N-CA-C	5.28	117.22	109.24
1	A	358	TYR	N-CA-C	5.26	122.00	110.80
1	C	492	TYR	CA-C-N	-5.26	115.94	123.20
1	C	492	TYR	C-N-CA	-5.26	115.94	123.20
2	B	583	ALA	N-CA-C	-5.22	99.67	110.80
2	D	672	SER	N-CA-C	5.22	121.92	110.80
1	C	377	TRP	N-CA-C	5.21	116.21	108.86
1	C	533	THR	N-CA-CB	-5.21	102.87	110.47
1	C	249	LYS	CG-CD-CE	-5.18	99.39	111.30
1	A	572	GLU	N-CA-C	-5.17	105.29	111.03
1	A	530	CYS	CA-C-N	-5.13	114.64	122.28
1	A	530	CYS	C-N-CA	-5.13	114.64	122.28
1	C	277	LYS	N-CA-C	-5.12	103.95	111.17
2	D	619	SER	N-CA-C	5.11	121.69	110.80
1	C	274	ASN	N-CA-C	5.10	118.77	112.54
2	D	581	ASN	N-CA-C	5.09	116.91	108.20
1	C	58	VAL	CB-CA-C	-5.09	104.60	110.91
2	D	673	LEU	N-CA-C	-5.08	105.37	112.03
2	B	672	SER	N-CA-C	5.06	121.58	110.80
1	C	290	TYR	N-CA-C	5.02	115.77	108.14
1	C	267	ASN	N-CA-C	5.01	117.36	110.35

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	CYS	Peptide
1	A	98	ASP	Peptide
2	B	277	ALA	Peptide
2	B	293	THR	Peptide
2	B	379	HIS	Peptide
2	B	380	LEU	Peptide
2	B	582	ALA	Peptide
2	B	584	ARG	Peptide
2	B	598	LYS	Peptide
2	B	608	SER	Peptide
1	C	158	ILE	Peptide
1	C	243	CYS	Peptide
1	C	98	ASP	Peptide
2	D	277	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	D	293	THR	Peptide
2	D	379	HIS	Peptide
2	D	380	LEU	Peptide
2	D	584	ARG	Peptide
2	D	598	LYS	Peptide
2	D	608	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4760	0	4722	235	0
1	C	4751	0	4709	258	0
2	B	3715	0	3674	265	0
2	D	3704	0	3660	242	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	16935	0	16765	983	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 29.

All (983) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LYS:CE	1:C:249:LYS:CD	1.79	1.60
2:B:413:LYS:CE	2:B:413:LYS:CD	1.87	1.52
1:A:249:LYS:CE	1:A:249:LYS:CD	1.85	1.50
2:B:413:LYS:CE	2:B:413:LYS:NZ	1.74	1.47
2:D:413:LYS:NZ	2:D:413:LYS:CE	1.76	1.45
2:D:413:LYS:CE	2:D:413:LYS:CD	1.97	1.43
2:B:608:SER:O	2:B:609:ILE:HG13	1.44	1.16
2:B:601:ARG:HG3	2:B:601:ARG:HH11	0.99	1.16
2:D:601:ARG:HG3	2:D:601:ARG:HH11	1.05	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:608:SER:O	2:D:609:ILE:HG13	1.48	1.12
2:B:584:ARG:HG3	2:B:585:ARG:H	1.01	1.11
1:C:487:ARG:HH11	1:C:487:ARG:HG2	1.14	1.10
2:D:253:ARG:HH11	2:D:253:ARG:HG3	1.17	1.07
2:D:584:ARG:HG3	2:D:585:ARG:H	0.95	1.07
2:B:427:THR:HG22	2:B:470:VAL:HG12	1.31	1.04
2:D:427:THR:HG22	2:D:470:VAL:HG12	1.38	1.04
1:C:533:THR:CG2	1:C:535:LEU:HB2	1.90	1.02
2:D:380:LEU:HD13	2:D:401:ASN:HB3	1.37	1.01
2:B:290:GLY:HA2	2:B:293:THR:N	1.74	1.01
1:C:356:PHE:HZ	2:D:488:ASP:HA	1.25	1.00
2:B:250:ARG:HG2	2:B:267:THR:OG1	1.59	0.99
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.27	0.98
2:D:250:ARG:HG2	2:D:267:THR:OG1	1.63	0.98
1:C:119:THR:HG21	1:C:168:PHE:H	1.29	0.98
2:D:584:ARG:HG3	2:D:585:ARG:N	1.78	0.97
2:D:584:ARG:CG	2:D:585:ARG:H	1.77	0.97
1:A:100:MET:CE	1:A:112:PHE:HB2	1.93	0.97
1:C:544:ILE:HG13	1:C:588:MET:HG2	1.47	0.97
2:B:301:GLU:HB3	2:B:371:TRP:CD1	2.00	0.96
2:B:463:HIS:NE2	2:B:484:THR:HG23	1.81	0.95
1:C:127:LEU:O	1:C:131:THR:HG22	1.66	0.95
1:C:533:THR:HG22	1:C:535:LEU:HB2	1.47	0.95
2:D:301:GLU:HB3	2:D:371:TRP:CD1	2.01	0.95
2:B:220:GLU:HB2	2:B:433:PRO:HG3	1.48	0.95
2:D:220:GLU:HB2	2:D:433:PRO:HG3	1.47	0.94
1:A:119:THR:HG21	1:A:168:PHE:H	1.31	0.93
1:A:127:LEU:O	1:A:131:THR:HG22	1.68	0.93
2:B:584:ARG:HG3	2:B:585:ARG:N	1.82	0.93
1:C:533:THR:HG22	1:C:535:LEU:H	1.33	0.93
2:B:238:ILE:HA	2:B:408:PHE:HB2	1.47	0.93
1:A:262:THR:HG21	1:A:268:PHE:CZ	2.04	0.93
1:A:100:MET:HE1	1:A:112:PHE:HB2	1.51	0.92
2:B:299:ASN:HD22	2:B:646:LYS:HZ2	1.16	0.92
1:C:533:THR:CG2	1:C:535:LEU:HD22	1.99	0.92
2:B:584:ARG:CG	2:B:585:ARG:H	1.82	0.92
2:D:238:ILE:HA	2:D:408:PHE:HB2	1.49	0.92
2:D:198:PHE:CE1	2:D:203:ILE:HD11	2.04	0.91
2:B:236:HIS:HB3	2:B:409:LYS:HG2	1.52	0.91
2:B:250:ARG:NE	2:B:250:ARG:HA	1.83	0.91
2:B:299:ASN:HD22	2:B:646:LYS:NZ	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:THR:CG2	2:B:470:VAL:HG12	2.00	0.91
1:C:100:MET:CE	1:C:112:PHE:HB2	1.99	0.91
1:A:466:LYS:CE	1:A:490:PRO:HB3	2.01	0.91
1:A:533:THR:HG21	1:A:535:LEU:HD22	1.50	0.90
2:B:380:LEU:HD13	2:B:401:ASN:HB3	1.52	0.90
1:A:323:GLU:O	1:A:324:PHE:HB2	1.72	0.90
2:B:601:ARG:HG3	2:B:601:ARG:NH1	1.80	0.90
2:D:188:LYS:O	2:D:192:GLU:HB2	1.71	0.89
2:D:601:ARG:HG3	2:D:601:ARG:NH1	1.85	0.89
2:D:463:HIS:NE2	2:D:484:THR:HG23	1.88	0.89
2:B:188:LYS:O	2:B:192:GLU:HB2	1.71	0.89
2:D:427:THR:HG21	2:D:470:VAL:H	1.39	0.88
1:A:68:LYS:H	1:A:108:ASN:HD21	1.18	0.88
2:B:234:VAL:HG21	2:B:412:GLU:HG2	1.54	0.88
1:C:68:LYS:H	1:C:108:ASN:HD21	1.17	0.88
2:D:563:ARG:HD2	2:D:649:GLU:HB3	1.55	0.88
2:D:250:ARG:HA	2:D:250:ARG:NE	1.87	0.87
1:C:323:GLU:O	1:C:324:PHE:HB2	1.72	0.87
2:D:527:ILE:HG22	2:D:559:ILE:CD1	2.06	0.86
1:C:358:TYR:HB2	2:D:508:ARG:HH22	1.40	0.86
2:B:601:ARG:HH11	2:B:601:ARG:CG	1.88	0.86
1:A:356:PHE:HZ	2:B:488:ASP:HA	1.40	0.86
2:B:295:ILE:O	2:B:295:ILE:HG13	1.76	0.86
2:B:380:LEU:HD22	2:B:401:ASN:HA	1.56	0.85
2:B:598:LYS:HD2	2:B:624:PRO:O	1.75	0.85
1:C:533:THR:HG21	1:C:535:LEU:HD22	1.56	0.85
1:A:289:SER:HB2	1:A:304:ASN:HD21	1.39	0.85
1:A:530:CYS:SG	1:A:533:THR:HB	2.17	0.85
1:C:356:PHE:CZ	2:D:488:ASP:HA	2.11	0.85
2:B:234:VAL:CG2	2:B:412:GLU:HG2	2.07	0.84
1:A:466:LYS:HE3	1:A:490:PRO:HB3	1.60	0.84
2:D:234:VAL:HG21	2:D:412:GLU:HG2	1.59	0.84
2:B:236:HIS:CB	2:B:409:LYS:HG2	2.08	0.84
2:D:234:VAL:CG2	2:D:412:GLU:HG2	2.08	0.83
1:C:262:THR:HG21	1:C:268:PHE:CZ	2.13	0.83
2:B:361:HIS:HD2	2:B:363:PHE:H	1.26	0.83
1:A:533:THR:CG2	1:A:535:LEU:HD22	2.08	0.83
2:B:301:GLU:HG3	2:B:301:GLU:O	1.79	0.83
1:C:97:ASP:HB2	1:C:99:TRP:CE3	2.14	0.82
1:C:500:ASN:HB2	1:C:539:THR:O	1.80	0.82
2:D:380:LEU:HD22	2:D:401:ASN:HA	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:MET:HG2	1:C:289:SER:HB3	1.61	0.81
1:A:533:THR:HG22	1:A:535:LEU:HB2	1.63	0.81
1:A:97:ASP:HB2	1:A:99:TRP:CE3	2.17	0.80
1:C:226:ARG:HG3	2:D:457:SER:OG	1.81	0.80
2:D:176:LEU:HG	2:D:177:ASN:H	1.44	0.80
2:B:384:LEU:HD22	2:B:398:ILE:HD11	1.64	0.80
2:D:427:THR:CG2	2:D:470:VAL:HG12	2.11	0.80
1:A:533:THR:CG2	1:A:535:LEU:HB2	2.11	0.80
1:C:487:ARG:HG2	1:C:487:ARG:NH1	1.92	0.80
2:B:413:LYS:CE	2:B:413:LYS:CG	2.60	0.80
1:C:289:SER:HB2	1:C:304:ASN:HD21	1.47	0.80
1:A:226:ARG:HG3	2:B:457:SER:OG	1.81	0.79
1:C:539:THR:HG23	1:C:540:THR:H	1.48	0.79
2:B:427:THR:HG21	2:B:470:VAL:N	1.98	0.79
2:D:198:PHE:HE1	2:D:203:ILE:CD1	1.96	0.79
2:D:585:ARG:HA	2:D:588:HIS:HB3	1.63	0.79
2:B:563:ARG:HD2	2:B:649:GLU:HB3	1.65	0.79
1:C:533:THR:HG21	1:C:535:LEU:HB2	1.65	0.79
1:A:503:LEU:HD12	1:A:504:GLU:N	1.98	0.79
1:C:108:ASN:HD22	1:C:120:ASN:HD21	1.28	0.78
2:B:427:THR:HG21	2:B:470:VAL:H	1.48	0.78
2:B:585:ARG:HA	2:B:588:HIS:HB3	1.65	0.78
2:D:295:ILE:HG13	2:D:295:ILE:O	1.81	0.78
2:D:198:PHE:HE1	2:D:203:ILE:HD11	1.48	0.78
1:A:284:MET:HG2	1:A:289:SER:HB3	1.66	0.78
1:C:249:LYS:CE	1:C:249:LYS:CG	2.61	0.78
2:B:176:LEU:HG	2:B:177:ASN:H	1.49	0.78
2:D:178:LYS:H	2:D:178:LYS:HD2	1.48	0.77
2:D:413:LYS:CE	2:D:413:LYS:CG	2.61	0.77
2:D:601:ARG:HH11	2:D:601:ARG:CG	1.93	0.77
1:A:48:ILE:O	1:A:50:CYS:N	2.18	0.77
2:B:178:LYS:H	2:B:178:LYS:HD2	1.47	0.77
1:A:48:ILE:HG22	1:A:51:ASN:H	1.49	0.76
1:A:533:THR:HG22	1:A:535:LEU:H	1.49	0.76
2:D:427:THR:HG21	2:D:470:VAL:N	2.00	0.76
2:D:600:LEU:HG	2:D:601:ARG:N	2.01	0.76
1:A:262:THR:CG2	1:A:268:PHE:HZ	1.99	0.75
2:B:198:PHE:CE1	2:B:203:ILE:HD11	2.21	0.75
1:C:100:MET:HE1	1:C:112:PHE:HB2	1.64	0.75
2:B:361:HIS:CD2	2:B:363:PHE:H	2.02	0.75
2:D:236:HIS:HB3	2:D:409:LYS:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:640:ILE:HG12	2:D:641:ASN:N	1.99	0.75
2:B:597:GLN:O	2:B:598:LYS:HG3	1.86	0.75
1:C:487:ARG:HH11	1:C:487:ARG:CG	1.97	0.75
1:A:506:THR:HG23	1:A:522:THR:HG21	1.67	0.74
2:B:346:MET:HE1	2:B:668:LEU:HD22	1.68	0.74
1:C:159:ARG:HH11	1:C:159:ARG:HB2	1.53	0.74
1:A:158:ILE:HG22	1:A:159:ARG:N	2.01	0.74
2:D:288:VAL:HG11	2:D:317:VAL:HG11	1.69	0.74
2:B:381:VAL:HG12	2:B:382:GLY:H	1.53	0.74
2:B:527:ILE:HG22	2:B:559:ILE:CD1	2.18	0.74
1:A:249:LYS:CE	1:A:249:LYS:CG	2.66	0.74
1:A:262:THR:CG2	1:A:268:PHE:CZ	2.71	0.74
1:C:262:THR:CG2	1:C:268:PHE:CZ	2.71	0.73
1:A:474:ASP:OD2	1:A:567:THR:HB	1.88	0.73
2:B:253:ARG:HG2	2:B:266:SER:HB3	1.71	0.72
1:C:21:LEU:HD22	1:C:348:VAL:HG23	1.70	0.72
1:A:159:ARG:HH11	1:A:159:ARG:HB2	1.52	0.72
1:A:100:MET:HE3	1:A:112:PHE:HB2	1.69	0.72
1:C:67:ASN:O	1:C:70:ASP:HB2	1.89	0.72
2:D:346:MET:HE1	2:D:668:LEU:HD22	1.71	0.72
2:B:640:ILE:HG12	2:B:641:ASN:N	2.05	0.72
1:C:48:ILE:HG22	1:C:51:ASN:H	1.55	0.72
2:B:239:ASN:HB3	2:B:242:GLU:CG	2.20	0.71
2:D:205:PRO:HD3	2:D:651:SER:OG	1.90	0.71
2:D:236:HIS:CB	2:D:409:LYS:HG2	2.20	0.71
2:B:607:TYR:OH	2:B:612:ASP:OD1	2.08	0.71
1:C:307:ALA:N	1:C:308:PRO:HD2	2.05	0.71
1:C:358:TYR:HB2	2:D:508:ARG:NH2	2.06	0.71
2:B:404:ASP:O	2:B:406:HIS:N	2.24	0.71
2:D:301:GLU:HB3	2:D:371:TRP:CG	2.25	0.71
1:A:67:ASN:O	1:A:70:ASP:HB2	1.90	0.71
1:A:466:LYS:HE3	1:A:490:PRO:CB	2.20	0.71
2:B:288:VAL:O	2:B:290:GLY:N	2.23	0.71
2:D:527:ILE:HG22	2:D:559:ILE:HD11	1.73	0.71
2:B:388:SER:OG	2:B:390:GLU:HG2	1.90	0.71
1:C:530:CYS:SG	1:C:533:THR:HB	2.30	0.71
1:A:262:THR:HG23	1:A:290:TYR:OH	1.91	0.71
2:B:600:LEU:HG	2:B:601:ARG:N	2.03	0.71
2:B:431:LEU:HG	2:B:437:VAL:CG2	2.21	0.71
1:A:138:ASN:ND2	1:A:140:ILE:H	1.89	0.70
1:A:289:SER:CB	1:A:304:ASN:HD21	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ILE:HD12	1:C:369:MET:HE1	1.74	0.70
1:C:302:ALA:O	1:C:304:ASN:N	2.25	0.70
2:D:253:ARG:HH11	2:D:253:ARG:CG	2.00	0.70
2:D:431:LEU:HG	2:D:437:VAL:CG2	2.22	0.70
1:A:473:PHE:HE2	1:A:498:MET:HG3	1.56	0.70
1:C:100:MET:HE3	1:C:112:PHE:HB2	1.74	0.70
1:C:412:LEU:HD23	1:C:430:LEU:HD22	1.74	0.70
2:D:301:GLU:O	2:D:301:GLU:HG3	1.91	0.70
2:B:234:VAL:HG23	2:B:412:GLU:H	1.58	0.69
2:B:301:GLU:HB3	2:B:371:TRP:CG	2.26	0.69
2:D:299:ASN:HD22	2:D:646:LYS:HZ2	1.38	0.69
1:A:563:TYR:HB3	1:A:567:THR:CG2	2.22	0.69
2:D:483:SER:HB3	2:D:526:TYR:CZ	2.27	0.69
1:A:72:GLU:HG2	1:A:127:LEU:HD13	1.75	0.69
2:D:239:ASN:HB3	2:D:242:GLU:CG	2.23	0.69
2:D:512:SER:HB3	2:D:515:VAL:HG23	1.74	0.69
2:B:353:CYS:HA	2:D:275:VAL:HG11	1.73	0.69
1:C:533:THR:HG22	1:C:535:LEU:CB	2.21	0.69
1:C:533:THR:HG23	1:C:535:LEU:HD22	1.74	0.69
2:B:661:ASN:HD21	2:B:665:LEU:H	1.41	0.68
1:C:262:THR:CG2	1:C:268:PHE:HZ	2.04	0.68
2:D:381:VAL:HG12	2:D:382:GLY:H	1.58	0.68
1:A:21:LEU:HD22	1:A:348:VAL:HG23	1.75	0.68
1:C:138:ASN:ND2	1:C:140:ILE:H	1.90	0.68
1:A:412:LEU:HD23	1:A:430:LEU:HD22	1.75	0.68
1:C:247:VAL:HG21	1:C:283:LEU:HD11	1.75	0.68
1:A:356:PHE:CZ	2:B:488:ASP:HA	2.24	0.68
1:A:304:ASN:C	1:A:306:ILE:H	2.02	0.68
1:C:108:ASN:ND2	1:C:120:ASN:HD21	1.92	0.68
2:D:527:ILE:CG2	2:D:559:ILE:HD11	2.23	0.68
2:D:608:SER:OG	2:D:611:ASP:HB2	1.94	0.68
1:C:142:SER:HB3	1:C:158:ILE:HD12	1.75	0.68
1:A:466:LYS:CE	1:A:490:PRO:CB	2.72	0.68
1:C:304:ASN:C	1:C:306:ILE:H	2.02	0.67
1:C:474:ASP:OD2	1:C:567:THR:HB	1.93	0.67
2:B:393:ILE:HD13	2:B:418:LEU:HD12	1.75	0.67
1:C:268:PHE:CG	1:C:285:SER:HB3	2.29	0.67
1:C:355:ALA:O	1:C:356:PHE:HD2	1.77	0.67
1:C:126:ASN:HB2	1:C:129:SER:HB2	1.76	0.67
1:C:533:THR:HG21	1:C:535:LEU:CD2	2.24	0.67
2:B:447:GLU:HB2	2:B:458:PHE:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:PHE:HE2	1:C:536:PRO:HD3	1.60	0.67
1:C:533:THR:CG2	1:C:535:LEU:CB	2.71	0.67
2:B:288:VAL:HG11	2:B:317:VAL:HG11	1.76	0.66
2:D:299:ASN:HD22	2:D:646:LYS:NZ	1.93	0.66
2:D:661:ASN:HD21	2:D:665:LEU:H	1.44	0.66
2:D:384:LEU:HD22	2:D:398:ILE:HD11	1.78	0.66
2:D:253:ARG:HG2	2:D:266:SER:HB3	1.76	0.66
1:C:72:GLU:HG2	1:C:127:LEU:HD13	1.77	0.66
2:D:298:LEU:HG	2:D:644:CYS:SG	2.36	0.66
2:D:640:ILE:HG12	2:D:641:ASN:H	1.58	0.66
2:B:236:HIS:HB3	2:B:409:LYS:CG	2.24	0.66
2:B:301:GLU:HB3	2:B:371:TRP:NE1	2.11	0.66
2:B:346:MET:HE1	2:B:668:LEU:CD2	2.25	0.66
1:C:42:PRO:HB2	1:C:386:LEU:HD13	1.77	0.66
2:D:234:VAL:HG23	2:D:412:GLU:H	1.59	0.66
1:A:126:ASN:HB2	1:A:129:SER:HB2	1.78	0.65
1:A:459:TYR:OH	1:A:488:GLU:O	2.14	0.65
2:B:295:ILE:HD11	2:B:644:CYS:SG	2.36	0.65
1:C:318:SER:O	1:C:322:ASN:HA	1.95	0.65
2:D:239:ASN:O	2:D:241:THR:N	2.29	0.65
2:B:616:ILE:HD12	2:B:616:ILE:H	1.60	0.65
2:D:554:THR:HG21	2:D:574:ASP:HB3	1.78	0.65
1:A:14:PHE:CD2	1:A:20:ASN:ND2	2.64	0.65
2:B:372:HIS:O	2:B:373:GLU:HB2	1.96	0.65
1:A:436:MET:HG3	1:A:440:MET:HE2	1.76	0.65
2:B:643:THR:O	2:B:644:CYS:SG	2.53	0.65
1:A:303:ASP:O	1:A:304:ASN:HB3	1.95	0.65
2:D:198:PHE:CE1	2:D:203:ILE:CD1	2.75	0.65
2:B:198:PHE:HE1	2:B:203:ILE:CD1	2.10	0.64
1:C:359:LYS:HG3	1:C:363:GLU:HG3	1.77	0.64
2:D:361:HIS:HD2	2:D:363:PHE:H	1.45	0.64
1:C:138:ASN:C	1:C:138:ASN:HD22	2.06	0.64
2:D:361:HIS:CD2	2:D:363:PHE:H	2.14	0.64
2:B:267:THR:HG21	2:B:289:GLY:HA2	1.80	0.64
1:A:363:GLU:O	1:A:364:GLN:CB	2.46	0.64
2:B:413:LYS:CD	2:B:413:LYS:NZ	2.61	0.64
1:C:25:ARG:HD2	1:C:95:PRO:C	2.23	0.64
2:D:607:TYR:OH	2:D:612:ASP:OD1	2.15	0.64
2:B:239:ASN:HB3	2:B:242:GLU:HG2	1.80	0.63
2:B:554:THR:HG21	2:B:574:ASP:HB3	1.80	0.63
2:B:275:VAL:HG11	2:D:353:CYS:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:SER:CB	1:C:304:ASN:HD21	2.11	0.63
2:D:616:ILE:H	2:D:616:ILE:HD12	1.63	0.63
1:C:25:ARG:HD2	1:C:95:PRO:O	1.97	0.63
1:C:304:ASN:O	1:C:306:ILE:N	2.30	0.63
1:A:215:GLN:H	1:A:215:GLN:NE2	1.97	0.63
1:C:159:ARG:O	1:C:161:ASN:N	2.30	0.63
2:D:640:ILE:O	2:D:661:ASN:HB2	1.99	0.63
2:B:302:GLU:CG	2:B:649:GLU:HB2	2.29	0.63
2:B:641:ASN:O	2:B:642:ILE:HG13	1.99	0.63
2:D:302:GLU:CG	2:D:649:GLU:HB2	2.29	0.63
2:D:523:ILE:HD13	2:D:582:ALA:HB1	1.80	0.63
1:A:108:ASN:HD22	1:A:120:ASN:HD21	1.46	0.62
1:A:358:TYR:HB2	2:B:508:ARG:HH22	1.64	0.62
1:C:284:MET:HG2	1:C:289:SER:CB	2.27	0.62
2:B:285:ILE:HG12	2:B:667:THR:HB	1.80	0.62
2:D:346:MET:HE1	2:D:668:LEU:CD2	2.28	0.62
1:A:359:LYS:HG3	1:A:363:GLU:HG3	1.80	0.62
2:D:220:GLU:CB	2:D:433:PRO:HG3	2.24	0.62
1:C:127:LEU:O	1:C:131:THR:CG2	2.45	0.62
1:C:232:LEU:HD13	1:C:241:LEU:HD23	1.81	0.62
2:B:608:SER:C	2:B:609:ILE:HG13	2.19	0.62
2:D:301:GLU:HB3	2:D:371:TRP:NE1	2.15	0.62
2:D:385:SER:HB3	2:D:428:PHE:HZ	1.64	0.62
2:D:404:ASP:O	2:D:406:HIS:N	2.31	0.62
1:A:268:PHE:CG	1:A:285:SER:HB3	2.35	0.61
2:D:380:LEU:O	2:D:381:VAL:O	2.18	0.61
2:B:506:VAL:HG12	2:B:507:SER:HB3	1.82	0.61
1:C:69:LEU:HD11	1:C:131:THR:HB	1.83	0.61
1:C:363:GLU:O	1:C:364:GLN:CB	2.47	0.61
2:D:527:ILE:CG2	2:D:559:ILE:CD1	2.78	0.61
2:D:641:ASN:O	2:D:642:ILE:HG13	2.00	0.61
1:A:127:LEU:O	1:A:131:THR:CG2	2.46	0.61
1:C:6:ASP:OD1	1:C:369:MET:HA	1.99	0.61
1:C:248:HIS:ND1	1:C:259:SER:HB3	2.15	0.61
1:A:20:ASN:O	1:A:31:LEU:HA	2.00	0.61
1:C:34:PHE:CD2	1:C:35:PRO:HA	2.36	0.61
1:C:48:ILE:HG23	1:C:54:ASN:HB2	1.82	0.61
2:D:605:TRP:CH2	2:D:665:LEU:HD13	2.35	0.61
2:B:176:LEU:O	2:B:177:ASN:CB	2.49	0.61
1:C:533:THR:HG22	1:C:535:LEU:N	2.11	0.61
1:A:119:THR:HG21	1:A:168:PHE:N	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ILE:HD13	2:B:582:ALA:HB1	1.81	0.61
1:C:506:THR:HG23	1:C:522:THR:HG21	1.82	0.61
1:A:412:LEU:HA	1:A:435:GLU:HG3	1.81	0.61
2:D:483:SER:HB3	2:D:526:TYR:CE1	2.35	0.61
2:B:605:TRP:CH2	2:B:665:LEU:HD13	2.36	0.60
1:A:215:GLN:H	1:A:215:GLN:HE21	1.48	0.60
2:B:545:ALA:O	2:B:547:HIS:HD2	1.84	0.60
1:C:48:ILE:O	1:C:50:CYS:N	2.31	0.60
1:A:356:PHE:C	1:A:356:PHE:CD2	2.78	0.60
1:A:473:PHE:CE2	1:A:498:MET:HG3	2.35	0.60
2:B:299:ASN:ND2	2:B:646:LYS:NZ	2.45	0.60
2:B:512:SER:HB3	2:B:515:VAL:HG23	1.83	0.60
2:D:250:ARG:HD2	2:D:252:LYS:O	2.01	0.60
2:D:388:SER:OG	2:D:390:GLU:HG2	2.00	0.60
2:B:220:GLU:CB	2:B:433:PRO:HG3	2.29	0.60
1:A:48:ILE:HG23	1:A:54:ASN:HB2	1.84	0.60
1:A:247:VAL:HG21	1:A:283:LEU:HD11	1.84	0.60
2:B:608:SER:OG	2:B:611:ASP:HB2	2.01	0.60
1:C:347:ILE:HB	1:C:369:MET:HE2	1.82	0.60
2:D:239:ASN:HB3	2:D:242:GLU:HG2	1.84	0.60
1:A:533:THR:HG21	1:A:535:LEU:CD2	2.28	0.60
2:B:301:GLU:O	2:B:301:GLU:CG	2.47	0.60
1:C:276:GLU:HB3	1:C:278:GLU:HB2	1.84	0.60
1:C:356:PHE:C	1:C:356:PHE:CD2	2.80	0.60
1:A:237:TYR:N	1:A:237:TYR:HD1	1.99	0.60
2:B:604:LYS:HB2	2:B:604:LYS:NZ	2.17	0.60
1:A:355:ALA:O	1:A:356:PHE:HD2	1.85	0.60
2:B:253:ARG:HH11	2:B:253:ARG:CG	2.05	0.60
1:C:359:LYS:HG3	1:C:363:GLU:CG	2.31	0.60
1:A:142:SER:HB3	1:A:158:ILE:HD12	1.83	0.60
1:A:302:ALA:O	1:A:304:ASN:N	2.35	0.60
2:B:205:PRO:HD3	2:B:651:SER:OG	2.01	0.60
1:A:333:ILE:HG21	1:A:336:ILE:HD11	1.83	0.59
2:B:432:SER:HB2	2:B:433:PRO:HD2	1.84	0.59
1:A:211:ALA:O	1:A:213:SER:N	2.35	0.59
1:A:363:GLU:O	1:A:364:GLN:HB2	2.02	0.59
2:D:604:LYS:NZ	2:D:604:LYS:HB2	2.17	0.59
1:C:512:PHE:CE2	1:C:536:PRO:HD3	2.37	0.59
1:C:533:THR:CG2	1:C:535:LEU:CD2	2.78	0.59
2:D:253:ARG:HG3	2:D:253:ARG:NH1	1.96	0.59
1:A:303:ASP:O	1:A:304:ASN:CB	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:610:LYS:HA	2:D:610:LYS:NZ	2.17	0.59
2:B:198:PHE:CE1	2:B:203:ILE:CD1	2.84	0.59
1:C:21:LEU:HD22	1:C:348:VAL:CG2	2.32	0.59
1:C:138:ASN:HD22	1:C:140:ILE:H	1.50	0.59
1:C:333:ILE:HG21	1:C:336:ILE:HD11	1.85	0.59
2:D:270:LYS:NZ	2:D:353:CYS:O	2.35	0.59
1:A:318:SER:O	1:A:322:ASN:HA	2.03	0.59
1:C:34:PHE:HD2	1:C:35:PRO:CA	2.16	0.59
2:B:250:ARG:NE	2:B:250:ARG:CA	2.63	0.59
1:C:363:GLU:O	1:C:364:GLN:HB2	2.02	0.59
1:C:563:TYR:HB3	1:C:567:THR:CG2	2.32	0.59
1:A:25:ARG:HD2	1:A:95:PRO:C	2.28	0.58
1:A:533:THR:HG22	1:A:535:LEU:CB	2.32	0.58
2:B:640:ILE:HG12	2:B:641:ASN:H	1.65	0.58
1:A:289:SER:HB2	1:A:304:ASN:ND2	2.14	0.58
2:D:267:THR:HG21	2:D:289:GLY:HA2	1.84	0.58
2:B:250:ARG:HA	2:B:250:ARG:CZ	2.32	0.58
2:B:301:GLU:CB	2:B:371:TRP:CG	2.86	0.58
1:C:211:ALA:O	1:C:213:SER:N	2.35	0.58
1:C:355:ALA:O	1:C:356:PHE:CD2	2.56	0.58
2:D:598:LYS:HD2	2:D:624:PRO:O	2.03	0.58
1:C:249:LYS:CD	1:C:249:LYS:NZ	2.65	0.58
1:A:69:LEU:HD11	1:A:131:THR:HB	1.86	0.58
1:A:138:ASN:HD22	1:A:140:ILE:H	1.50	0.58
1:A:304:ASN:O	1:A:306:ILE:N	2.34	0.58
1:C:237:TYR:N	1:C:237:TYR:HD1	2.01	0.58
2:D:288:VAL:CG1	2:D:317:VAL:HG11	2.33	0.58
2:D:431:LEU:HG	2:D:437:VAL:HG23	1.86	0.58
2:D:506:VAL:HG12	2:D:507:SER:HB3	1.85	0.58
1:A:541:HIS:CE1	1:A:557:ARG:HH21	2.21	0.58
1:A:503:LEU:HD12	1:A:504:GLU:H	1.69	0.58
2:B:301:GLU:CB	2:B:371:TRP:CD1	2.81	0.58
2:D:565:HIS:HD2	2:D:567:MET:H	1.52	0.58
1:A:533:THR:HG21	1:A:535:LEU:HB2	1.86	0.58
2:B:239:ASN:O	2:B:241:THR:N	2.37	0.58
2:B:431:LEU:HG	2:B:437:VAL:HG23	1.86	0.58
1:A:411:LYS:HG2	1:A:417:TYR:OH	2.04	0.57
1:C:528:LYS:O	1:C:537:ILE:HG22	2.04	0.57
1:C:270:ILE:O	1:C:270:ILE:HG13	2.03	0.57
2:D:368:ASP:OD2	2:D:427:THR:HG23	2.04	0.57
1:A:159:ARG:HB2	1:A:159:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:ILE:CG2	2:B:559:ILE:HD11	2.33	0.57
2:B:565:HIS:HD2	2:B:567:MET:H	1.52	0.57
1:C:515:ASP:OD1	1:C:517:GLU:N	2.31	0.57
2:B:385:SER:HB3	2:B:428:PHE:HZ	1.68	0.57
1:C:412:LEU:HA	1:C:435:GLU:HG3	1.87	0.57
2:D:611:ASP:O	2:D:612:ASP:HB2	2.03	0.57
1:A:237:TYR:N	1:A:237:TYR:CD1	2.73	0.57
1:A:347:ILE:HD12	1:A:369:MET:HE1	1.86	0.57
1:C:248:HIS:ND1	1:C:259:SER:CB	2.67	0.57
2:D:301:GLU:CB	2:D:371:TRP:CG	2.87	0.57
1:A:276:GLU:HB3	1:A:278:GLU:HB2	1.87	0.57
1:A:517:GLU:C	1:A:529:ARG:HD2	2.29	0.57
1:C:527:TRP:CE2	1:C:538:LEU:HD11	2.40	0.57
2:D:346:MET:HB3	2:D:353:CYS:HB2	1.87	0.56
2:B:176:LEU:CG	2:B:177:ASN:H	2.18	0.56
1:C:215:GLN:H	1:C:215:GLN:HE21	1.53	0.56
1:C:289:SER:HB2	1:C:304:ASN:ND2	2.18	0.56
2:D:250:ARG:NE	2:D:250:ARG:CA	2.66	0.56
2:D:600:LEU:HD12	2:D:621:GLU:H	1.70	0.56
1:C:237:TYR:N	1:C:237:TYR:CD1	2.74	0.56
2:D:301:GLU:O	2:D:301:GLU:CG	2.53	0.56
2:D:393:ILE:HD13	2:D:418:LEU:HD12	1.87	0.56
1:A:90:VAL:HG22	1:A:103:LEU:HB3	1.88	0.56
2:D:223:TYR:HD2	2:D:224:ASN:HD22	1.53	0.56
2:D:563:ARG:HD2	2:D:649:GLU:CB	2.31	0.56
1:A:359:LYS:HG3	1:A:363:GLU:CG	2.35	0.56
1:A:479:LEU:HD21	1:A:492:TYR:CD2	2.40	0.56
1:C:20:ASN:O	1:C:31:LEU:HA	2.06	0.56
1:A:289:SER:CB	1:A:304:ASN:ND2	2.68	0.56
2:B:527:ILE:HG22	2:B:559:ILE:HD11	1.88	0.56
2:B:611:ASP:O	2:B:612:ASP:HB2	2.05	0.56
1:A:97:ASP:CB	1:A:99:TRP:CE3	2.89	0.56
1:A:232:LEU:HD13	1:A:241:LEU:HD23	1.88	0.56
1:C:123:SER:O	1:C:130:ARG:HD3	2.05	0.56
1:C:419:ILE:HD12	1:C:464:ASN:ND2	2.21	0.56
2:B:640:ILE:O	2:B:661:ASN:HB2	2.05	0.55
2:D:298:LEU:O	2:D:646:LYS:HD2	2.06	0.55
2:D:211:VAL:HG12	2:D:522:GLN:HE21	1.72	0.55
2:D:223:TYR:HB2	2:D:375:CYS:HA	1.88	0.55
2:B:301:GLU:HB3	2:B:371:TRP:CE2	2.42	0.55
2:D:352:HIS:O	2:D:353:CYS:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:413:LYS:NZ	2:D:413:LYS:CD	2.70	0.55
1:A:6:ASP:OD1	1:A:369:MET:HA	2.05	0.55
1:A:232:LEU:HD13	1:A:241:LEU:CD2	2.36	0.55
2:D:295:ILE:HD11	2:D:644:CYS:SG	2.46	0.55
1:A:68:LYS:H	1:A:108:ASN:ND2	1.98	0.55
1:A:163:GLU:O	1:A:165:THR:N	2.39	0.55
2:B:384:LEU:CD2	2:B:398:ILE:HD11	2.35	0.55
2:B:483:SER:HB3	2:B:526:TYR:CZ	2.42	0.55
1:C:264:SER:HB3	1:C:268:PHE:HE2	1.71	0.55
2:D:248:LYS:H	2:D:319:GLN:HE21	1.54	0.55
1:C:292:VAL:HA	1:C:299:HIS:O	2.06	0.55
1:A:48:ILE:HG21	1:A:51:ASN:O	2.07	0.55
1:C:519:VAL:HG11	1:C:536:PRO:HG3	1.88	0.55
2:B:393:ILE:HG23	2:B:418:LEU:HB2	1.89	0.55
1:C:215:GLN:H	1:C:215:GLN:NE2	2.05	0.55
1:C:264:SER:C	1:C:266:GLU:H	2.15	0.55
2:B:483:SER:HB3	2:B:526:TYR:CE1	2.42	0.54
1:A:34:PHE:CD2	1:A:35:PRO:HA	2.42	0.54
1:C:412:LEU:HD22	1:C:454:PHE:HA	1.89	0.54
1:C:158:ILE:HG22	1:C:159:ARG:N	2.22	0.54
1:A:25:ARG:HD2	1:A:95:PRO:O	2.07	0.54
1:C:527:TRP:CD2	1:C:538:LEU:HD11	2.42	0.54
2:B:363:PHE:HB3	2:B:388:SER:HB2	1.89	0.54
2:B:565:HIS:CD2	2:B:567:MET:HB2	2.41	0.54
2:D:363:PHE:HB3	2:D:388:SER:HB2	1.89	0.54
2:D:365:GLU:HG3	2:D:389:GLN:NE2	2.22	0.54
2:B:253:ARG:HG3	2:B:253:ARG:NH1	2.05	0.54
2:B:532:ALA:HA	2:B:555:THR:HG22	1.88	0.54
1:C:138:ASN:HD22	1:C:139:PRO:N	2.06	0.54
2:D:176:LEU:O	2:D:177:ASN:CB	2.56	0.54
1:A:159:ARG:O	1:A:161:ASN:N	2.40	0.54
1:A:248:HIS:ND1	1:A:259:SER:HB3	2.22	0.54
1:A:264:SER:C	1:A:266:GLU:H	2.14	0.54
2:B:431:LEU:HG	2:B:437:VAL:HG22	1.89	0.54
2:D:285:ILE:HG12	2:D:667:THR:HB	1.90	0.54
2:D:301:GLU:CB	2:D:371:TRP:CD1	2.84	0.54
2:B:211:VAL:HG12	2:B:522:GLN:HE21	1.72	0.54
2:B:297:TRP:HD1	2:B:298:LEU:O	1.91	0.54
1:A:502:PHE:CZ	1:A:503:LEU:HD23	2.43	0.53
2:D:236:HIS:HB3	2:D:409:LYS:CG	2.34	0.53
2:D:545:ALA:O	2:D:547:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:O	1:A:268:PHE:HD2	1.92	0.53
2:B:585:ARG:HB2	2:B:585:ARG:HH11	1.71	0.53
2:D:297:TRP:HD1	2:D:298:LEU:H	1.57	0.53
2:D:447:GLU:HB2	2:D:458:PHE:CE2	2.44	0.53
1:A:304:ASN:O	1:A:305:ILE:HG12	2.08	0.53
2:D:231:ASN:O	2:D:415:SER:HA	2.07	0.53
2:D:234:VAL:HG21	2:D:412:GLU:CG	2.35	0.53
2:D:288:VAL:HG11	2:D:317:VAL:CG1	2.37	0.53
2:D:289:GLY:O	2:D:293:THR:N	2.42	0.53
2:D:605:TRP:CZ3	2:D:616:ILE:HG13	2.43	0.53
1:A:264:SER:HB3	1:A:268:PHE:HE2	1.73	0.53
2:D:297:TRP:HD1	2:D:298:LEU:N	2.07	0.53
2:D:399:ILE:O	2:D:400:ASP:HB2	2.08	0.53
1:A:138:ASN:HD22	1:A:138:ASN:C	2.17	0.53
1:A:466:LYS:HE2	1:A:490:PRO:HB3	1.90	0.53
2:B:250:ARG:HD2	2:B:252:LYS:O	2.09	0.53
1:C:436:MET:HG3	1:C:440:MET:HE2	1.91	0.53
2:D:302:GLU:HG3	2:D:649:GLU:HB2	1.90	0.53
2:B:527:ILE:CG2	2:B:559:ILE:CD1	2.86	0.53
1:C:379:ILE:HG22	1:C:437:ARG:HD2	1.90	0.53
1:A:248:HIS:ND1	1:A:259:SER:CB	2.72	0.53
2:B:616:ILE:HD12	2:B:616:ILE:N	2.24	0.53
2:B:289:GLY:O	2:B:293:THR:N	2.42	0.53
1:C:232:LEU:HD13	1:C:241:LEU:CD2	2.39	0.53
1:C:520:THR:OG1	1:C:526:THR:HB	2.09	0.53
2:B:473:ALA:HB2	2:B:526:TYR:CZ	2.44	0.52
1:C:289:SER:CB	1:C:304:ASN:ND2	2.72	0.52
2:B:610:LYS:NZ	2:B:610:LYS:HA	2.25	0.52
2:D:431:LEU:HG	2:D:437:VAL:HG22	1.92	0.52
2:D:432:SER:HB2	2:D:433:PRO:HD2	1.91	0.52
1:A:428:ASN:OD1	1:A:573:ARG:NH1	2.42	0.52
2:B:220:GLU:O	2:B:221:SER:HB3	2.10	0.52
2:D:610:LYS:HA	2:D:610:LYS:CE	2.40	0.52
2:B:441:LYS:O	2:B:441:LYS:HG2	2.10	0.52
2:B:380:LEU:O	2:B:381:VAL:O	2.28	0.52
1:C:544:ILE:HD11	1:C:588:MET:SD	2.50	0.52
1:A:284:MET:HG2	1:A:289:SER:CB	2.37	0.52
1:A:563:TYR:HB3	1:A:567:THR:HG22	1.92	0.52
1:A:193:ASP:O	1:A:208:THR:HG23	2.10	0.52
2:B:597:GLN:C	2:B:598:LYS:HG3	2.35	0.52
2:D:297:TRP:CD1	2:D:298:LEU:H	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:HIS:HA	1:A:259:SER:HB3	1.92	0.52
1:A:292:VAL:HA	1:A:299:HIS:O	2.09	0.52
2:D:385:SER:HB3	2:D:428:PHE:CZ	2.45	0.51
1:A:358:TYR:HB2	2:B:508:ARG:NH2	2.25	0.51
2:B:368:ASP:OD2	2:B:427:THR:HG23	2.10	0.51
2:B:454:GLU:O	2:B:456:PRO:HD3	2.10	0.51
1:C:303:ASP:OD1	1:C:305:ILE:HG23	2.10	0.51
1:C:443:ASN:OD1	1:C:449:PRO:HA	2.10	0.51
2:B:203:ILE:O	2:B:651:SER:OG	2.27	0.51
1:C:517:GLU:C	1:C:529:ARG:HD2	2.36	0.51
1:A:307:ALA:N	1:A:308:PRO:HD2	2.26	0.51
2:B:298:LEU:O	2:B:299:ASN:HB2	2.11	0.51
2:B:365:GLU:HG3	2:B:389:GLN:NE2	2.25	0.51
2:B:585:ARG:HH11	2:B:585:ARG:CB	2.23	0.51
2:B:588:HIS:HE1	2:B:590:ILE:CD1	2.24	0.51
2:B:604:LYS:HG3	2:B:604:LYS:O	2.10	0.51
2:B:661:ASN:HD22	2:B:661:ASN:C	2.18	0.51
2:D:301:GLU:HB3	2:D:371:TRP:CE2	2.45	0.51
1:A:533:THR:CG2	1:A:535:LEU:CD2	2.87	0.51
2:B:405:VAL:HG13	2:B:406:HIS:N	2.26	0.51
2:D:176:LEU:CG	2:D:177:ASN:H	2.18	0.51
1:C:327:TYR:CD2	1:C:353:ARG:HD3	2.45	0.51
1:C:541:HIS:CE1	1:C:557:ARG:HE	2.28	0.51
1:A:125:GLY:O	1:A:130:ARG:HG3	2.11	0.51
2:B:614:TYR:HE2	2:B:639:GLY:O	1.94	0.51
2:D:250:ARG:HA	2:D:250:ARG:CZ	2.41	0.51
2:D:196:PHE:HE2	2:D:599:SER:HA	1.76	0.51
2:D:250:ARG:HD3	2:D:250:ARG:C	2.36	0.51
1:A:155:PHE:HE1	1:A:174:ILE:HD12	1.76	0.50
1:A:277:LYS:O	1:A:278:GLU:HG2	2.10	0.50
1:A:278:GLU:O	1:A:279:SER:C	2.54	0.50
2:B:288:VAL:CG1	2:B:317:VAL:HG11	2.41	0.50
1:C:407:SER:HB3	1:C:410:LYS:HG3	1.93	0.50
2:D:298:LEU:C	2:D:298:LEU:HD12	2.37	0.50
2:D:578:ILE:HD13	2:D:601:ARG:HB2	1.93	0.50
1:A:297:GLU:HA	1:A:297:GLU:OE2	2.11	0.50
1:A:424:GLN:OE1	1:A:573:ARG:HB2	2.10	0.50
1:C:159:ARG:HB2	1:C:159:ARG:NH1	2.22	0.50
1:C:307:ALA:N	1:C:308:PRO:CD	2.74	0.50
1:A:355:ALA:O	1:A:356:PHE:CD2	2.64	0.50
2:B:298:LEU:HD12	2:B:298:LEU:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:O	1:C:173:SER:HA	2.12	0.50
1:C:483:ALA:HB2	1:C:513:THR:HG22	1.94	0.50
2:B:176:LEU:O	2:B:177:ASN:HB3	2.11	0.50
2:D:608:SER:C	2:D:609:ILE:HG13	2.25	0.50
1:A:79:LEU:HD23	2:B:502:THR:HB	1.93	0.50
1:A:108:ASN:ND2	1:A:120:ASN:HD21	2.10	0.50
2:D:273:PHE:N	2:D:274:PRO:CD	2.75	0.50
2:D:345:LYS:HB2	2:D:356:VAL:HG21	1.94	0.50
1:A:347:ILE:HB	1:A:369:MET:HE2	1.93	0.50
1:A:379:ILE:HG22	1:A:437:ARG:HD2	1.94	0.50
1:C:537:ILE:HG23	1:C:537:ILE:O	2.11	0.50
1:A:362:SER:O	1:A:363:GLU:CB	2.60	0.50
1:A:435:GLU:CD	1:A:435:GLU:H	2.20	0.50
2:B:607:TYR:CG	2:B:608:SER:N	2.80	0.50
1:A:89:ARG:HH11	1:A:89:ARG:CG	2.24	0.49
2:B:239:ASN:CB	2:B:242:GLU:HG2	2.41	0.49
2:D:176:LEU:O	2:D:177:ASN:HB3	2.12	0.49
2:D:233:THR:O	2:D:234:VAL:HG13	2.12	0.49
1:A:437:ARG:HA	1:A:440:MET:HE3	1.94	0.49
1:A:466:LYS:HE2	1:A:490:PRO:CB	2.43	0.49
1:A:249:LYS:CD	1:A:249:LYS:NZ	2.72	0.49
2:B:661:ASN:C	2:B:661:ASN:ND2	2.70	0.49
1:C:362:SER:O	1:C:363:GLU:CB	2.60	0.49
1:A:94:SER:HB3	1:A:97:ASP:O	2.12	0.49
2:B:223:TYR:HB2	2:B:375:CYS:HA	1.95	0.49
2:B:588:HIS:HE1	2:B:590:ILE:HD12	1.77	0.49
1:C:268:PHE:CD2	1:C:285:SER:HB3	2.46	0.49
2:B:377:ALA:HB1	2:B:378:PRO:HD2	1.93	0.49
2:B:527:ILE:HD13	2:B:568:VAL:HG21	1.94	0.49
1:C:48:ILE:HG21	1:C:51:ASN:O	2.12	0.49
1:C:210:SER:C	1:C:212:SER:H	2.20	0.49
1:C:321:TRP:HZ2	1:C:325:ASN:HD22	1.61	0.49
2:D:168:ASP:HA	2:D:171:GLU:HB2	1.94	0.49
1:A:138:ASN:HD22	1:A:139:PRO:N	2.10	0.49
2:B:302:GLU:HG3	2:B:649:GLU:HB2	1.95	0.49
2:B:610:LYS:HA	2:B:610:LYS:CE	2.42	0.49
1:C:16:ASP:OD1	1:C:16:ASP:N	2.44	0.49
1:C:537:ILE:HD11	1:C:542:VAL:HG11	1.94	0.49
2:D:247:ILE:HG22	2:D:247:ILE:O	2.12	0.49
2:D:616:ILE:HD12	2:D:616:ILE:N	2.27	0.49
1:A:441:PHE:HA	1:A:444:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:PHE:HE1	2:B:203:ILE:HD12	1.76	0.49
2:B:233:THR:O	2:B:234:VAL:HG13	2.13	0.49
2:B:527:ILE:HD12	2:B:561:VAL:HG11	1.95	0.49
1:C:304:ASN:O	1:C:305:ILE:HG12	2.13	0.49
1:A:18:LYS:HE2	1:A:90:VAL:HG12	1.94	0.48
1:A:563:TYR:HB3	1:A:567:THR:HG23	1.93	0.48
1:C:262:THR:HG21	1:C:268:PHE:CE2	2.47	0.48
1:C:428:ASN:OD1	1:C:573:ARG:NH1	2.46	0.48
1:A:100:MET:HE1	1:A:112:PHE:CB	2.35	0.48
2:B:370:LYS:O	2:B:385:SER:HB2	2.13	0.48
2:D:405:VAL:HG13	2:D:406:HIS:N	2.28	0.48
1:A:3:LEU:HD11	1:A:370:PHE:O	2.13	0.48
1:C:322:ASN:O	1:C:323:GLU:O	2.31	0.48
1:C:344:SER:HB3	1:C:394:ILE:HG21	1.95	0.48
2:D:239:ASN:CB	2:D:242:GLU:HG2	2.43	0.48
2:B:216:PRO:O	2:B:433:PRO:HD3	2.12	0.48
2:B:605:TRP:CZ3	2:B:616:ILE:HG13	2.48	0.48
1:C:94:SER:HB3	1:C:97:ASP:O	2.13	0.48
2:D:340:CYS:HB2	2:D:359:ILE:O	2.13	0.48
2:B:399:ILE:O	2:B:400:ASP:HB2	2.12	0.48
2:D:357:GLN:OE1	2:D:400:ASP:HB3	2.13	0.48
2:D:532:ALA:HA	2:D:555:THR:HG22	1.94	0.48
2:B:235:TYR:CG	2:B:236:HIS:N	2.81	0.48
2:B:253:ARG:HG2	2:B:266:SER:CB	2.43	0.48
2:B:384:LEU:HD22	2:B:398:ILE:CD1	2.37	0.48
1:C:243:CYS:HB3	1:C:244:PRO:CD	2.42	0.48
1:C:553:ILE:HB	1:C:571:LEU:HD22	1.96	0.48
1:C:378:THR:HG22	1:C:401:LYS:HB2	1.95	0.48
2:D:661:ASN:C	2:D:661:ASN:HD22	2.21	0.48
1:A:210:SER:C	1:A:212:SER:H	2.22	0.48
1:C:242:THR:HG21	1:C:268:PHE:O	2.14	0.48
2:B:385:SER:HB3	2:B:428:PHE:CZ	2.48	0.48
2:B:533:SER:O	2:B:551:SER:HA	2.14	0.48
1:A:183:ASP:HB3	1:A:200:SER:HB2	1.96	0.48
1:A:304:ASN:C	1:A:305:ILE:HG12	2.38	0.48
2:B:223:TYR:HD2	2:B:224:ASN:HD22	1.60	0.48
1:A:159:ARG:O	1:A:166:PRO:O	2.32	0.47
2:B:234:VAL:CB	2:B:412:GLU:HG2	2.44	0.47
2:B:601:ARG:NH1	2:B:604:LYS:HB3	2.29	0.47
2:D:301:GLU:HB3	2:D:371:TRP:CD2	2.49	0.47
1:A:42:PRO:HB2	1:A:386:LEU:HD13	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:THR:OG1	1:A:526:THR:HB	2.14	0.47
1:C:441:PHE:HA	1:C:444:MET:HE3	1.96	0.47
1:A:68:LYS:N	1:A:108:ASN:HD21	2.00	0.47
2:D:231:ASN:OD1	2:D:231:ASN:N	2.47	0.47
2:D:235:TYR:CG	2:D:236:HIS:N	2.80	0.47
1:A:322:ASN:O	1:A:323:GLU:O	2.33	0.47
1:C:448:LYS:HE3	1:C:448:LYS:HB3	1.55	0.47
1:C:500:ASN:O	1:C:502:PHE:N	2.47	0.47
2:D:384:LEU:HD22	2:D:398:ILE:CD1	2.44	0.47
1:A:515:ASP:OD1	1:A:517:GLU:N	2.41	0.47
1:C:21:LEU:HD13	1:C:31:LEU:CD2	2.45	0.47
1:C:278:GLU:O	1:C:279:SER:C	2.58	0.47
1:C:466:LYS:HA	1:C:469:LEU:HD12	1.96	0.47
1:C:496:LEU:HD12	1:C:496:LEU:HA	1.51	0.47
1:C:550:GLN:HG2	1:C:580:TYR:CE1	2.49	0.47
2:D:239:ASN:CG	2:D:242:GLU:HG2	2.40	0.47
2:D:454:GLU:O	2:D:456:PRO:HD3	2.14	0.47
1:A:89:ARG:HH11	1:A:89:ARG:HG2	1.80	0.47
1:A:303:ASP:CG	1:A:305:ILE:HG23	2.40	0.47
1:C:230:THR:CG2	1:C:267:ASN:HB2	2.45	0.47
1:C:424:GLN:OE1	1:C:573:ARG:HB2	2.14	0.47
2:D:297:TRP:HD1	2:D:298:LEU:O	1.98	0.47
2:B:267:THR:CG2	2:B:289:GLY:HA2	2.43	0.47
2:B:299:ASN:HD22	2:B:646:LYS:HZ3	1.60	0.47
2:B:352:HIS:O	2:B:353:CYS:HB3	2.15	0.47
2:B:600:LEU:HD12	2:B:621:GLU:H	1.79	0.47
2:D:346:MET:CB	2:D:353:CYS:HB2	2.44	0.47
1:A:34:PHE:HD2	1:A:35:PRO:CA	2.28	0.47
1:A:402:LEU:HD22	1:A:438:ILE:HG23	1.96	0.47
2:B:361:HIS:HB2	2:B:363:PHE:CD1	2.49	0.47
1:C:321:TRP:O	1:C:322:ASN:C	2.58	0.47
2:D:230:LYS:HA	2:D:230:LYS:HD3	1.65	0.47
1:A:41:GLN:O	1:A:56:PHE:HA	2.14	0.46
1:A:260:LEU:HG	1:A:261:LYS:O	2.15	0.46
1:A:412:LEU:HD22	1:A:454:PHE:HA	1.97	0.46
2:B:273:PHE:N	2:B:274:PRO:CD	2.78	0.46
1:C:163:GLU:O	1:C:165:THR:N	2.47	0.46
1:C:268:PHE:HB2	1:C:284:MET:O	2.15	0.46
1:C:314:PHE:O	1:C:314:PHE:CD1	2.68	0.46
1:C:357:LYS:O	1:C:359:LYS:N	2.48	0.46
2:D:178:LYS:HD2	2:D:178:LYS:N	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:HIS:HB2	2:D:363:PHE:CD1	2.49	0.46
2:D:604:LYS:HG3	2:D:604:LYS:O	2.14	0.46
2:D:661:ASN:C	2:D:661:ASN:ND2	2.72	0.46
1:A:59:LYS:HD2	1:A:59:LYS:HA	1.69	0.46
1:C:125:GLY:O	1:C:130:ARG:HG3	2.14	0.46
2:B:357:GLN:OE1	2:B:400:ASP:HB3	2.16	0.46
2:B:642:ILE:HA	2:B:661:ASN:HA	1.96	0.46
2:D:520:CYS:HB2	2:D:527:ILE:HD12	1.98	0.46
2:D:648:ASN:ND2	2:D:650:THR:H	2.13	0.46
1:A:264:SER:O	1:A:266:GLU:N	2.48	0.46
2:B:230:LYS:HA	2:B:230:LYS:HD3	1.58	0.46
2:B:247:ILE:HG22	2:B:247:ILE:O	2.15	0.46
1:C:124:LYS:HG3	1:C:125:GLY:H	1.81	0.46
1:A:48:ILE:C	1:A:50:CYS:N	2.74	0.46
1:A:188:ILE:HG23	1:A:195:LEU:HD11	1.97	0.46
2:B:578:ILE:HD13	2:B:601:ARG:HB2	1.98	0.46
1:C:183:ASP:HB3	1:C:200:SER:HB2	1.98	0.46
1:C:264:SER:O	1:C:266:GLU:N	2.48	0.46
1:C:347:ILE:HD12	1:C:369:MET:CE	2.42	0.46
2:D:239:ASN:HB3	2:D:242:GLU:HB2	1.97	0.46
2:D:372:HIS:O	2:D:373:GLU:HB2	2.16	0.46
2:D:579:ILE:O	2:D:599:SER:HB3	2.15	0.46
2:D:601:ARG:NH1	2:D:604:LYS:HB3	2.31	0.46
1:C:159:ARG:O	1:C:166:PRO:O	2.33	0.46
1:C:481:ILE:HG12	1:C:534:LEU:HD12	1.97	0.46
2:D:585:ARG:HH11	2:D:585:ARG:HB2	1.81	0.46
1:C:18:LYS:HE2	1:C:90:VAL:HG12	1.98	0.46
1:C:21:LEU:HD13	1:C:31:LEU:HD23	1.98	0.46
1:C:117:MET:HG3	1:C:118:LEU:N	2.30	0.46
1:A:284:MET:HE3	1:A:284:MET:HB3	1.88	0.46
2:B:239:ASN:HB3	2:B:242:GLU:HB2	1.98	0.46
2:B:239:ASN:CG	2:B:242:GLU:HG2	2.41	0.46
2:B:297:TRP:HD1	2:B:298:LEU:H	1.64	0.46
2:B:301:GLU:HB3	2:B:371:TRP:CD2	2.50	0.46
2:B:545:ALA:O	2:B:547:HIS:CD2	2.66	0.46
2:D:545:ALA:O	2:D:547:HIS:CD2	2.69	0.46
1:C:78:GLY:C	1:C:80:LEU:H	2.23	0.46
1:C:230:THR:HG21	1:C:267:ASN:HB2	1.97	0.46
1:C:541:HIS:CE1	1:C:557:ARG:HG3	2.50	0.46
2:D:247:ILE:CD1	2:D:340:CYS:HB3	2.46	0.46
1:A:18:LYS:O	1:A:18:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASN:OD1	1:A:449:PRO:HA	2.17	0.45
2:B:356:VAL:O	2:B:406:HIS:HA	2.17	0.45
1:C:100:MET:HE2	1:C:100:MET:HB3	1.86	0.45
1:C:303:ASP:O	1:C:304:ASN:HB3	2.16	0.45
1:C:537:ILE:O	1:C:538:LEU:HD23	2.16	0.45
2:B:288:VAL:HG11	2:B:317:VAL:CG1	2.44	0.45
2:D:234:VAL:CB	2:D:412:GLU:HG2	2.45	0.45
2:D:311:GLN:HE22	2:D:650:THR:HG21	1.82	0.45
2:D:377:ALA:HB1	2:D:378:PRO:HD2	1.97	0.45
2:D:473:ALA:HB2	2:D:526:TYR:CZ	2.51	0.45
1:A:18:LYS:O	1:A:19:ASN:CB	2.64	0.45
1:A:303:ASP:OD1	1:A:305:ILE:HG23	2.16	0.45
2:B:607:TYR:OH	2:B:612:ASP:HA	2.15	0.45
1:C:369:MET:HE2	1:C:369:MET:HB3	1.91	0.45
1:C:537:ILE:CG1	1:C:542:VAL:HG11	2.46	0.45
2:D:393:ILE:HG23	2:D:418:LEU:HB2	1.98	0.45
2:B:172:ARG:HA	2:B:172:ARG:HD3	1.79	0.45
2:B:361:HIS:CD2	2:B:363:PHE:HB2	2.51	0.45
2:B:376:HIS:HB2	2:B:377:ALA:H	1.56	0.45
1:C:96:ILE:HG22	1:C:97:ASP:OD2	2.16	0.45
2:B:231:ASN:O	2:B:415:SER:HA	2.16	0.45
2:B:231:ASN:OD1	2:B:231:ASN:N	2.50	0.45
2:B:584:ARG:CG	2:B:585:ARG:N	2.54	0.45
1:C:3:LEU:HD11	1:C:370:PHE:O	2.17	0.45
1:C:18:LYS:O	1:C:19:ASN:CB	2.63	0.45
1:C:90:VAL:HG22	1:C:103:LEU:HB3	1.99	0.45
2:D:198:PHE:HE1	2:D:203:ILE:HD12	1.77	0.45
1:A:533:THR:CG2	1:A:535:LEU:CB	2.88	0.45
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.72	0.45
1:C:510:GLU:O	1:C:512:PHE:N	2.50	0.45
2:D:642:ILE:HA	2:D:661:ASN:HA	1.99	0.45
1:A:268:PHE:HB2	1:A:284:MET:O	2.17	0.45
2:B:579:ILE:O	2:B:599:SER:HB3	2.17	0.45
2:B:270:LYS:NZ	2:B:353:CYS:O	2.49	0.45
2:B:361:HIS:HD2	2:B:363:PHE:N	2.04	0.45
2:D:288:VAL:O	2:D:289:GLY:C	2.60	0.45
2:D:297:TRP:CD1	2:D:298:LEU:N	2.83	0.45
1:A:92:LYS:HB2	1:A:135:PHE:CE1	2.52	0.45
1:A:235:VAL:CG2	1:A:272:PRO:HB3	2.47	0.45
1:C:97:ASP:CB	1:C:99:TRP:CE3	2.95	0.45
1:C:539:THR:HG23	1:C:540:THR:N	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:TYR:HB3	1:C:567:THR:HG23	1.98	0.45
2:D:203:ILE:O	2:D:651:SER:OG	2.34	0.45
2:D:303:ASN:H	2:D:650:THR:HG21	1.81	0.45
1:A:15:GLU:HG3	1:A:34:PHE:CD1	2.52	0.44
1:A:26:ASP:HA	1:A:384:VAL:HG23	1.99	0.44
2:B:297:TRP:CD1	2:B:298:LEU:H	2.35	0.44
1:C:243:CYS:CB	1:C:244:PRO:CD	2.95	0.44
2:D:370:LYS:O	2:D:385:SER:HB2	2.17	0.44
2:B:216:PRO:HD3	2:B:474:TYR:CG	2.52	0.44
2:D:569:LEU:HG	2:D:647:TRP:CZ2	2.51	0.44
1:A:155:PHE:CE1	1:A:174:ILE:HD12	2.51	0.44
2:B:234:VAL:HG21	2:B:412:GLU:CG	2.37	0.44
2:B:247:ILE:CD1	2:B:340:CYS:HB3	2.47	0.44
1:C:34:PHE:CD2	1:C:35:PRO:CA	2.96	0.44
2:D:235:TYR:CD1	2:D:236:HIS:N	2.85	0.44
1:C:157:SER:HB2	1:C:169:TYR:CE2	2.52	0.44
1:C:297:GLU:OE2	1:C:297:GLU:HA	2.17	0.44
1:A:242:THR:HG21	1:A:268:PHE:O	2.17	0.44
1:A:402:LEU:HD22	1:A:438:ILE:CG2	2.48	0.44
2:B:425:ILE:HG12	2:B:440:PHE:CE2	2.52	0.44
2:D:376:HIS:O	2:D:377:ALA:HB3	2.17	0.44
1:A:20:ASN:HB3	1:A:32:THR:OG1	2.17	0.44
2:B:563:ARG:HD2	2:B:649:GLU:CB	2.40	0.44
2:B:648:ASN:ND2	2:B:650:THR:H	2.15	0.44
1:C:262:THR:O	1:C:262:THR:HG22	2.17	0.44
2:D:216:PRO:HD3	2:D:474:TYR:CG	2.53	0.44
2:B:401:ASN:O	2:B:403:THR:N	2.47	0.44
2:B:512:SER:HB2	2:B:531:GLY:HA2	2.00	0.44
1:C:92:LYS:HB2	1:C:135:PHE:CE1	2.53	0.44
1:C:115:ASN:O	1:C:116:LYS:C	2.61	0.44
1:C:304:ASN:OD1	1:C:306:ILE:HB	2.18	0.44
1:C:349:TYR:HE1	1:C:351:MET:HE2	1.82	0.44
2:D:262:ASP:OD1	2:D:613:LYS:HE2	2.17	0.44
1:A:458:LEU:HD12	1:A:458:LEU:HA	1.71	0.44
2:B:299:ASN:ND2	2:B:646:LYS:HZ3	2.16	0.44
2:B:640:ILE:CG1	2:B:641:ASN:H	2.26	0.44
2:D:557:THR:HB	2:D:642:ILE:O	2.18	0.44
1:A:412:LEU:HA	1:A:435:GLU:CG	2.48	0.44
2:B:427:THR:HG22	2:B:428:PHE:N	2.32	0.44
1:C:89:ARG:HD3	2:D:501:THR:HA	2.00	0.44
1:C:235:VAL:CG2	1:C:272:PRO:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLU:O	1:C:268:PHE:HD2	2.00	0.44
2:D:512:SER:HB2	2:D:531:GLY:HA2	2.00	0.44
1:A:21:LEU:HD22	1:A:348:VAL:CG2	2.47	0.43
1:A:39:ILE:HD12	1:A:61:PHE:CD1	2.53	0.43
2:B:346:MET:HB3	2:B:353:CYS:HB2	1.99	0.43
2:B:473:ALA:HB2	2:B:526:TYR:OH	2.18	0.43
1:C:136:GLU:HG2	1:C:190:TRP:H	1.83	0.43
1:C:262:THR:HG23	1:C:290:TYR:OH	2.18	0.43
1:C:412:LEU:HA	1:C:435:GLU:CG	2.48	0.43
1:A:302:ALA:O	1:A:303:ASP:C	2.60	0.43
2:B:225:LYS:O	2:B:451:THR:HG22	2.18	0.43
1:C:138:ASN:ND2	1:C:138:ASN:C	2.75	0.43
1:C:155:PHE:HE1	1:C:174:ILE:HD12	1.82	0.43
1:C:175:ARG:HA	1:C:175:ARG:HD2	1.84	0.43
1:A:230:THR:CG2	1:A:267:ASN:HB2	2.48	0.43
1:A:533:THR:HG22	1:A:535:LEU:N	2.26	0.43
2:B:248:LYS:H	2:B:319:GLN:HE21	1.66	0.43
1:C:18:LYS:O	1:C:18:LYS:HG2	2.18	0.43
1:C:188:ILE:HG23	1:C:195:LEU:HD11	2.00	0.43
1:A:545:CYS:HA	1:A:546:PRO:HD3	1.82	0.43
2:B:297:TRP:HD1	2:B:298:LEU:N	2.15	0.43
2:B:381:VAL:HG12	2:B:382:GLY:N	2.27	0.43
1:C:411:LYS:HG2	1:C:417:TYR:OH	2.19	0.43
2:D:585:ARG:HH11	2:D:585:ARG:CB	2.31	0.43
1:A:78:GLY:C	1:A:80:LEU:H	2.26	0.43
1:A:530:CYS:O	1:A:551:ARG:O	2.37	0.43
1:C:126:ASN:O	1:C:127:LEU:CB	2.65	0.43
1:C:303:ASP:CG	1:C:305:ILE:HG23	2.43	0.43
2:D:220:GLU:O	2:D:221:SER:HB3	2.18	0.43
1:A:289:SER:C	1:A:304:ASN:HD22	2.27	0.43
2:B:290:GLY:CA	2:B:293:THR:N	2.63	0.43
2:B:410:MET:O	2:B:411:CYS:C	2.60	0.43
2:B:571:GLY:HA2	2:B:576:SER:O	2.19	0.43
1:C:41:GLN:O	1:C:56:PHE:HA	2.18	0.43
2:D:607:TYR:CG	2:D:608:SER:N	2.79	0.43
2:B:239:ASN:HB3	2:B:242:GLU:CB	2.49	0.43
2:B:585:ARG:CB	2:B:585:ARG:NH1	2.81	0.43
1:A:321:TRP:CG	1:A:321:TRP:O	2.71	0.43
2:B:582:ALA:O	2:B:583:ALA:HB2	2.18	0.43
1:A:268:PHE:CD2	1:A:285:SER:HB3	2.53	0.43
2:B:418:LEU:HD23	2:B:453:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:HD23	1:C:55:LEU:HA	1.71	0.43
1:C:284:MET:HA	1:C:289:SER:HB3	2.01	0.43
1:C:460:GLU:HA	1:C:460:GLU:OE2	2.19	0.43
2:D:233:THR:HG23	2:D:414:PRO:HA	2.01	0.43
2:D:250:ARG:C	2:D:250:ARG:CD	2.92	0.43
1:A:34:PHE:CD2	1:A:35:PRO:CA	3.01	0.43
1:A:369:MET:HE2	1:A:369:MET:HB3	1.91	0.43
2:B:340:CYS:HB2	2:B:359:ILE:O	2.19	0.43
2:B:372:HIS:O	2:B:373:GLU:CB	2.61	0.43
1:C:59:LYS:HD2	1:C:59:LYS:HA	1.59	0.43
1:C:251:ASP:HB3	1:C:254:ASN:OD1	2.19	0.43
1:C:426:TYR:CE2	1:C:461:TYR:HB2	2.54	0.43
1:A:133:HIS:ND1	2:B:501:THR:HG21	2.34	0.42
1:A:262:THR:O	1:A:262:THR:HG22	2.19	0.42
1:A:272:PRO:HA	1:A:281:ILE:HG22	2.01	0.42
1:C:396:ASN:O	1:C:397:GLN:HB2	2.19	0.42
2:D:294:ASP:HB3	2:D:662:SER:O	2.19	0.42
1:C:26:ASP:HA	1:C:384:VAL:HG23	2.01	0.42
1:C:126:ASN:O	1:C:127:LEU:HB3	2.19	0.42
2:D:614:TYR:HE2	2:D:639:GLY:O	2.03	0.42
1:A:262:THR:HG21	1:A:268:PHE:CE2	2.50	0.42
2:B:277:ALA:C	2:B:279:GLY:N	2.77	0.42
2:B:358:THR:OG1	2:B:406:HIS:HE1	2.02	0.42
1:C:553:ILE:HB	1:C:571:LEU:CD2	2.49	0.42
1:A:396:ASN:O	1:A:397:GLN:HB2	2.18	0.42
2:B:303:ASN:H	2:B:650:THR:HG21	1.83	0.42
2:B:393:ILE:HD12	2:B:428:PHE:CD1	2.54	0.42
1:C:65:PHE:CE2	1:C:102:VAL:HG11	2.54	0.42
1:C:247:VAL:HG21	1:C:283:LEU:CD1	2.48	0.42
1:C:530:CYS:O	1:C:551:ARG:O	2.38	0.42
2:D:172:ARG:HA	2:D:172:ARG:HD3	1.84	0.42
2:D:223:TYR:CD2	2:D:223:TYR:C	2.97	0.42
2:D:458:PHE:CD1	2:D:458:PHE:C	2.98	0.42
1:A:5:LYS:HD3	1:A:51:ASN:ND2	2.34	0.42
1:A:80:LEU:C	1:A:82:SER:H	2.26	0.42
1:A:315:LYS:O	1:A:318:SER:HB3	2.19	0.42
2:B:297:TRP:CD1	2:B:298:LEU:O	2.73	0.42
2:B:549:LEU:HD12	2:B:549:LEU:HA	1.94	0.42
2:B:669:GLU:HG2	2:B:670:TYR:N	2.34	0.42
1:C:226:ARG:NH1	2:D:455:VAL:O	2.51	0.42
1:A:347:ILE:HD12	1:A:369:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLU:O	2:B:246:MET:HB2	2.20	0.42
2:B:376:HIS:O	2:B:377:ALA:HB3	2.20	0.42
2:B:470:VAL:O	2:B:470:VAL:HG13	2.18	0.42
2:D:405:VAL:HG13	2:D:406:HIS:H	1.84	0.42
2:D:425:ILE:HG12	2:D:440:PHE:CE2	2.54	0.42
2:B:235:TYR:CD1	2:B:236:HIS:N	2.87	0.42
2:B:366:VAL:HG13	2:B:386:PHE:HB2	2.01	0.42
2:B:373:GLU:OE2	2:B:563:ARG:NH2	2.52	0.42
1:C:303:ASP:O	1:C:304:ASN:CB	2.68	0.42
2:D:512:SER:HB3	2:D:515:VAL:CG2	2.46	0.42
2:D:640:ILE:CG1	2:D:641:ASN:H	2.21	0.42
1:A:448:LYS:O	1:A:449:PRO:C	2.61	0.42
2:B:528:TYR:N	2:B:528:TYR:CD2	2.87	0.42
1:C:143:SER:HB2	1:C:156:PHE:O	2.20	0.42
2:D:641:ASN:HD21	2:D:662:SER:HB3	1.85	0.42
1:A:148:ASN:OD1	1:A:152:GLU:HB3	2.20	0.42
1:A:459:TYR:CE2	1:A:487:ARG:HG2	2.55	0.42
1:C:277:LYS:O	1:C:278:GLU:HG2	2.19	0.42
1:C:442:LEU:O	1:C:445:THR:HB	2.20	0.42
1:C:522:THR:HG23	1:C:523:THR:N	2.35	0.42
1:A:325:ASN:HD22	1:A:325:ASN:HA	1.72	0.42
1:A:327:TYR:CD2	1:A:353:ARG:HD3	2.54	0.42
2:B:196:PHE:CZ	2:B:622:VAL:HG13	2.55	0.42
1:C:321:TRP:O	1:C:321:TRP:CG	2.73	0.42
2:D:196:PHE:CZ	2:D:622:VAL:HG13	2.54	0.42
2:D:610:LYS:HA	2:D:610:LYS:HZ1	1.83	0.42
1:A:515:ASP:OD1	1:A:515:ASP:C	2.63	0.41
1:A:153:LEU:O	1:A:173:SER:HA	2.20	0.41
1:A:475:LEU:HD13	1:A:475:LEU:HA	1.76	0.41
2:B:298:LEU:HG	2:B:644:CYS:SG	2.60	0.41
1:C:528:LYS:HB2	1:C:537:ILE:HG21	2.01	0.41
2:D:420:LEU:HD12	2:D:420:LEU:HA	1.82	0.41
1:C:48:ILE:CG2	1:C:54:ASN:HB2	2.50	0.41
1:A:126:ASN:O	1:A:127:LEU:CB	2.68	0.41
2:B:196:PHE:HE2	2:B:599:SER:HA	1.84	0.41
2:B:405:VAL:HG13	2:B:406:HIS:H	1.85	0.41
1:C:165:THR:O	1:C:166:PRO:C	2.62	0.41
1:C:321:TRP:CD1	1:C:327:TYR:HB2	2.56	0.41
1:C:358:TYR:CB	2:D:508:ARG:NH2	2.79	0.41
1:C:519:VAL:CG1	1:C:536:PRO:HG3	2.51	0.41
1:C:545:CYS:HA	1:C:546:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:CG	1:A:89:ARG:NH1	2.83	0.41
1:A:354:VAL:HB	1:A:355:ALA:H	1.51	0.41
1:A:571:LEU:HD23	1:A:571:LEU:HA	1.85	0.41
2:B:168:ASP:HA	2:B:171:GLU:HB2	2.02	0.41
2:B:250:ARG:HD3	2:B:252:LYS:N	2.36	0.41
1:C:3:LEU:HD12	1:C:4:LEU:H	1.86	0.41
1:C:41:GLN:HA	1:C:42:PRO:HD3	1.87	0.41
1:C:112:PHE:CD2	1:C:117:MET:HA	2.55	0.41
2:D:216:PRO:O	2:D:433:PRO:HD3	2.20	0.41
2:D:239:ASN:HB3	2:D:242:GLU:CB	2.49	0.41
2:D:584:ARG:HH21	2:D:585:ARG:HD3	1.85	0.41
1:A:321:TRP:HZ2	1:A:325:ASN:HD22	1.67	0.41
1:A:529:ARG:NH1	1:A:534:LEU:O	2.53	0.41
2:B:257:LEU:O	2:B:616:ILE:HD12	2.21	0.41
2:B:388:SER:C	2:B:390:GLU:H	2.29	0.41
1:C:80:LEU:C	1:C:82:SER:H	2.29	0.41
2:D:277:ALA:C	2:D:279:GLY:N	2.77	0.41
2:D:302:GLU:OE2	2:D:302:GLU:HA	2.21	0.41
2:D:418:LEU:HD23	2:D:453:PRO:HB3	2.02	0.41
2:D:427:THR:HG21	2:D:469:SER:HA	2.01	0.41
2:D:580:THR:HB	2:D:599:SER:CB	2.51	0.41
2:D:623:TYR:HA	2:D:624:PRO:HD3	1.74	0.41
2:B:300:ILE:HD12	2:B:300:ILE:HG21	1.88	0.41
2:D:258:ILE:CD1	2:D:271:ILE:HG21	2.50	0.41
1:A:16:ASP:OD1	1:A:16:ASP:N	2.54	0.41
1:A:175:ARG:HA	1:A:175:ARG:HD2	1.86	0.41
1:A:407:SER:HB3	1:A:410:LYS:HD2	2.02	0.41
1:A:138:ASN:HD22	1:A:139:PRO:HD2	1.86	0.41
1:A:143:SER:HB2	1:A:156:PHE:O	2.21	0.41
1:A:262:THR:HG23	1:A:290:TYR:HH	1.85	0.41
1:A:276:GLU:O	1:A:277:LYS:C	2.64	0.41
1:A:448:LYS:HB3	1:A:448:LYS:HE3	1.41	0.41
1:A:459:TYR:OH	1:A:463:ILE:HD11	2.20	0.41
2:B:585:ARG:NH1	2:B:585:ARG:HB3	2.36	0.41
1:C:325:ASN:C	1:C:327:TYR:N	2.77	0.41
2:D:273:PHE:N	2:D:274:PRO:HD3	2.36	0.41
2:D:358:THR:OG1	2:D:406:HIS:HE1	2.04	0.41
2:D:366:VAL:HG13	2:D:386:PHE:HB2	2.02	0.41
2:D:395:PHE:CD2	2:D:395:PHE:N	2.88	0.41
2:D:441:LYS:O	2:D:441:LYS:HG2	2.20	0.41
2:D:582:ALA:O	2:D:583:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:661:ASN:HD22	2:D:661:ASN:H	1.69	0.41
1:A:230:THR:HG21	1:A:267:ASN:HB2	2.01	0.41
2:B:253:ARG:CG	2:B:253:ARG:NH1	2.74	0.41
2:B:383:CYS:HB2	2:B:397:GLU:HA	2.02	0.41
2:B:559:ILE:HG21	2:B:559:ILE:HD13	1.81	0.41
1:C:276:GLU:O	1:C:277:LYS:C	2.63	0.41
1:C:382:ARG:HG2	1:C:382:ARG:HH11	1.86	0.41
2:D:203:ILE:HG22	2:D:651:SER:HA	2.03	0.41
1:A:138:ASN:HD22	1:A:139:PRO:CD	2.34	0.40
1:A:145:VAL:HG22	1:A:190:TRP:CZ3	2.56	0.40
1:A:321:TRP:O	1:A:322:ASN:C	2.64	0.40
2:B:588:HIS:HE1	2:B:590:ILE:CG1	2.34	0.40
1:C:10:ASP:OD1	1:C:365:SER:HB3	2.22	0.40
1:C:155:PHE:HE1	1:C:174:ILE:CD1	2.34	0.40
1:C:563:TYR:HB3	1:C:567:THR:HG22	2.02	0.40
1:A:124:LYS:HG3	1:A:125:GLY:H	1.85	0.40
1:C:81:ASN:HA	1:C:106:ASN:ND2	2.37	0.40
1:C:340:PRO:HB2	1:C:383:ALA:HB2	2.02	0.40
1:C:435:GLU:CD	1:C:435:GLU:H	2.29	0.40
1:A:5:LYS:HB3	1:A:51:ASN:HA	2.04	0.40
1:A:243:CYS:HB3	1:A:244:PRO:CD	2.50	0.40
2:B:442:ASN:OD1	2:B:444:PHE:HD1	2.04	0.40
2:B:661:ASN:ND2	2:B:665:LEU:H	2.14	0.40
1:C:556:LYS:HD2	1:C:575:ASN:ND2	2.36	0.40
2:B:184:LEU:HD12	2:B:184:LEU:HA	1.93	0.40
2:B:465:SER:O	2:B:466:TYR:C	2.64	0.40
1:C:302:ALA:O	1:C:303:ASP:C	2.64	0.40
2:B:420:LEU:HD12	2:B:420:LEU:HA	1.92	0.40
2:B:641:ASN:HD22	2:B:642:ILE:N	2.20	0.40
1:C:499:LYS:O	1:C:561:ASN:ND2	2.53	0.40
2:D:196:PHE:O	2:D:579:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/588 (100%)	475 (81%)	74 (13%)	36 (6%)	1	9
1	C	584/588 (99%)	475 (81%)	69 (12%)	40 (7%)	1	7
2	B	462/524 (88%)	362 (78%)	68 (15%)	32 (7%)	1	7
2	D	459/524 (88%)	356 (78%)	76 (17%)	27 (6%)	1	10
All	All	2090/2224 (94%)	1668 (80%)	287 (14%)	135 (6%)	1	8

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	124	LYS
1	A	159	ARG
1	A	164	ASN
1	A	166	PRO
1	A	212	SER
1	A	278	GLU
1	A	303	ASP
1	A	305	ILE
1	A	320	ILE
1	A	321	TRP
1	A	323	GLU
1	A	324	PHE
1	A	354	VAL
1	A	358	TYR
1	A	361	ALA
1	A	363	GLU
1	A	364	GLN
2	B	177	ASN
2	B	222	ALA
2	B	223	TYR
2	B	235	TYR
2	B	238	ILE
2	B	289	GLY
2	B	379	HIS
2	B	380	LEU
2	B	381	VAL
2	B	400	ASP
2	B	405	VAL
2	B	583	ALA

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Mol	Chain	Res	Type
2	B	584	ARG
2	B	610	LYS
2	B	640	ILE
2	B	674	GLU
1	C	80	LEU
1	C	124	LYS
1	C	126	ASN
1	C	127	LEU
1	C	159	ARG
1	C	164	ASN
1	C	166	PRO
1	C	212	SER
1	C	278	GLU
1	C	303	ASP
1	C	305	ILE
1	C	320	ILE
1	C	321	TRP
1	C	323	GLU
1	C	324	PHE
1	C	354	VAL
1	C	358	TYR
1	C	361	ALA
1	C	363	GLU
1	C	364	GLN
1	C	501	SER
2	D	222	ALA
2	D	223	TYR
2	D	235	TYR
2	D	238	ILE
2	D	379	HIS
2	D	380	LEU
2	D	381	VAL
2	D	400	ASP
2	D	405	VAL
2	D	583	ALA
2	D	584	ARG
2	D	610	LYS
2	D	640	ILE
1	A	49	ASN
1	A	126	ASN
1	A	127	LEU
1	A	322	ASN

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Mol	Chain	Res	Type
2	B	339	SER
2	B	402	ALA
2	B	611	ASP
1	C	322	ASN
1	C	416	ASN
2	D	177	ASN
2	D	339	SER
2	D	424	LEU
2	D	611	ASP
1	A	99	TRP
1	A	210	SER
1	A	416	ASN
2	B	233	THR
2	B	378	PRO
2	B	423	SER
2	B	589	GLY
2	B	641	ASN
2	B	672	SER
1	C	160	LYS
1	C	163	GLU
1	C	402	LEU
1	C	488	GLU
2	D	233	THR
2	D	378	PRO
2	D	402	ALA
2	D	423	SER
2	D	641	ASN
2	D	672	SER
1	A	19	ASN
1	A	163	GLU
2	B	251	THR
2	B	424	LEU
2	B	532	ALA
1	C	49	ASN
1	C	99	TRP
1	C	210	SER
1	C	211	ALA
1	C	215	GLN
1	C	236	ASP
1	C	265	LEU
1	C	359	LYS
2	D	251	THR

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Mol	Chain	Res	Type
2	D	530	ASP
2	D	532	ALA
1	A	158	ILE
1	A	211	ALA
1	A	215	GLN
1	A	236	ASP
1	A	359	LYS
1	A	402	LEU
2	B	530	ASP
1	C	19	ASN
1	C	158	ILE
1	C	243	CYS
1	A	84	PRO
1	A	265	LEU
2	B	308	LYS
2	B	466	TYR
1	C	511	SER
1	C	84	PRO
2	B	609	ILE
2	D	609	ILE
1	A	243	CYS

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	543/544 (100%)	437 (80%)	106 (20%)	1	8
1	C	542/544 (100%)	432 (80%)	110 (20%)	1	7
2	B	415/465 (89%)	323 (78%)	92 (22%)	1	5
2	D	414/465 (89%)	320 (77%)	94 (23%)	1	5
All	All	1914/2018 (95%)	1512 (79%)	402 (21%)	1	6

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	19	ASN
1	A	22	THR
1	A	31	LEU
1	A	33	THR
1	A	48	ILE
1	A	49	ASN
1	A	57	HIS
1	A	59	LYS
1	A	63	LEU
1	A	83	GLN
1	A	85	VAL
1	A	89	ARG
1	A	97	ASP
1	A	100	MET
1	A	115	ASN
1	A	117	MET
1	A	119	THR
1	A	131	THR
1	A	140	ILE
1	A	145	VAL
1	A	159	ARG
1	A	160	LYS
1	A	162	SER
1	A	163	GLU
1	A	165	THR
1	A	178	ASP
1	A	181	SER
1	A	182	LYS
1	A	183	ASP
1	A	189	VAL
1	A	193	ASP
1	A	194	VAL
1	A	207	MET
1	A	215	GLN
1	A	219	ARG
1	A	226	ARG
1	A	237	TYR
1	A	247	VAL
1	A	249	LYS
1	A	254	ASN
1	A	255	TYR
1	A	257	ILE

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Mol	Chain	Res	Type
1	A	258	SER
1	A	269	HIS
1	A	270	ILE
1	A	277	LYS
1	A	280	THR
1	A	284	MET
1	A	287	LYS
1	A	295	GLU
1	A	305	ILE
1	A	312	LYS
1	A	313	LYS
1	A	319	THR
1	A	325	ASN
1	A	331	LEU
1	A	344	SER
1	A	352	GLU
1	A	354	VAL
1	A	356	PHE
1	A	358	TYR
1	A	362	SER
1	A	368	ILE
1	A	384	VAL
1	A	397	GLN
1	A	399	LEU
1	A	404	GLU
1	A	408	MET
1	A	412	LEU
1	A	414	ASN
1	A	435	GLU
1	A	437	ARG
1	A	448	LYS
1	A	450	SER
1	A	451	ILE
1	A	458	LEU
1	A	463	ILE
1	A	472	SER
1	A	475	LEU
1	A	478	VAL
1	A	484	ILE
1	A	491	ILE
1	A	493	ASN
1	A	498	MET

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Mol	Chain	Res	Type
1	A	501	SER
1	A	503	LEU
1	A	506	THR
1	A	510	GLU
1	A	513	THR
1	A	517	GLU
1	A	523	THR
1	A	526	THR
1	A	533	THR
1	A	535	LEU
1	A	538	LEU
1	A	539	THR
1	A	544	ILE
1	A	545	CYS
1	A	549	LYS
1	A	551	ARG
1	A	567	THR
1	A	573	ARG
1	A	577	ILE
1	A	579	VAL
1	A	581	CYS
2	B	172	ARG
2	B	178	LYS
2	B	179	GLU
2	B	183	LEU
2	B	184	LEU
2	B	219	LYS
2	B	220	GLU
2	B	221	SER
2	B	224	ASN
2	B	226	VAL
2	B	227	ILE
2	B	231	ASN
2	B	234	VAL
2	B	235	TYR
2	B	236	HIS
2	B	237	GLU
2	B	238	ILE
2	B	246	MET
2	B	249	LEU
2	B	250	ARG
2	B	251	THR

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Mol	Chain	Res	Type
2	B	253	ARG
2	B	256	LEU
2	B	257	LEU
2	B	258	ILE
2	B	265	VAL
2	B	266	SER
2	B	271	ILE
2	B	282	ARG
2	B	293	THR
2	B	295	ILE
2	B	300	ILE
2	B	301	GLU
2	B	302	GLU
2	B	304	THR
2	B	306	ILE
2	B	308	LYS
2	B	313	LEU
2	B	338	SER
2	B	343	ILE
2	B	348	THR
2	B	354	VAL
2	B	365	GLU
2	B	376	HIS
2	B	381	VAL
2	B	383	CYS
2	B	388	SER
2	B	393	ILE
2	B	394	ASN
2	B	396	LEU
2	B	399	ILE
2	B	401	ASN
2	B	403	THR
2	B	415	SER
2	B	437	VAL
2	B	447	GLU
2	B	451	THR
2	B	454	GLU
2	B	455	VAL
2	B	464	ASP
2	B	480	THR
2	B	481	VAL
2	B	484	THR

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Mol	Chain	Res	Type
2	B	507	SER
2	B	510	ARG
2	B	517	VAL
2	B	518	VAL
2	B	525	SER
2	B	533	SER
2	B	546	VAL
2	B	549	LEU
2	B	554	THR
2	B	557	THR
2	B	559	ILE
2	B	563	ARG
2	B	584	ARG
2	B	585	ARG
2	B	586	LEU
2	B	587	LEU
2	B	597	GLN
2	B	600	LEU
2	B	601	ARG
2	B	604	LYS
2	B	609	ILE
2	B	610	LYS
2	B	616	ILE
2	B	640	ILE
2	B	648	ASN
2	B	651	SER
2	B	661	ASN
2	B	667	THR
2	B	668	LEU
1	C	4	LEU
1	C	8	LEU
1	C	18	LYS
1	C	19	ASN
1	C	22	THR
1	C	33	THR
1	C	48	ILE
1	C	49	ASN
1	C	57	HIS
1	C	59	LYS
1	C	63	LEU
1	C	83	GLN
1	C	85	VAL

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Mol	Chain	Res	Type
1	C	89	ARG
1	C	97	ASP
1	C	100	MET
1	C	115	ASN
1	C	117	MET
1	C	119	THR
1	C	131	THR
1	C	141	GLU
1	C	145	VAL
1	C	159	ARG
1	C	160	LYS
1	C	162	SER
1	C	163	GLU
1	C	165	THR
1	C	166	PRO
1	C	169	TYR
1	C	178	ASP
1	C	181	SER
1	C	182	LYS
1	C	183	ASP
1	C	189	VAL
1	C	193	ASP
1	C	194	VAL
1	C	207	MET
1	C	215	GLN
1	C	219	ARG
1	C	226	ARG
1	C	237	TYR
1	C	243	CYS
1	C	247	VAL
1	C	254	ASN
1	C	257	ILE
1	C	258	SER
1	C	269	HIS
1	C	270	ILE
1	C	277	LYS
1	C	280	THR
1	C	284	MET
1	C	287	LYS
1	C	305	ILE
1	C	312	LYS
1	C	313	LYS

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Mol	Chain	Res	Type
1	C	319	THR
1	C	325	ASN
1	C	331	LEU
1	C	344	SER
1	C	352	GLU
1	C	354	VAL
1	C	356	PHE
1	C	358	TYR
1	C	362	SER
1	C	368	ILE
1	C	384	VAL
1	C	397	GLN
1	C	399	LEU
1	C	401	LYS
1	C	407	SER
1	C	409	ASN
1	C	412	LEU
1	C	414	ASN
1	C	435	GLU
1	C	437	ARG
1	C	448	LYS
1	C	450	SER
1	C	451	ILE
1	C	458	LEU
1	C	463	ILE
1	C	472	SER
1	C	475	LEU
1	C	478	VAL
1	C	481	ILE
1	C	484	ILE
1	C	487	ARG
1	C	488	GLU
1	C	495	THR
1	C	497	LEU
1	C	500	ASN
1	C	502	PHE
1	C	503	LEU
1	C	506	THR
1	C	510	GLU
1	C	511	SER
1	C	513	THR
1	C	517	GLU

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Mol	Chain	Res	Type
1	C	523	THR
1	C	526	THR
1	C	533	THR
1	C	535	LEU
1	C	537	ILE
1	C	540	THR
1	C	544	ILE
1	C	549	LYS
1	C	551	ARG
1	C	567	THR
1	C	579	VAL
1	C	587	VAL
1	C	588	MET
2	D	172	ARG
2	D	178	LYS
2	D	179	GLU
2	D	183	LEU
2	D	184	LEU
2	D	219	LYS
2	D	220	GLU
2	D	221	SER
2	D	224	ASN
2	D	226	VAL
2	D	227	ILE
2	D	231	ASN
2	D	234	VAL
2	D	235	TYR
2	D	236	HIS
2	D	237	GLU
2	D	238	ILE
2	D	246	MET
2	D	249	LEU
2	D	250	ARG
2	D	251	THR
2	D	253	ARG
2	D	256	LEU
2	D	257	LEU
2	D	258	ILE
2	D	265	VAL
2	D	266	SER
2	D	271	ILE
2	D	282	ARG

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Mol	Chain	Res	Type
2	D	293	THR
2	D	295	ILE
2	D	300	ILE
2	D	301	GLU
2	D	302	GLU
2	D	304	THR
2	D	306	ILE
2	D	308	LYS
2	D	313	LEU
2	D	338	SER
2	D	343	ILE
2	D	348	THR
2	D	353	CYS
2	D	354	VAL
2	D	365	GLU
2	D	366	VAL
2	D	376	HIS
2	D	381	VAL
2	D	383	CYS
2	D	388	SER
2	D	393	ILE
2	D	394	ASN
2	D	396	LEU
2	D	399	ILE
2	D	401	ASN
2	D	403	THR
2	D	404	ASP
2	D	415	SER
2	D	427	THR
2	D	447	GLU
2	D	454	GLU
2	D	455	VAL
2	D	464	ASP
2	D	480	THR
2	D	481	VAL
2	D	484	THR
2	D	507	SER
2	D	510	ARG
2	D	517	VAL
2	D	518	VAL
2	D	525	SER
2	D	533	SER

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Mol	Chain	Res	Type
2	D	546	VAL
2	D	549	LEU
2	D	550	VAL
2	D	557	THR
2	D	559	ILE
2	D	563	ARG
2	D	584	ARG
2	D	585	ARG
2	D	586	LEU
2	D	587	LEU
2	D	600	LEU
2	D	601	ARG
2	D	604	LYS
2	D	609	ILE
2	D	610	LYS
2	D	613	LYS
2	D	616	ILE
2	D	640	ILE
2	D	651	SER
2	D	661	ASN
2	D	667	THR
2	D	668	LEU
2	D	674	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	51	ASN
1	A	57	HIS
1	A	67	ASN
1	A	76	GLN
1	A	106	ASN
1	A	108	ASN
1	A	138	ASN
1	A	161	ASN
1	A	215	GLN
1	A	304	ASN
1	A	325	ASN
1	A	396	ASN
1	A	397	GLN
1	A	416	ASN

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Mol	Chain	Res	Type
1	A	493	ASN
1	A	541	HIS
1	A	575	ASN
2	B	204	GLN
2	B	224	ASN
2	B	287	ASN
2	B	299	ASN
2	B	311	GLN
2	B	342	GLN
2	B	357	GLN
2	B	361	HIS
2	B	389	GLN
2	B	401	ASN
2	B	406	HIS
2	B	522	GLN
2	B	547	HIS
2	B	565	HIS
2	B	588	HIS
2	B	638	HIS
2	B	641	ASN
2	B	648	ASN
2	B	661	ASN
1	C	41	GLN
1	C	51	ASN
1	C	57	HIS
1	C	67	ASN
1	C	76	GLN
1	C	106	ASN
1	C	108	ASN
1	C	120	ASN
1	C	138	ASN
1	C	161	ASN
1	C	215	GLN
1	C	267	ASN
1	C	304	ASN
1	C	325	ASN
1	C	397	GLN
1	C	416	ASN
1	C	541	HIS
1	C	575	ASN
2	D	224	ASN
2	D	299	ASN

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Mol	Chain	Res	Type
2	D	311	GLN
2	D	357	GLN
2	D	361	HIS
2	D	389	GLN
2	D	401	ASN
2	D	406	HIS
2	D	522	GLN
2	D	547	HIS
2	D	565	HIS
2	D	638	HIS
2	D	641	ASN
2	D	648	ASN
2	D	661	ASN

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	587/588 (99%)	0.09	4 (0%) 84 69	61, 71, 71, 81	0
1	C	586/588 (99%)	0.19	3 (0%) 87 76	60, 71, 71, 87	0
2	B	472/524 (90%)	0.16	4 (0%) 82 67	70, 71, 71, 72	0
2	D	469/524 (89%)	0.06	5 (1%) 78 61	71, 71, 71, 75	0
All	All	2114/2224 (95%)	0.13	16 (0%) 82 67	60, 71, 71, 87	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	300	ILE	3.3
2	B	590	ILE	2.8
2	D	300	ILE	2.6
1	A	362	SER	2.4
2	D	306	ILE	2.4
2	D	402	ALA	2.4
2	D	236	HIS	2.3
1	C	538	LEU	2.3
2	D	380	LEU	2.3
1	A	259	SER	2.3
1	C	541	HIS	2.2
1	A	320	ILE	2.2
1	C	160	LYS	2.2
1	A	323	GLU	2.1
2	B	306	ILE	2.0
2	B	236	HIS	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.