



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:03 PM UTC

PDB ID : 4FQU / pdb_00004fqu
Title : Glutathionyl-Hydroquinone Reductase PcpF of *Sphingobium chlorophenolicum*
Authors : Green, A.R.; Hayes, R.P.; Xun, L.; Kang, C.
Deposited on : 2012-06-25
Resolution : 3.00 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

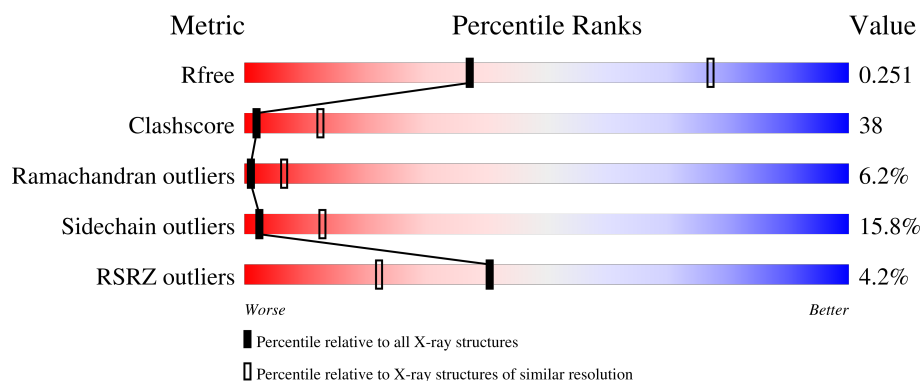
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	313	4% 50% 35% 12%
1	B	313	3% 50% 35% 11%
1	C	313	4% 40% 44% 12%
1	D	313	4% 37% 45% 16%
1	E	313	4% 41% 42% 14%

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Mol	Chain	Length	Quality of chain	
1	F	313		..
1	G	313		..
1	H	313		..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19729 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 Putative glutathione transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2491	1592	435	458	6			
1	B	303	Total	C	N	O	S	0	0	0
			2420	1549	424	441	6			
1	C	312	Total	C	N	O	S	0	0	0
			2482	1584	435	457	6			
1	D	312	Total	C	N	O	S	0	0	0
			2481	1586	432	457	6			
1	E	312	Total	C	N	O	S	0	0	0
			2484	1587	435	456	6			
1	F	308	Total	C	N	O	S	0	0	0
			2444	1559	429	450	6			
1	G	305	Total	C	N	O	S	0	0	0
			2428	1551	426	445	6			
1	H	309	Total	C	N	O	S	0	0	0
			2444	1561	430	447	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	5	Total	O	0	0
			5	5		
2	C	9	Total	O	0	0
			9	9		
2	D	3	Total	O	0	0
			3	3		
2	E	1	Total	O	0	0
			1	1		
2	F	13	Total	O	0	0
			13	13		

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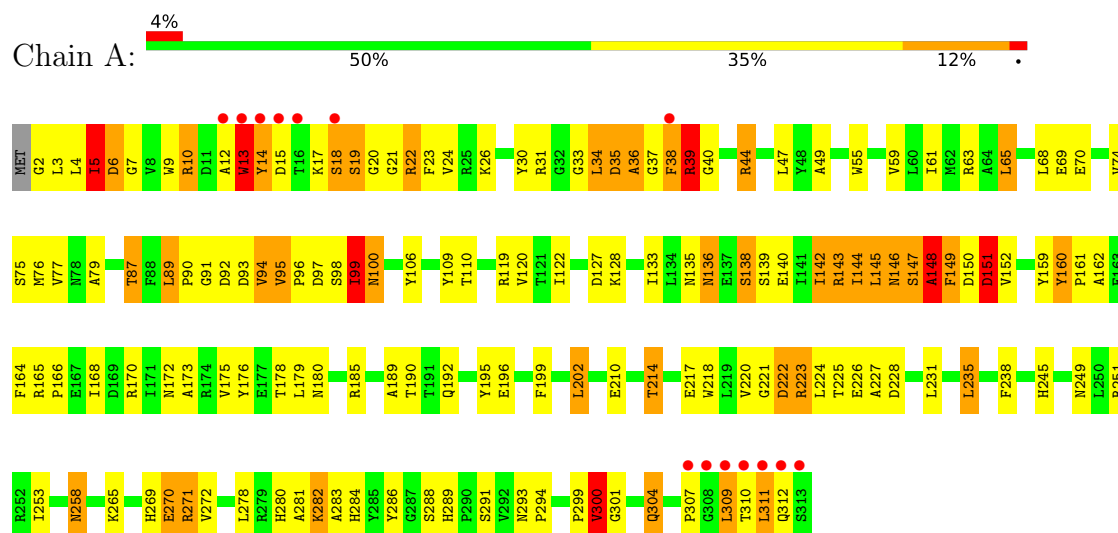
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	1	Total	O	0	0
			1	1		

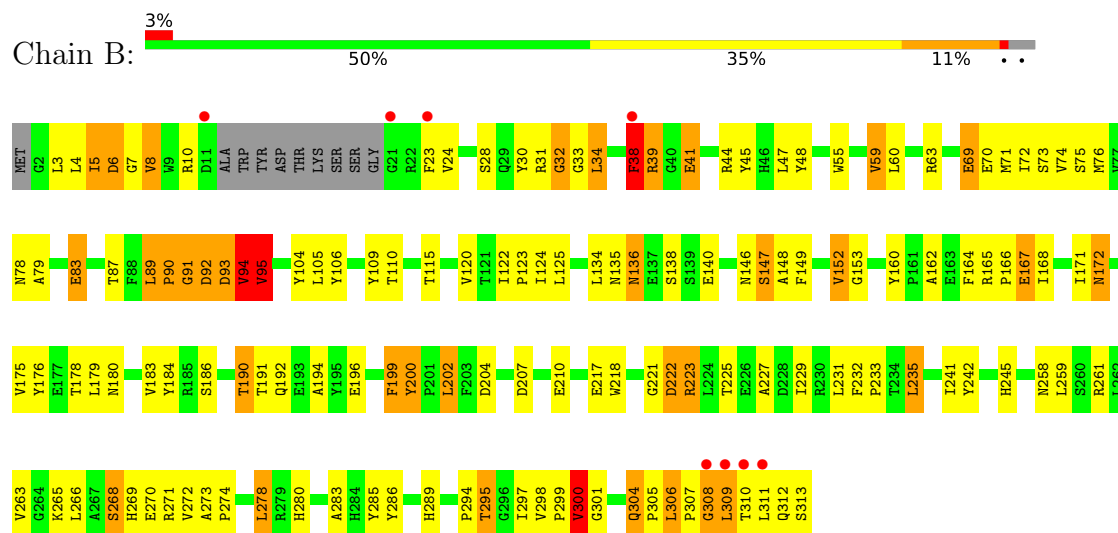
3 Residue-property plots

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.

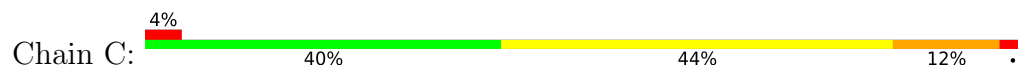
• Molecule 1: Putative glutathione transferase

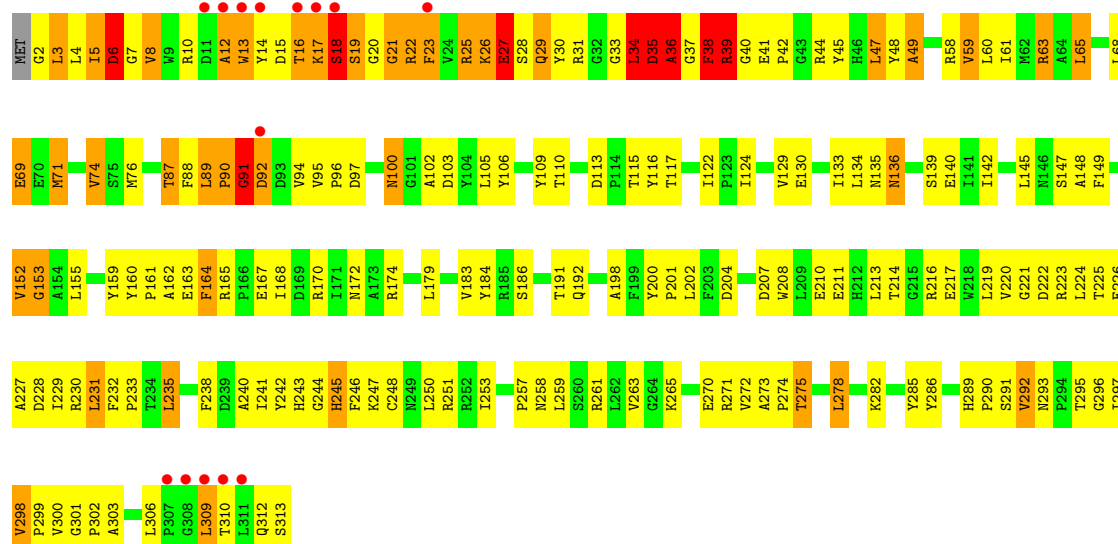


• Molecule 1: Putative glutathione transferase

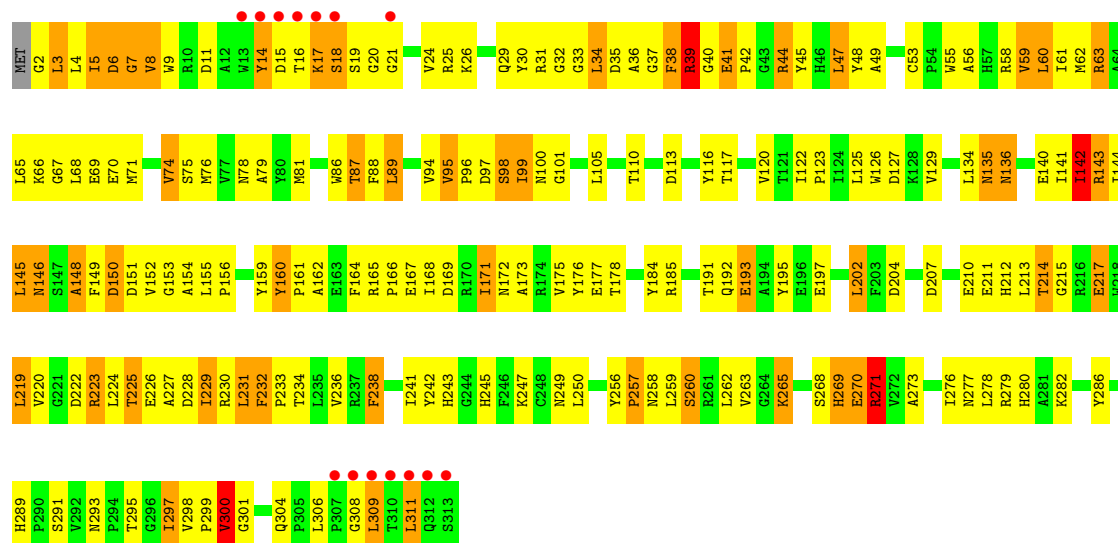


• Molecule 1: Putative glutathione transferase

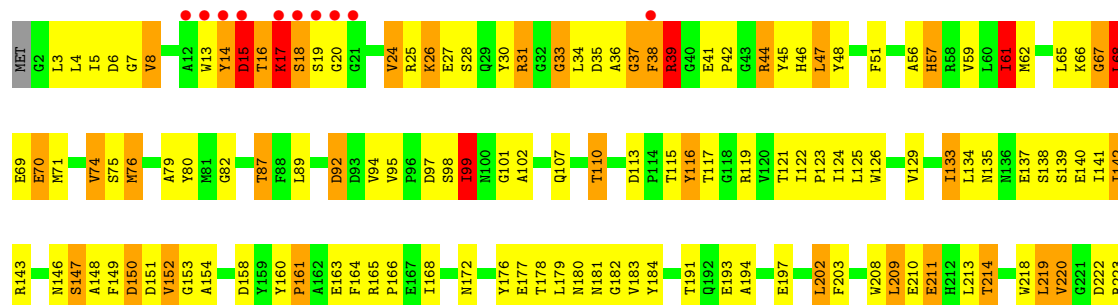
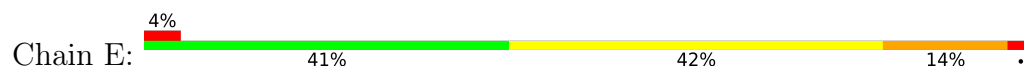


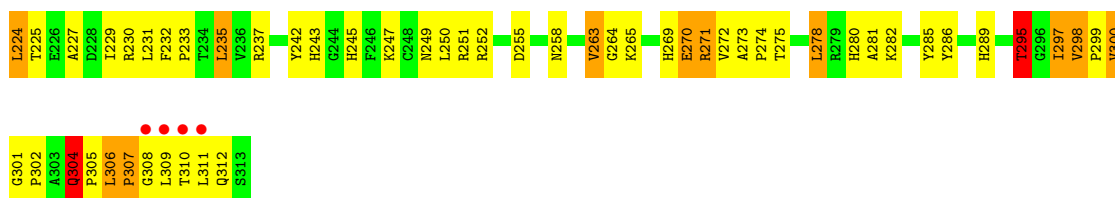


• Molecule 1: Putative glutathione transferase

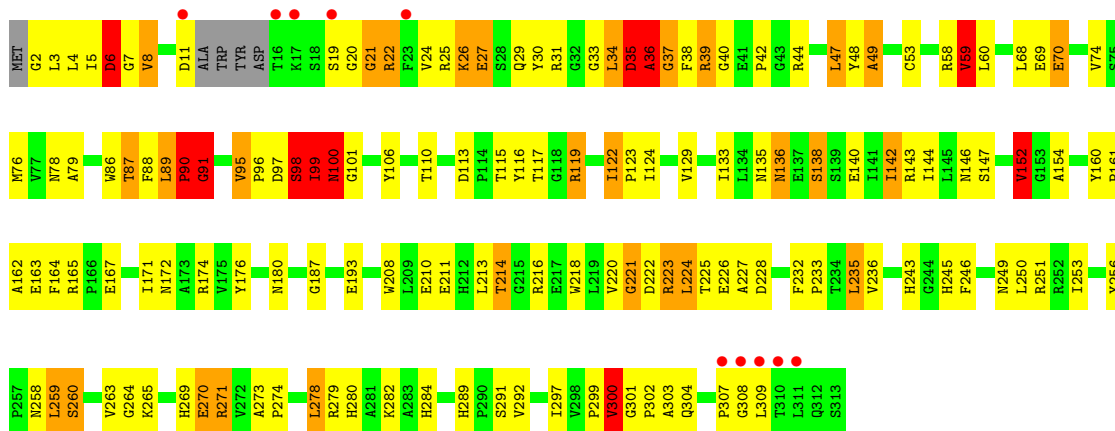


• Molecule 1: Putative glutathione transferase

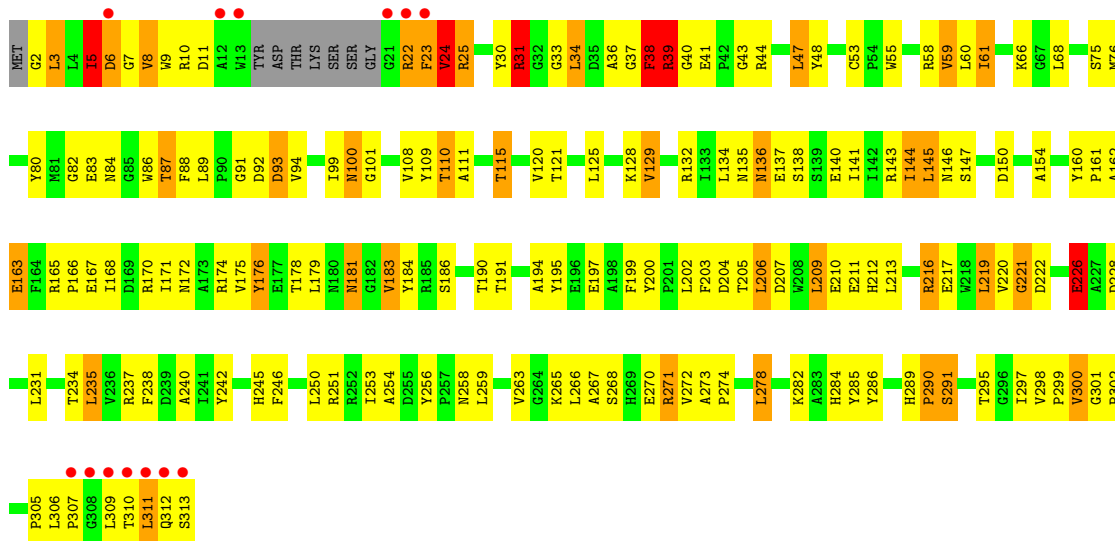




• Molecule 1: Putative glutathione transferase

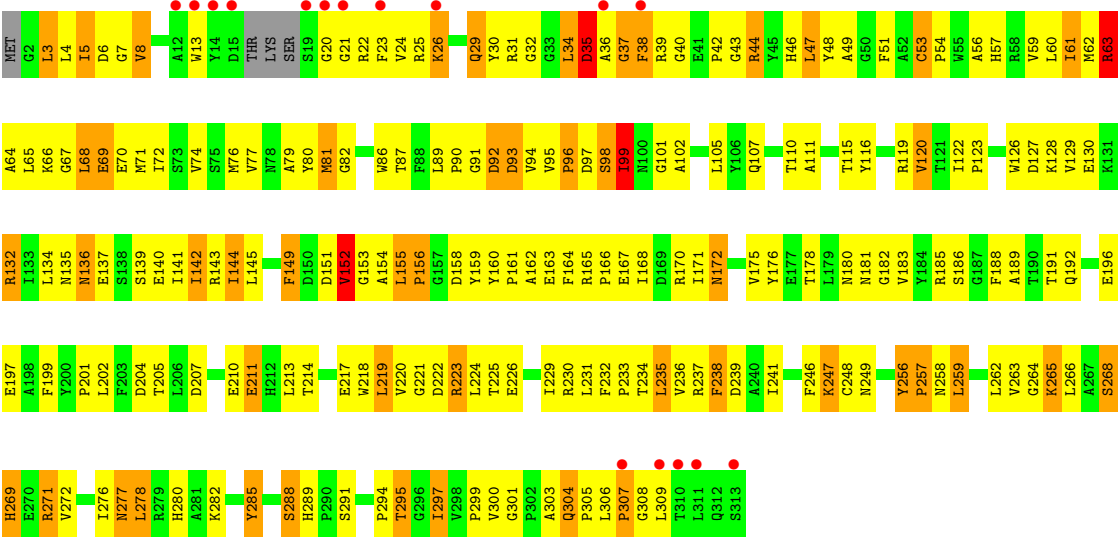


• Molecule 1: Putative glutathione transferase



• Molecule 1: Putative glutathione transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	242.84Å 242.84Å 242.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.9 (49.57-3.00) 87.5 (49.57-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.256 0.195 , 0.251	Depositor DCC
R_{free} test set	2007 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19729	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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	1.17	10/2562 (0.4%)	1.34	27/3490 (0.8%)
1	B	1.00	3/2488 (0.1%)	1.27	21/3387 (0.6%)
1	C	0.98	0/2552	1.28	20/3476 (0.6%)
1	D	0.90	2/2552 (0.1%)	1.25	26/3478 (0.7%)
1	E	1.01	2/2554 (0.1%)	1.27	18/3479 (0.5%)
1	F	1.13	7/2511 (0.3%)	1.30	23/3418 (0.7%)
1	G	0.84	0/2495	1.19	13/3397 (0.4%)
1	H	0.78	0/2511	1.11	15/3419 (0.4%)
All	All	0.99	24/20225 (0.1%)	1.25	163/27544 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	9

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ALA	CA-CB	7.79	1.64	1.52
1	F	99	ILE	CA-CB	7.77	1.65	1.54
1	A	148	ALA	CA-C	7.27	1.61	1.53
1	A	283	ALA	CA-CB	-7.26	1.42	1.53
1	A	310	THR	CA-CB	7.15	1.58	1.53
1	F	36	ALA	CA-C	6.85	1.61	1.52
1	A	173	ALA	CA-CB	-6.75	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	133	ILE	CA-CB	-6.58	1.46	1.54
1	A	19	SER	CA-C	6.55	1.58	1.52
1	B	38	PHE	CA-C	6.55	1.61	1.52
1	F	39	ARG	C-O	6.37	1.32	1.24
1	D	298	VAL	CA-C	-6.14	1.47	1.53
1	A	39	ARG	CA-C	6.08	1.60	1.52
1	E	297	ILE	CA-CB	-6.07	1.48	1.54
1	A	168	ILE	CA-CB	-6.04	1.47	1.54
1	F	304	GLN	C-N	5.89	1.38	1.33
1	B	283	ALA	CA-CB	-5.82	1.44	1.53
1	F	36	ALA	CA-CB	-5.72	1.43	1.53
1	F	37	GLY	C-O	5.67	1.31	1.23
1	A	99	ILE	CA-CB	5.29	1.61	1.54
1	B	263	VAL	CA-CB	-5.26	1.48	1.54
1	A	144	ILE	CA-CB	-5.12	1.48	1.54
1	E	298	VAL	CA-C	-5.04	1.48	1.53
1	D	142	ILE	CA-CB	5.01	1.62	1.54

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ASP	N-CA-C	-12.47	96.78	114.12
1	A	149	PHE	N-CA-C	-12.36	96.94	112.88
1	G	24	VAL	N-CA-C	11.52	121.23	111.90
1	A	95	VAL	CA-C-N	10.37	131.01	119.92
1	A	95	VAL	C-N-CA	10.37	131.01	119.92
1	D	6	ASP	N-CA-C	-9.96	98.76	112.30
1	E	304	GLN	CA-C-N	9.05	128.70	119.56
1	E	304	GLN	C-N-CA	9.05	128.70	119.56
1	H	74	VAL	N-CA-C	8.84	120.01	108.35
1	B	93	ASP	N-CA-C	8.51	123.22	113.01
1	C	89	LEU	CA-C-N	8.13	130.01	119.84
1	C	89	LEU	C-N-CA	8.13	130.01	119.84
1	F	29	GLN	N-CA-C	7.90	122.74	113.18
1	B	94	VAL	N-CA-C	7.84	125.64	109.34
1	B	95	VAL	N-CA-C	7.74	125.60	108.88
1	F	89	LEU	CA-C-N	7.70	129.46	119.84
1	F	89	LEU	C-N-CA	7.70	129.46	119.84
1	C	113	ASP	CA-C-N	-7.58	113.09	120.83
1	C	113	ASP	C-N-CA	-7.58	113.09	120.83
1	E	33	GLY	N-CA-C	-7.56	98.47	112.37
1	D	222	ASP	N-CA-C	-7.40	101.29	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	91	GLY	N-CA-C	-7.35	100.01	110.88
1	F	95	VAL	CA-C-N	7.34	127.30	120.03
1	F	95	VAL	C-N-CA	7.34	127.30	120.03
1	D	298	VAL	CB-CA-C	-7.24	102.53	110.85
1	D	95	VAL	CA-C-N	7.19	128.83	119.84
1	D	95	VAL	C-N-CA	7.19	128.83	119.84
1	F	144	ILE	CB-CA-C	-7.04	102.96	111.97
1	G	129	VAL	N-CA-C	7.03	117.03	110.42
1	B	222	ASP	N-CA-C	-7.02	104.71	112.72
1	B	95	VAL	CA-C-N	7.00	128.59	119.84
1	B	95	VAL	C-N-CA	7.00	128.59	119.84
1	A	148	ALA	N-CA-C	6.91	120.98	107.57
1	A	293	ASN	CA-C-N	6.86	126.67	119.05
1	A	293	ASN	C-N-CA	6.86	126.67	119.05
1	H	95	VAL	CA-C-N	6.86	128.41	119.84
1	H	95	VAL	C-N-CA	6.86	128.41	119.84
1	C	298	VAL	CB-CA-C	-6.82	103.01	110.85
1	F	91	GLY	N-CA-C	6.80	129.29	113.18
1	H	29	GLN	N-CA-C	6.77	121.63	113.23
1	C	91	GLY	N-CA-C	6.67	128.98	113.18
1	C	153	GLY	N-CA-C	6.66	122.51	113.99
1	C	222	ASP	N-CA-C	-6.65	103.48	112.26
1	F	59	VAL	N-CA-C	6.54	117.30	110.62
1	G	55	TRP	N-CA-C	-6.41	104.38	111.36
1	F	292	VAL	CB-CA-C	-6.40	105.16	111.30
1	E	24	VAL	N-CA-C	6.32	115.44	106.53
1	G	175	VAL	CB-CA-C	-6.32	103.79	111.88
1	B	89	LEU	CA-C-N	6.30	127.72	119.84
1	B	89	LEU	C-N-CA	6.30	127.72	119.84
1	E	295	THR	N-CA-C	-6.25	104.36	112.23
1	D	39	ARG	N-CA-C	6.23	118.89	109.23
1	A	55	TRP	N-CA-C	-6.23	104.03	111.69
1	A	77	VAL	CB-CA-C	-6.21	104.76	111.59
1	D	101	GLY	N-CA-C	-6.20	106.14	115.32
1	B	304	GLN	CA-C-N	6.12	127.49	119.84
1	B	304	GLN	C-N-CA	6.12	127.49	119.84
1	F	49	ALA	N-CA-C	6.10	116.48	108.07
1	E	298	VAL	CA-C-N	6.09	126.10	119.89
1	E	298	VAL	C-N-CA	6.09	126.10	119.89
1	A	160	TYR	CA-C-N	6.07	127.02	119.98
1	A	160	TYR	C-N-CA	6.07	127.02	119.98
1	G	206	LEU	N-CA-C	-6.06	104.36	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	SER	N-CA-C	-6.04	105.87	113.72
1	H	53	CYS	CA-C-N	6.03	125.65	119.56
1	H	53	CYS	C-N-CA	6.03	125.65	119.56
1	F	36	ALA	N-CA-C	6.03	123.64	110.80
1	D	273	ALA	CA-C-N	-6.01	113.61	120.89
1	D	273	ALA	C-N-CA	-6.01	113.61	120.89
1	E	222	ASP	N-CA-C	-6.01	104.59	112.41
1	B	83	GLU	N-CA-C	-6.00	105.94	113.20
1	E	181	ASN	N-CA-C	-6.00	106.12	113.50
1	A	217	GLU	N-CA-C	-5.97	106.63	114.04
1	D	7	GLY	CA-C-N	5.97	132.45	121.70
1	D	7	GLY	C-N-CA	5.97	132.45	121.70
1	D	300	VAL	N-CA-C	-5.97	105.17	112.76
1	H	222	ASP	N-CA-C	-5.95	105.84	112.57
1	H	217	GLU	N-CA-C	-5.94	105.95	113.43
1	D	160	TYR	CA-C-N	5.92	125.86	119.76
1	D	160	TYR	C-N-CA	5.92	125.86	119.76
1	C	302	PRO	CA-C-O	-5.87	114.95	121.23
1	C	293	ASN	CA-C-N	5.84	125.70	119.28
1	C	293	ASN	C-N-CA	5.84	125.70	119.28
1	F	6	ASP	CA-C-N	5.84	125.52	119.92
1	F	6	ASP	C-N-CA	5.84	125.52	119.92
1	E	45	TYR	N-CA-C	5.83	118.41	108.90
1	B	171	ILE	N-CA-C	-5.82	104.85	110.72
1	A	220	VAL	N-CA-C	5.81	116.44	107.78
1	D	270	GLU	N-CA-C	-5.81	102.69	110.24
1	A	7	GLY	N-CA-C	-5.80	107.25	115.43
1	A	77	VAL	N-CA-C	5.77	116.33	110.05
1	F	221	GLY	CA-C-N	-5.75	114.60	123.17
1	F	221	GLY	C-N-CA	-5.75	114.60	123.17
1	B	300	VAL	N-CA-C	5.71	121.22	109.34
1	D	304	GLN	CA-C-N	5.69	127.78	120.89
1	D	304	GLN	C-N-CA	5.69	127.78	120.89
1	B	55	TRP	N-CA-C	-5.68	104.78	110.97
1	B	200	TYR	N-CA-C	-5.67	106.28	113.77
1	F	6	ASP	N-CA-C	-5.61	105.51	112.47
1	H	289	HIS	CA-C-N	5.61	125.30	119.64
1	H	289	HIS	C-N-CA	5.61	125.30	119.64
1	B	221	GLY	CA-C-N	-5.59	113.72	122.73
1	B	221	GLY	C-N-CA	-5.59	113.72	122.73
1	G	121	THR	N-CA-C	5.58	117.75	108.99
1	E	133	ILE	CB-CA-C	-5.57	104.57	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	98	SER	N-CA-C	-5.54	102.82	110.35
1	B	94	VAL	CA-C-N	5.49	132.29	122.13
1	B	94	VAL	C-N-CA	5.49	132.29	122.13
1	E	76	MET	CG-SD-CE	-5.49	88.83	100.90
1	C	49	ALA	N-CA-C	5.46	115.33	108.45
1	D	217	GLU	N-CA-C	-5.44	107.19	113.88
1	C	164	PHE	N-CA-C	5.44	119.76	113.18
1	G	221	GLY	CA-C-N	-5.43	114.46	123.37
1	G	221	GLY	C-N-CA	-5.43	114.46	123.37
1	A	270	GLU	N-CA-C	-5.43	99.24	110.80
1	F	259	LEU	N-CA-C	-5.42	105.45	111.36
1	D	89	LEU	CA-C-N	5.41	126.60	119.84
1	D	89	LEU	C-N-CA	5.41	126.60	119.84
1	G	254	ALA	N-CA-C	-5.39	105.56	111.82
1	C	29	GLN	N-CA-C	5.38	119.97	113.41
1	C	103	ASP	N-CA-C	-5.38	106.85	113.41
1	A	7	GLY	CA-C-N	-5.37	115.65	123.06
1	A	7	GLY	C-N-CA	-5.37	115.65	123.06
1	F	101	GLY	N-CA-C	5.36	121.30	113.48
1	A	39	ARG	N-CA-C	5.36	122.21	110.80
1	C	39	ARG	N-CA-C	-5.36	99.39	110.80
1	A	89	LEU	CA-C-N	5.34	126.52	119.84
1	A	89	LEU	C-N-CA	5.34	126.52	119.84
1	H	249	ASN	N-CA-C	5.33	117.71	110.88
1	H	132	ARG	N-CA-C	5.28	115.10	108.45
1	G	226	GLU	N-CA-C	-5.25	106.13	112.54
1	A	258	ASN	N-CA-C	5.25	117.00	111.28
1	A	151	ASP	N-CA-CB	-5.24	101.63	110.49
1	C	35	ASP	N-CA-C	5.24	121.96	110.80
1	G	61	ILE	CB-CA-C	-5.21	105.30	111.97
1	G	31	ARG	N-CA-C	5.21	118.75	111.30
1	E	61	ILE	CB-CA-C	-5.21	105.15	111.87
1	D	70	GLU	N-CA-C	-5.20	105.76	112.68
1	A	94	VAL	N-CA-C	5.20	116.29	109.58
1	E	74	VAL	CB-CA-C	-5.19	103.43	110.90
1	F	304	GLN	CA-C-N	5.18	127.00	121.00
1	F	304	GLN	C-N-CA	5.18	127.00	121.00
1	C	302	PRO	N-CA-C	-5.16	103.08	111.03
1	E	285	TYR	N-CA-C	5.14	116.57	111.07
1	B	272	VAL	N-CA-C	5.14	115.36	110.53
1	A	133	ILE	N-CA-C	5.13	116.13	108.54
1	D	223	ARG	N-CA-C	5.13	117.66	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	113	ASP	CA-C-N	5.12	126.24	119.84
1	E	113	ASP	C-N-CA	5.12	126.24	119.84
1	F	113	ASP	CA-C-N	5.11	126.23	119.84
1	F	113	ASP	C-N-CA	5.11	126.23	119.84
1	D	276	ILE	CB-CA-C	-5.09	104.00	110.98
1	C	74	VAL	N-CA-C	5.07	116.91	108.99
1	A	5	ILE	CA-C-N	-5.07	114.36	122.62
1	A	5	ILE	C-N-CA	-5.07	114.36	122.62
1	A	6	ASP	N-CA-C	-5.06	102.82	110.06
1	D	232	PHE	CA-C-N	-5.06	114.61	119.87
1	D	232	PHE	C-N-CA	-5.06	114.61	119.87
1	H	256	TYR	CA-C-N	5.04	126.14	119.84
1	H	256	TYR	C-N-CA	5.04	126.14	119.84
1	D	74	VAL	CB-CA-C	-5.04	102.63	110.69
1	E	74	VAL	N-CA-C	5.04	116.85	108.99
1	F	270	GLU	N-CA-C	-5.00	103.55	110.35

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ALA	Peptide
1	A	39	ARG	Peptide
1	A	40	GLY	Peptide
1	C	36	ALA	Peptide
1	C	6	ASP	Peptide
1	D	300	VAL	Peptide
1	E	6	ASP	Peptide
1	F	21	GLY	Peptide
1	F	6	ASP	Peptide

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	2491	0	2406	185	0
1	B	2420	0	2340	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2482	0	2392	211	0
1	D	2481	0	2383	241	0
1	E	2484	0	2385	200	0
1	F	2444	0	2354	150	0
1	G	2428	0	2344	162	0
1	H	2444	0	2351	222	0
2	A	21	0	0	3	0
2	B	5	0	0	0	0
2	C	9	0	0	4	0
2	D	3	0	0	1	0
2	E	1	0	0	0	0
2	F	13	0	0	1	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
All	All	19729	0	18955	1483	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 38.

All (1483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HE	1:A:148:ALA:C	1.39	1.31
1:C:49:ALA:HB3	1:C:76:MET:HE1	1.26	1.18
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.06	1.14
1:A:221:GLY:HA3	2:A:401:HOH:O	1.46	1.12
1:C:213:LEU:HD21	1:C:219:LEU:HD23	1.29	1.12
1:H:23:PHE:CB	1:H:24:VAL:HA	1.73	1.12
1:B:39:ARG:HB3	1:B:39:ARG:NH1	1.63	1.11
1:A:37:GLY:HA2	1:A:38:PHE:CB	1.76	1.11
1:A:23:PHE:CE2	1:F:26:LYS:HB2	1.86	1.09
1:A:39:ARG:NE	1:A:148:ALA:C	2.10	1.09
1:E:7:GLY:HA3	1:E:8:VAL:CB	1.82	1.08
1:D:214:THR:HG23	1:D:215:GLY:H	1.16	1.06
1:E:31:ARG:HH11	1:E:31:ARG:HG2	1.11	1.06
1:H:23:PHE:HB3	1:H:24:VAL:HA	1.12	1.06
1:B:39:ARG:HH22	1:B:44:ARG:CZ	1.69	1.05
1:F:119:ARG:HG3	1:F:119:ARG:HH11	1.17	1.05
1:B:39:ARG:HH11	1:B:39:ARG:CB	1.69	1.04
1:C:152:VAL:HG12	1:C:153:GLY:H	0.88	1.04
1:F:19:SER:HB3	1:F:20:GLY:HA2	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:VAL:HG12	1:C:153:GLY:N	1.63	1.03
1:D:60:LEU:HD21	1:D:76:MET:HE1	1.41	1.02
1:D:143:ARG:HG3	1:D:143:ARG:HH11	1.19	1.02
1:A:37:GLY:CA	1:A:38:PHE:HB3	1.89	1.01
1:D:37:GLY:HA2	1:D:38:PHE:HB3	1.38	1.00
1:A:17:LYS:HA	1:A:18:SER:HB3	1.41	1.00
1:C:152:VAL:CG1	1:C:153:GLY:H	1.75	1.00
1:C:38:PHE:O	1:C:38:PHE:CD1	2.15	1.00
1:D:87:THR:HG21	1:D:89:LEU:HG	1.41	0.99
1:A:270:GLU:O	1:A:271:ARG:HB2	1.62	0.98
1:D:39:ARG:HG3	1:D:40:GLY:N	1.71	0.98
1:F:87:THR:HG23	1:F:89:LEU:H	1.24	0.98
1:F:270:GLU:O	1:F:271:ARG:HB2	1.61	0.98
1:D:136:ASN:HD22	1:D:136:ASN:C	1.68	0.98
1:A:39:ARG:HH21	1:A:149:PHE:H	1.01	0.98
1:A:143:ARG:HH11	1:A:143:ARG:CG	1.76	0.98
1:G:167:GLU:HG3	1:G:170:ARG:NH1	1.78	0.98
1:B:245:HIS:HE1	1:B:289:HIS:HD2	1.08	0.98
1:H:271:ARG:HH11	1:H:271:ARG:HG2	1.29	0.98
1:D:71:MET:SD	1:D:149:PHE:CZ	2.58	0.97
1:H:23:PHE:HB3	1:H:24:VAL:CA	1.94	0.97
1:C:38:PHE:O	1:C:38:PHE:HD1	1.45	0.96
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.27	0.96
1:H:6:ASP:H	1:H:7:GLY:HA2	1.29	0.96
1:A:19:SER:N	1:A:20:GLY:HA2	1.81	0.96
1:G:39:ARG:HA	1:G:39:ARG:NE	1.82	0.95
1:B:39:ARG:HB3	1:B:39:ARG:HH11	0.79	0.95
1:C:7:GLY:HA2	1:C:8:VAL:O	1.66	0.95
1:G:174:ARG:O	1:G:178:THR:HG22	1.65	0.94
1:A:245:HIS:HE1	1:A:289:HIS:CD2	1.86	0.94
1:E:87:THR:HG23	1:E:89:LEU:H	1.29	0.94
1:C:27:GLU:CD	1:C:28:SER:H	1.75	0.93
1:B:38:PHE:HB2	1:B:39:ARG:C	1.92	0.93
1:A:22:ARG:HH11	1:A:22:ARG:HG2	1.30	0.93
1:B:78:ASN:ND2	1:B:91:GLY:HA3	1.82	0.93
1:G:191:THR:HG23	1:G:194:ALA:H	1.33	0.93
1:A:14:TYR:N	1:A:15:ASP:HA	1.84	0.92
1:A:39:ARG:HG2	1:A:148:ALA:O	1.68	0.92
1:B:38:PHE:HB2	1:B:39:ARG:O	1.69	0.92
1:B:38:PHE:HB2	1:B:39:ARG:CA	2.00	0.91
1:A:222:ASP:N	2:A:401:HOH:O	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:GLY:HA2	1:D:38:PHE:CB	1.98	0.91
1:A:143:ARG:HG3	1:A:143:ARG:NH1	1.78	0.90
1:F:37:GLY:HA2	1:F:39:ARG:H	1.34	0.90
1:G:167:GLU:HG3	1:G:170:ARG:HH12	1.36	0.90
1:B:41:GLU:CD	1:B:41:GLU:H	1.77	0.90
1:D:143:ARG:HH11	1:D:143:ARG:CG	1.84	0.90
1:E:300:VAL:HG12	1:F:250:LEU:HD13	1.51	0.90
1:F:99:ILE:HD12	1:F:99:ILE:O	1.71	0.89
1:A:37:GLY:HA2	1:A:38:PHE:HB3	0.94	0.89
1:B:270:GLU:O	1:B:271:ARG:HB2	1.73	0.89
1:A:245:HIS:HE1	1:A:289:HIS:HD2	1.15	0.89
1:H:42:PRO:HD3	1:H:152:VAL:HG11	1.55	0.89
1:D:47:LEU:HB3	1:D:74:VAL:HG12	1.53	0.88
1:H:34:LEU:H	1:H:144:ILE:HD11	1.36	0.88
1:H:38:PHE:HD2	1:H:38:PHE:O	1.56	0.88
1:A:223:ARG:CB	1:A:223:ARG:HH11	1.87	0.88
1:E:270:GLU:O	1:E:271:ARG:HB2	1.74	0.88
1:E:300:VAL:CG1	1:F:250:LEU:HD13	2.03	0.88
1:A:49:ALA:HB3	1:A:76:MET:HE1	1.54	0.87
1:C:49:ALA:HB3	1:C:76:MET:CE	2.03	0.87
1:D:150:ASP:HA	1:D:154:ALA:HB3	1.55	0.87
1:A:39:ARG:NH1	1:A:147:SER:N	2.21	0.87
1:A:39:ARG:NH2	1:A:149:PHE:H	1.73	0.87
1:B:199:PHE:HD2	1:B:199:PHE:H	1.22	0.87
1:G:213:LEU:HD21	1:G:219:LEU:HD23	1.55	0.86
1:A:22:ARG:HH11	1:A:22:ARG:CG	1.87	0.86
1:C:210:GLU:OE2	1:C:257:PRO:HD2	1.75	0.86
1:D:87:THR:HG22	1:D:89:LEU:H	1.38	0.86
1:E:31:ARG:HG2	1:E:31:ARG:NH1	1.87	0.86
1:C:87:THR:CG2	1:C:89:LEU:H	1.88	0.86
1:A:5:ILE:HG21	1:A:10:ARG:HH11	1.41	0.85
1:A:19:SER:H	1:A:20:GLY:HA2	1.37	0.85
1:D:217:GLU:HB3	1:D:265:LYS:NZ	1.90	0.85
1:F:37:GLY:HA2	1:F:39:ARG:HG3	1.59	0.85
1:H:155:LEU:HB3	1:H:156:PRO:HD2	1.56	0.85
1:D:87:THR:CG2	1:D:89:LEU:HG	2.05	0.85
1:H:306:LEU:HB3	1:H:307:PRO:HD2	1.56	0.85
1:B:245:HIS:HE1	1:B:289:HIS:CD2	1.95	0.85
1:H:37:GLY:N	1:H:38:PHE:HB3	1.91	0.85
1:H:226:GLU:HA	1:H:229:ILE:HD12	1.58	0.85
1:B:191:THR:HG23	1:B:194:ALA:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ARG:HH11	1:E:31:ARG:CG	1.90	0.84
1:A:17:LYS:HA	1:A:18:SER:CB	2.04	0.84
1:D:81:MET:HE3	1:D:86:TRP:CE2	2.11	0.84
1:H:63:ARG:HG2	1:H:63:ARG:HH11	1.39	0.84
1:D:282:LYS:NZ	1:D:301:GLY:HA3	1.92	0.84
1:H:6:ASP:O	1:H:115:THR:HA	1.77	0.84
1:A:299:PRO:C	1:A:301:GLY:H	1.83	0.84
1:H:271:ARG:HH11	1:H:271:ARG:CG	1.90	0.84
1:C:33:GLY:O	1:C:34:LEU:HB2	1.79	0.83
1:H:304:GLN:H	1:H:304:GLN:NE2	1.76	0.83
1:F:224:LEU:HD12	1:F:225:THR:N	1.92	0.83
1:A:39:ARG:HE	1:A:149:PHE:N	1.75	0.83
1:A:23:PHE:HE2	1:F:26:LYS:HB2	1.43	0.83
1:D:59:VAL:HG12	1:D:142:ILE:HD13	1.60	0.83
1:H:304:GLN:H	1:H:304:GLN:HE21	1.26	0.83
1:C:42:PRO:HG3	1:C:152:VAL:HG11	1.60	0.83
1:C:39:ARG:HB3	1:C:41:GLU:OE1	1.78	0.82
1:D:269:HIS:ND1	1:D:270:GLU:O	2.11	0.82
1:D:202:LEU:HD12	1:D:202:LEU:C	2.04	0.82
1:A:223:ARG:HH11	1:A:223:ARG:HB3	1.44	0.82
1:G:31:ARG:HH11	1:G:31:ARG:CG	1.92	0.82
1:H:79:ALA:HB2	1:H:280:HIS:CE1	2.14	0.82
1:E:14:TYR:O	1:E:15:ASP:HB3	1.79	0.82
1:H:91:GLY:O	1:H:94:VAL:HG23	1.80	0.82
1:E:245:HIS:HE1	1:E:289:HIS:HD2	1.26	0.82
1:A:74:VAL:CG1	1:A:76:MET:HE3	2.09	0.82
1:D:164:PHE:C	1:D:166:PRO:HD2	2.03	0.82
1:E:13:TRP:O	1:E:14:TYR:HB2	1.78	0.82
1:G:22:ARG:HD3	1:G:23:PHE:H	1.43	0.82
1:D:63:ARG:HH11	1:D:63:ARG:CG	1.92	0.81
1:B:38:PHE:HB2	1:B:39:ARG:HA	1.61	0.81
1:C:63:ARG:HG2	1:C:63:ARG:HH11	1.46	0.81
1:E:33:GLY:O	1:E:34:LEU:HB2	1.78	0.81
1:H:241:ILE:HD13	1:H:285:TYR:CD1	2.15	0.81
1:B:41:GLU:OE1	1:B:44:ARG:HD2	1.80	0.81
1:B:30:TYR:O	1:B:135:ASN:HA	1.81	0.80
1:H:6:ASP:N	1:H:7:GLY:HA2	1.94	0.80
1:E:152:VAL:HG12	1:E:152:VAL:O	1.78	0.80
1:B:312:GLN:HG2	1:B:313:SER:H	1.45	0.80
1:C:136:ASN:H	1:C:136:ASN:HD22	1.29	0.80
1:C:16:THR:HG21	1:C:20:GLY:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PHE:O	2:D:402:HOH:O	1.99	0.80
1:A:39:ARG:HH12	1:A:147:SER:N	1.80	0.80
1:G:213:LEU:HD12	1:G:259:LEU:HD23	1.62	0.80
1:H:20:GLY:HA3	1:H:22:ARG:H	1.47	0.79
1:C:87:THR:HG23	1:C:89:LEU:H	1.47	0.79
1:D:122:ILE:HB	1:D:123:PRO:HA	1.65	0.79
1:A:39:ARG:HH21	1:A:149:PHE:N	1.79	0.79
1:A:99:ILE:HD12	1:A:99:ILE:O	1.82	0.79
1:D:270:GLU:O	1:D:271:ARG:HB2	1.81	0.79
1:E:17:LYS:HA	1:E:18:SER:CB	2.12	0.79
1:F:37:GLY:CA	1:F:39:ARG:H	1.96	0.79
1:F:214:THR:HA	1:F:258:ASN:ND2	1.97	0.79
1:D:214:THR:HA	1:D:258:ASN:ND2	1.98	0.79
1:H:166:PRO:HG2	1:H:167:GLU:H	1.48	0.78
1:D:214:THR:CG2	1:D:215:GLY:H	1.96	0.78
1:D:256:TYR:O	1:D:260:SER:HB2	1.83	0.78
1:E:202:LEU:C	1:E:202:LEU:HD12	2.07	0.78
1:F:87:THR:CG2	1:F:89:LEU:H	1.96	0.78
1:A:20:GLY:HA3	1:A:21:GLY:C	2.09	0.78
1:D:217:GLU:HB3	1:D:265:LYS:HZ2	1.49	0.78
1:F:245:HIS:HE1	1:F:289:HIS:HD2	1.31	0.78
1:C:39:ARG:HB3	1:C:41:GLU:CD	2.09	0.78
1:G:39:ARG:NH2	1:G:41:GLU:OE1	2.16	0.78
1:D:87:THR:CG2	1:D:89:LEU:H	1.97	0.78
1:E:150:ASP:N	1:E:154:ALA:HB3	1.99	0.78
1:H:282:LYS:NZ	1:H:301:GLY:HA3	1.99	0.77
1:G:204:ASP:O	1:G:207:ASP:HB2	1.84	0.77
1:B:7:GLY:HA2	1:B:8:VAL:CB	2.15	0.77
1:C:265:LYS:HA	1:C:310:THR:HG21	1.67	0.77
1:D:15:ASP:C	1:D:17:LYS:H	1.93	0.77
1:G:34:LEU:HD11	1:G:140:GLU:HB3	1.65	0.77
1:B:76:MET:HB2	1:B:95:VAL:HG13	1.65	0.77
1:G:7:GLY:HA2	1:G:8:VAL:CB	2.14	0.77
1:H:162:ALA:HA	1:H:165:ARG:HD2	1.66	0.77
1:H:218:TRP:CZ2	1:H:265:LYS:HE2	2.20	0.77
1:D:226:GLU:HA	1:D:229:ILE:HG13	1.65	0.77
1:E:150:ASP:H	1:E:154:ALA:HB3	1.48	0.77
1:E:282:LYS:NZ	1:E:301:GLY:HA3	1.99	0.77
1:B:39:ARG:NH2	1:B:44:ARG:CZ	2.47	0.76
1:C:30:TYR:O	1:C:135:ASN:HA	1.84	0.76
1:H:94:VAL:HG12	1:H:96:PRO:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:LEU:HD21	1:H:122:ILE:HG23	1.65	0.76
1:D:214:THR:HG23	1:D:215:GLY:N	1.96	0.76
1:E:125:LEU:HD23	1:E:134:LEU:HD23	1.68	0.76
1:F:22:ARG:HH11	1:F:22:ARG:HB3	1.50	0.76
1:G:33:GLY:O	1:G:34:LEU:HB2	1.85	0.76
1:A:300:VAL:HB	1:B:199:PHE:CZ	2.21	0.75
1:G:5:ILE:O	1:G:6:ASP:HB2	1.85	0.75
1:B:196:GLU:HA	1:B:199:PHE:HE2	1.52	0.75
1:F:245:HIS:HE1	1:F:289:HIS:CD2	2.03	0.75
1:C:37:GLY:HA2	1:C:38:PHE:CB	2.17	0.75
1:C:87:THR:HG23	1:C:89:LEU:HG	1.67	0.74
1:G:286:TYR:HB2	1:G:298:VAL:HG22	1.69	0.74
1:H:149:PHE:HD1	1:H:149:PHE:N	1.86	0.74
1:F:36:ALA:C	1:F:38:PHE:HB3	2.12	0.74
1:A:223:ARG:HB3	1:A:223:ARG:NH1	2.01	0.74
1:H:164:PHE:O	1:H:168:ILE:HG13	1.88	0.74
1:B:71:MET:HE1	1:B:153:GLY:HA3	1.70	0.74
1:B:245:HIS:CE1	1:B:289:HIS:HD2	2.00	0.74
1:G:6:ASP:O	1:G:115:THR:HA	1.87	0.74
1:H:37:GLY:C	1:H:39:ARG:H	1.93	0.74
1:E:224:LEU:HD12	1:E:225:THR:N	2.03	0.74
1:A:245:HIS:CE1	1:A:289:HIS:HD2	2.02	0.74
1:B:79:ALA:HB2	1:B:280:HIS:CE1	2.23	0.74
1:E:56:ALA:HA	1:E:123:PRO:HG3	1.70	0.73
1:E:62:MET:HE3	1:E:146:ASN:HB2	1.70	0.73
1:G:179:LEU:O	1:G:183:VAL:HG13	1.88	0.73
1:H:37:GLY:H	1:H:38:PHE:CB	2.01	0.73
1:H:176:TYR:HA	1:H:180:ASN:HB2	1.69	0.73
1:B:38:PHE:HB3	1:B:148:ALA:HB1	1.70	0.73
1:E:46:HIS:HB3	1:E:126:TRP:HB3	1.70	0.73
1:G:37:GLY:HA2	1:G:38:PHE:CD2	2.23	0.73
1:D:245:HIS:HE1	1:D:289:HIS:CD2	2.06	0.73
1:F:22:ARG:O	1:F:22:ARG:HG2	1.87	0.73
1:D:41:GLU:HG2	1:D:42:PRO:HD2	1.70	0.73
1:G:231:LEU:HG	1:G:235:LEU:HD22	1.71	0.73
1:F:269:HIS:ND1	1:F:270:GLU:O	2.22	0.73
1:B:6:ASP:H	1:B:7:GLY:HA2	1.53	0.72
1:C:37:GLY:HA2	1:C:38:PHE:CG	2.24	0.72
1:H:51:PHE:CD1	1:H:277:ASN:HB3	2.24	0.72
1:E:19:SER:CB	1:E:20:GLY:HA3	2.19	0.72
1:H:192:GLN:O	1:H:196:GLU:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:CG2	1:D:6:ASP:N	2.52	0.72
1:H:37:GLY:HA2	1:H:39:ARG:HG3	1.71	0.72
1:D:245:HIS:HE1	1:D:289:HIS:HD2	1.35	0.72
1:G:38:PHE:HD1	1:G:39:ARG:O	1.71	0.72
1:C:270:GLU:O	1:C:271:ARG:HB2	1.87	0.72
1:D:38:PHE:HD1	1:D:39:ARG:H	1.35	0.72
1:D:193:GLU:O	1:D:197:GLU:HG3	1.90	0.72
1:F:270:GLU:O	1:F:271:ARG:CB	2.35	0.72
1:E:37:GLY:HA3	1:E:38:PHE:CD2	2.24	0.72
1:E:37:GLY:HA3	1:E:38:PHE:HD2	1.53	0.72
1:A:39:ARG:CZ	1:A:147:SER:C	2.62	0.71
1:H:5:ILE:HG22	1:H:8:VAL:CB	2.20	0.71
1:A:218:TRP:CZ2	1:A:265:LYS:HE3	2.25	0.71
1:B:93:ASP:O	1:B:94:VAL:HG13	1.90	0.71
1:D:5:ILE:HG22	1:D:8:VAL:CB	2.20	0.71
1:B:33:GLY:H	1:B:134:LEU:HD11	1.55	0.71
1:C:5:ILE:CG2	1:C:6:ASP:H	2.03	0.71
1:D:162:ALA:HA	1:D:165:ARG:HG3	1.73	0.71
1:G:216:ARG:HH11	1:G:216:ARG:HG2	1.56	0.71
1:B:305:PRO:HB2	1:B:306:LEU:HD13	1.72	0.70
1:D:49:ALA:O	1:D:76:MET:HA	1.91	0.70
1:B:41:GLU:CD	1:B:41:GLU:N	2.48	0.70
1:D:143:ARG:HG3	1:D:143:ARG:NH1	1.96	0.70
1:A:282:LYS:HE2	1:A:301:GLY:HA3	1.73	0.70
1:A:299:PRO:C	1:A:301:GLY:N	2.50	0.70
1:D:63:ARG:HG2	1:D:63:ARG:NH1	2.01	0.70
1:A:39:ARG:NH1	1:A:144:ILE:O	2.25	0.70
1:C:7:GLY:HA2	1:C:8:VAL:C	2.16	0.70
1:E:37:GLY:HA2	1:E:38:PHE:HB3	1.73	0.70
1:H:172:ASN:HB3	1:H:230:ARG:HH21	1.57	0.70
1:D:39:ARG:NH1	1:D:149:PHE:CD1	2.60	0.70
1:D:144:ILE:HG22	1:D:145:LEU:HD23	1.73	0.70
1:B:90:PRO:O	1:B:91:GLY:O	2.10	0.70
1:B:39:ARG:HG3	1:H:207:ASP:OD2	1.92	0.69
1:E:178:THR:O	1:E:202:LEU:HB2	1.92	0.69
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.56	0.69
1:C:23:PHE:CE2	1:E:27:GLU:HB3	2.27	0.69
1:E:163:GLU:HG2	1:E:164:PHE:CD1	2.26	0.69
1:H:89:LEU:HB3	1:H:90:PRO:HD2	1.73	0.69
1:B:39:ARG:HH22	1:B:44:ARG:NE	1.90	0.69
1:A:39:ARG:NE	1:A:148:ALA:N	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HD3	1:A:148:ALA:H	1.57	0.69
1:G:136:ASN:HD22	1:G:136:ASN:H	1.40	0.69
1:D:202:LEU:HD12	1:D:202:LEU:O	1.93	0.69
1:B:23:PHE:CG	1:B:23:PHE:O	2.45	0.69
1:E:117:THR:HG22	1:E:117:THR:O	1.93	0.69
1:F:30:TYR:H	1:F:136:ASN:HD21	1.41	0.69
1:F:97:ASP:C	1:F:98:SER:O	2.34	0.69
1:H:241:ILE:HD13	1:H:285:TYR:HD1	1.57	0.69
1:A:5:ILE:CG2	1:A:10:ARG:HH11	2.06	0.69
1:D:38:PHE:HD1	1:D:39:ARG:N	1.90	0.69
1:G:212:HIS:O	1:G:216:ARG:HD2	1.93	0.69
1:G:216:ARG:HG2	1:G:216:ARG:NH1	2.07	0.69
1:C:200:TYR:CZ	1:D:300:VAL:HG21	2.29	0.68
1:E:147:SER:O	1:E:149:PHE:N	2.27	0.68
1:A:39:ARG:NE	1:A:148:ALA:CA	2.56	0.68
1:F:264:GLY:HA3	1:F:308:GLY:O	1.92	0.68
1:G:286:TYR:CZ	1:G:299:PRO:HG2	2.27	0.68
1:E:307:PRO:HG2	1:E:308:GLY:H	1.58	0.68
1:G:38:PHE:CD1	1:G:39:ARG:O	2.47	0.68
1:H:40:GLY:HA3	1:H:149:PHE:CE1	2.29	0.68
1:C:5:ILE:HG23	1:C:6:ASP:N	2.07	0.68
1:E:62:MET:HE2	1:E:142:ILE:CD1	2.23	0.68
1:F:143:ARG:NH2	1:F:226:GLU:OE2	2.27	0.68
1:D:207:ASP:HB3	1:G:37:GLY:O	1.92	0.68
1:F:19:SER:HB3	1:F:20:GLY:CA	2.21	0.68
1:A:74:VAL:HG11	1:A:76:MET:HE3	1.76	0.68
1:B:39:ARG:HG2	1:B:41:GLU:OE2	1.93	0.68
1:F:22:ARG:HB3	1:F:22:ARG:NH1	2.07	0.68
1:C:20:GLY:N	1:C:21:GLY:CA	2.56	0.68
1:F:119:ARG:HH11	1:F:119:ARG:CG	1.98	0.68
1:H:38:PHE:O	1:H:38:PHE:CD2	2.43	0.68
1:H:66:LYS:O	1:H:68:LEU:HD12	1.93	0.68
1:D:5:ILE:CG2	1:D:6:ASP:H	2.07	0.67
1:E:152:VAL:O	1:E:152:VAL:CG1	2.42	0.67
1:F:19:SER:CB	1:F:20:GLY:HA2	2.13	0.67
1:H:149:PHE:N	1:H:149:PHE:CD1	2.58	0.67
1:H:87:THR:OG1	1:H:89:LEU:HG	1.94	0.67
1:B:270:GLU:O	1:B:271:ARG:CB	2.43	0.67
1:E:164:PHE:C	1:E:166:PRO:HD2	2.18	0.67
1:G:39:ARG:HE	1:G:40:GLY:HA2	1.60	0.67
1:G:87:THR:HG23	1:G:89:LEU:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:PRO:C	1:H:301:GLY:H	2.02	0.67
1:C:49:ALA:CB	1:C:76:MET:HE1	2.17	0.67
1:G:31:ARG:HH11	1:G:31:ARG:HG3	1.60	0.67
1:H:37:GLY:N	1:H:38:PHE:CB	2.57	0.67
1:A:22:ARG:HG2	1:A:22:ARG:NH1	2.08	0.67
1:C:241:ILE:HD13	1:C:285:TYR:CD1	2.30	0.67
1:F:38:PHE:C	1:F:40:GLY:H	2.01	0.66
1:B:196:GLU:HA	1:B:199:PHE:CE2	2.29	0.66
1:C:27:GLU:CD	1:C:28:SER:N	2.49	0.66
1:C:213:LEU:HD21	1:C:219:LEU:CD2	2.18	0.66
1:H:202:LEU:C	1:H:202:LEU:HD23	2.20	0.66
1:A:30:TYR:HB2	1:A:136:ASN:ND2	2.10	0.66
1:C:39:ARG:H	1:C:39:ARG:NH1	1.94	0.66
1:D:5:ILE:HG23	1:D:6:ASP:N	2.10	0.66
1:E:183:VAL:HG11	1:E:242:TYR:CD2	2.31	0.66
1:E:47:LEU:C	1:E:47:LEU:HD22	2.21	0.66
1:B:199:PHE:HA	1:B:202:LEU:HB3	1.76	0.66
1:H:158:ASP:O	1:H:161:PRO:HD3	1.95	0.66
1:B:136:ASN:HD22	1:B:136:ASN:H	1.43	0.66
1:B:89:LEU:O	1:B:91:GLY:N	2.28	0.66
1:C:243:HIS:HA	1:C:248:CYS:O	1.95	0.66
1:D:165:ARG:N	1:D:166:PRO:HD2	2.11	0.65
1:C:5:ILE:CG2	1:C:6:ASP:N	2.58	0.65
1:D:79:ALA:HB2	1:D:280:HIS:CE1	2.31	0.65
1:H:63:ARG:HG2	1:H:63:ARG:NH1	2.06	0.65
1:H:304:GLN:HE21	1:H:304:GLN:N	1.94	0.65
1:E:237:ARG:HG3	1:E:237:ARG:HH11	1.61	0.65
1:H:23:PHE:CB	1:H:24:VAL:CA	2.63	0.65
1:C:23:PHE:CD1	1:C:23:PHE:C	2.73	0.65
1:C:37:GLY:HA2	1:C:38:PHE:HB3	1.77	0.65
1:F:34:LEU:O	1:F:35:ASP:CB	2.45	0.65
1:F:34:LEU:O	1:F:35:ASP:OD2	2.15	0.65
1:D:14:TYR:C	1:D:14:TYR:CD2	2.75	0.65
1:D:220:VAL:HB	1:D:225:THR:HG21	1.78	0.65
1:D:232:PHE:O	1:D:236:VAL:HG12	1.97	0.65
1:F:4:LEU:HD21	1:F:106:TYR:HB2	1.78	0.65
1:G:270:GLU:O	1:G:271:ARG:HB2	1.97	0.65
1:H:172:ASN:HB3	1:H:230:ARG:NH2	2.12	0.65
1:D:60:LEU:HD21	1:D:76:MET:CE	2.24	0.65
1:F:228:ASP:OD1	2:F:405:HOH:O	2.14	0.65
1:C:39:ARG:H	1:C:39:ARG:CZ	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:HG23	1:E:133:ILE:HG23	1.78	0.65
1:F:299:PRO:C	1:F:301:GLY:H	2.04	0.65
1:E:191:THR:HG22	1:E:193:GLU:N	2.12	0.64
1:E:107:GLN:HA	1:E:110:THR:HG22	1.80	0.64
1:B:6:ASP:N	1:B:7:GLY:HA2	2.11	0.64
1:D:99:ILE:HG13	1:D:100:ASN:N	2.13	0.64
1:E:95:VAL:HG12	1:E:95:VAL:O	1.98	0.64
1:G:245:HIS:HE1	1:G:289:HIS:HD2	1.44	0.64
1:H:165:ARG:N	1:H:166:PRO:HD2	2.12	0.64
1:C:20:GLY:N	1:C:21:GLY:HA3	2.12	0.64
1:D:299:PRO:C	1:D:301:GLY:N	2.56	0.64
1:B:199:PHE:CD2	1:B:200:TYR:N	2.65	0.64
1:E:158:ASP:O	1:E:161:PRO:HD3	1.97	0.64
1:G:68:LEU:HD12	1:G:145:LEU:HD13	1.80	0.64
1:G:150:ASP:HA	1:G:154:ALA:HB3	1.78	0.64
1:H:213:LEU:HD12	1:H:258:ASN:HB3	1.78	0.64
1:A:30:TYR:O	1:A:135:ASN:HA	1.98	0.64
1:C:231:LEU:O	1:C:231:LEU:HG	1.95	0.64
1:A:300:VAL:HB	1:B:199:PHE:HZ	1.62	0.64
1:C:18:SER:O	1:C:19:SER:HB2	1.98	0.64
1:H:51:PHE:HD1	1:H:277:ASN:HB3	1.61	0.64
1:H:271:ARG:HG2	1:H:271:ARG:NH1	2.07	0.64
1:A:61:ILE:HG22	1:A:65:LEU:HD22	1.80	0.64
1:H:42:PRO:CD	1:H:152:VAL:HG11	2.26	0.64
1:B:31:ARG:HD2	1:B:140:GLU:OE1	1.98	0.63
1:B:78:ASN:HD22	1:B:91:GLY:HA3	1.63	0.63
1:C:217:GLU:OE1	1:C:265:LYS:HE2	1.97	0.63
1:B:271:ARG:NH1	1:B:271:ARG:HG2	2.13	0.63
1:E:79:ALA:HB2	1:E:280:HIS:CE1	2.33	0.63
1:C:14:TYR:N	1:C:15:ASP:HA	2.12	0.63
1:F:31:ARG:NH1	1:F:140:GLU:OE2	2.31	0.63
1:B:93:ASP:HB3	1:B:280:HIS:ND1	2.13	0.63
1:B:162:ALA:HA	1:B:165:ARG:NE	2.12	0.63
1:D:25:ARG:HH12	1:D:29:GLN:HG2	1.64	0.63
1:F:38:PHE:HD1	1:F:38:PHE:O	1.79	0.63
1:E:68:LEU:HD12	1:E:68:LEU:N	2.13	0.63
1:F:7:GLY:HA2	1:F:8:VAL:O	1.97	0.63
1:A:249:ASN:OD1	1:B:301:GLY:HA3	1.99	0.63
1:C:61:ILE:HG22	1:C:65:LEU:HD22	1.81	0.63
1:D:172:ASN:HA	1:D:175:VAL:HG12	1.81	0.63
1:H:136:ASN:H	1:H:136:ASN:HD22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PHE:HD2	1:B:199:PHE:N	1.94	0.62
1:E:245:HIS:CE1	1:E:289:HIS:HD2	2.15	0.62
1:F:48:TYR:HB2	1:F:124:ILE:HB	1.79	0.62
1:E:295:THR:OG1	1:E:297:ILE:HG13	2.00	0.62
1:G:168:ILE:HG12	1:G:220:VAL:HG21	1.80	0.62
1:A:39:ARG:CZ	1:A:148:ALA:N	2.62	0.62
1:F:172:ASN:HD21	1:F:227:ALA:HA	1.64	0.62
1:G:197:GLU:OE2	1:H:115:THR:HG21	1.98	0.62
1:H:305:PRO:HB2	1:H:306:LEU:HD12	1.82	0.62
1:B:39:ARG:NH2	1:B:44:ARG:NE	2.46	0.62
1:F:87:THR:HG23	1:F:89:LEU:HG	1.80	0.62
1:G:245:HIS:HE1	1:G:289:HIS:CD2	2.17	0.62
1:C:191:THR:C	1:D:297:ILE:HD11	2.25	0.62
1:H:155:LEU:HB3	1:H:156:PRO:CD	2.25	0.62
1:C:44:ARG:HD3	1:C:45:TYR:CE2	2.33	0.62
1:C:48:TYR:HB2	1:C:124:ILE:HB	1.80	0.62
1:G:22:ARG:HD3	1:G:23:PHE:N	2.15	0.62
1:D:38:PHE:CD1	1:D:39:ARG:N	2.65	0.62
1:H:37:GLY:H	1:H:38:PHE:HB3	1.60	0.62
1:H:120:VAL:HG12	1:H:120:VAL:O	1.97	0.62
1:B:165:ARG:N	1:B:166:PRO:HD2	2.15	0.62
1:D:56:ALA:O	1:D:60:LEU:HD12	1.99	0.62
1:F:245:HIS:CE1	1:F:289:HIS:HD2	2.17	0.62
1:A:148:ALA:HA	1:A:150:ASP:H	1.65	0.61
1:F:37:GLY:CA	1:F:39:ARG:HG3	2.29	0.61
1:A:39:ARG:HH12	1:A:146:ASN:C	2.08	0.61
1:C:238:PHE:CD1	1:C:253:ILE:HG12	2.35	0.61
1:A:99:ILE:O	1:A:100:ASN:HB2	1.99	0.61
1:D:309:LEU:HD12	1:D:311:LEU:HD12	1.81	0.61
1:A:49:ALA:HB3	1:A:76:MET:CE	2.26	0.61
1:B:300:VAL:H	1:B:301:GLY:HA3	1.64	0.61
1:E:191:THR:HG22	1:E:193:GLU:H	1.64	0.61
1:F:3:LEU:HD13	1:F:24:VAL:HG11	1.81	0.61
1:G:31:ARG:CG	1:G:31:ARG:NH1	2.59	0.61
1:E:150:ASP:H	1:E:154:ALA:CB	2.12	0.61
1:F:25:ARG:HG2	1:F:27:GLU:HG2	1.83	0.61
1:F:37:GLY:HA2	1:F:39:ARG:N	2.10	0.61
1:G:37:GLY:HA2	1:G:38:PHE:CB	2.31	0.61
1:G:210:GLU:HB2	1:G:256:TYR:HD1	1.66	0.61
1:H:6:ASP:N	1:H:7:GLY:CA	2.64	0.61
1:H:164:PHE:C	1:H:166:PRO:HD2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.66	0.61
1:A:106:TYR:HA	1:A:120:VAL:HG11	1.83	0.60
1:A:165:ARG:N	1:A:166:PRO:HD2	2.15	0.60
1:B:176:TYR:HA	1:B:180:ASN:HB2	1.82	0.60
1:F:136:ASN:H	1:F:136:ASN:HD22	1.49	0.60
1:G:39:ARG:HA	1:G:39:ARG:CZ	2.30	0.60
1:H:98:SER:O	1:H:99:ILE:HG12	2.02	0.60
1:H:163:GLU:C	1:H:164:PHE:HD2	2.09	0.60
1:D:39:ARG:HD3	1:D:149:PHE:HA	1.82	0.60
1:D:97:ASP:OD2	1:D:100:ASN:HB2	2.00	0.60
1:F:37:GLY:C	1:F:39:ARG:H	2.09	0.60
1:G:132:ARG:HG3	1:G:132:ARG:HH11	1.66	0.60
1:G:213:LEU:HD21	1:G:219:LEU:CD2	2.29	0.60
1:C:172:ASN:ND2	2:C:407:HOH:O	2.33	0.60
1:D:71:MET:SD	1:D:149:PHE:CE2	2.95	0.60
1:D:5:ILE:HG22	1:D:6:ASP:H	1.67	0.60
1:D:39:ARG:CD	1:D:149:PHE:HA	2.31	0.60
1:B:38:PHE:CB	1:B:39:ARG:HA	2.27	0.60
1:E:87:THR:HG23	1:E:89:LEU:N	2.11	0.60
1:E:149:PHE:O	1:E:151:ASP:N	2.34	0.60
1:F:33:GLY:O	1:F:34:LEU:HB2	2.02	0.60
1:G:31:ARG:HH11	1:G:31:ARG:HG2	1.65	0.60
1:G:310:THR:O	1:G:311:LEU:HB2	2.01	0.60
1:C:5:ILE:HG23	1:C:6:ASP:H	1.63	0.60
1:E:37:GLY:HA2	1:E:38:PHE:CB	2.29	0.60
1:G:87:THR:HG23	1:G:89:LEU:HG	1.84	0.60
1:D:39:ARG:HH11	1:D:149:PHE:HB2	1.65	0.60
1:G:210:GLU:CD	1:G:258:ASN:HB2	2.26	0.60
1:D:39:ARG:CZ	1:D:149:PHE:CD1	2.84	0.59
1:D:211:GLU:O	1:D:214:THR:HB	2.01	0.59
1:C:200:TYR:OH	1:D:300:VAL:CG2	2.50	0.59
1:C:271:ARG:HH11	1:C:271:ARG:HG2	1.67	0.59
1:C:152:VAL:CG1	1:C:153:GLY:N	2.40	0.59
1:D:229:ILE:O	1:D:233:PRO:HD3	2.01	0.59
1:F:99:ILE:O	1:F:99:ILE:CD1	2.47	0.59
1:B:95:VAL:O	1:B:95:VAL:HG22	2.01	0.59
1:B:202:LEU:HD12	1:B:202:LEU:C	2.27	0.59
1:E:163:GLU:HG2	1:E:164:PHE:CE1	2.38	0.59
1:G:37:GLY:HA2	1:G:38:PHE:CG	2.38	0.59
1:A:231:LEU:HG	1:A:235:LEU:HD22	1.83	0.59
1:B:93:ASP:O	1:B:93:ASP:OD2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:CZ2	1:B:265:LYS:HD3	2.37	0.59
1:C:39:ARG:HG2	1:C:44:ARG:NH1	2.16	0.59
1:C:192:GLN:HA	1:D:297:ILE:HG12	1.84	0.59
1:H:56:ALA:HA	1:H:123:PRO:HD3	1.84	0.59
1:F:2:GLY:O	1:F:3:LEU:HD23	2.03	0.59
1:D:178:THR:O	1:D:202:LEU:HB2	2.02	0.59
1:E:213:LEU:HD21	1:E:219:LEU:HD23	1.85	0.59
1:D:39:ARG:NH1	1:D:149:PHE:HB2	2.17	0.59
1:C:38:PHE:O	1:C:39:ARG:O	2.20	0.58
1:D:202:LEU:C	1:D:202:LEU:CD1	2.76	0.58
1:A:300:VAL:HB	1:B:199:PHE:CE1	2.38	0.58
1:C:282:LYS:NZ	1:C:301:GLY:HA3	2.18	0.58
1:C:295:THR:HG23	2:C:405:HOH:O	2.02	0.58
1:G:132:ARG:HG3	1:G:132:ARG:NH1	2.17	0.58
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.85	0.58
1:C:12:ALA:HB1	1:E:13:TRP:CE3	2.38	0.58
1:E:15:ASP:O	1:E:15:ASP:CG	2.46	0.58
1:A:39:ARG:CG	1:A:148:ALA:O	2.48	0.58
1:C:97:ASP:OD1	1:C:102:ALA:HB3	2.04	0.58
1:E:3:LEU:HD13	1:E:24:VAL:HG11	1.84	0.58
1:H:40:GLY:CA	1:H:149:PHE:CE1	2.86	0.58
1:C:179:LEU:HD12	1:C:202:LEU:CD2	2.33	0.58
1:E:70:GLU:N	1:E:70:GLU:CD	2.62	0.58
1:F:5:ILE:C	1:F:7:GLY:N	2.60	0.58
1:H:34:LEU:N	1:H:144:ILE:HD11	2.11	0.58
1:H:42:PRO:HB3	1:H:71:MET:HG3	1.86	0.58
1:H:137:GLU:HB3	1:H:140:GLU:HG3	1.84	0.58
1:H:304:GLN:NE2	1:H:304:GLN:N	2.51	0.58
1:E:67:GLY:O	1:E:69:GLU:N	2.35	0.58
1:G:22:ARG:HG2	1:H:185:ARG:NH2	2.18	0.58
1:H:136:ASN:HD22	1:H:136:ASN:N	1.99	0.58
1:B:6:ASP:N	1:B:7:GLY:CA	2.67	0.58
1:C:63:ARG:HG2	1:C:63:ARG:NH1	2.10	0.58
1:E:66:LYS:O	1:E:68:LEU:N	2.32	0.58
1:F:36:ALA:C	1:F:38:PHE:CB	2.77	0.58
1:A:143:ARG:CG	1:A:143:ARG:NH1	2.47	0.58
1:D:68:LEU:HD22	1:D:149:PHE:CD1	2.39	0.58
1:E:282:LYS:HZ1	1:E:301:GLY:HA3	1.65	0.58
1:F:42:PRO:HD3	1:F:152:VAL:HG11	1.86	0.58
1:H:47:LEU:C	1:H:47:LEU:HD22	2.28	0.58
1:A:87:THR:OG1	1:A:89:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PHE:CD2	1:B:199:PHE:N	2.65	0.58
1:D:4:LEU:HD22	1:D:7:GLY:HA2	1.86	0.57
1:D:219:LEU:HB2	1:D:228:ASP:OD2	2.04	0.57
1:E:286:TYR:HB2	1:E:298:VAL:HG22	1.86	0.57
1:F:30:TYR:H	1:F:136:ASN:ND2	2.02	0.57
1:G:140:GLU:O	1:G:144:ILE:HG13	2.04	0.57
1:D:15:ASP:O	1:D:17:LYS:N	2.37	0.57
1:F:119:ARG:HG3	1:F:119:ARG:NH1	1.97	0.57
1:D:30:TYR:O	1:D:135:ASN:HA	2.05	0.57
1:G:7:GLY:CA	1:G:8:VAL:CB	2.82	0.57
1:C:309:LEU:HD22	1:C:310:THR:H	1.70	0.57
1:E:38:PHE:HD1	1:E:39:ARG:H	1.51	0.57
1:H:67:GLY:O	1:H:69:GLU:N	2.38	0.57
1:A:13:TRP:C	1:A:15:ASP:HA	2.28	0.57
1:E:62:MET:HB2	1:E:142:ILE:HD11	1.87	0.57
1:E:210:GLU:CD	1:E:258:ASN:HB2	2.29	0.57
1:H:168:ILE:HG12	1:H:220:VAL:HG21	1.86	0.57
1:B:152:VAL:CG1	1:B:152:VAL:O	2.52	0.57
1:A:39:ARG:HH12	1:A:146:ASN:N	2.03	0.57
1:A:109:TYR:CD1	1:A:120:VAL:HG13	2.39	0.57
1:E:92:ASP:N	1:E:92:ASP:OD1	2.37	0.57
1:E:107:GLN:O	1:E:110:THR:HG22	2.04	0.57
1:C:47:LEU:HB3	1:C:74:VAL:HG12	1.87	0.57
1:B:217:GLU:OE1	1:B:311:LEU:HD21	2.05	0.57
1:D:113:ASP:OD1	1:D:113:ASP:C	2.48	0.57
1:D:136:ASN:C	1:D:136:ASN:ND2	2.42	0.57
1:G:216:ARG:HH11	1:G:216:ARG:CG	2.16	0.57
1:A:245:HIS:CE1	1:A:289:HIS:CD2	2.79	0.57
1:C:172:ASN:HD21	1:C:227:ALA:HA	1.70	0.57
1:C:224:LEU:HD12	1:C:225:THR:N	2.20	0.57
1:A:162:ALA:HA	1:A:165:ARG:HG3	1.87	0.56
1:C:167:GLU:HG3	1:C:170:ARG:NH1	2.20	0.56
1:B:39:ARG:CZ	1:B:41:GLU:CD	2.79	0.56
1:D:97:ASP:C	1:D:98:SER:O	2.47	0.56
1:D:149:PHE:O	1:D:154:ALA:HB2	2.05	0.56
1:E:61:ILE:HD13	1:E:272:VAL:HG13	1.86	0.56
1:E:300:VAL:CG1	1:E:300:VAL:O	2.54	0.56
1:E:307:PRO:CG	1:E:308:GLY:H	2.16	0.56
1:F:224:LEU:HD12	1:F:224:LEU:C	2.30	0.56
1:G:61:ILE:HG23	1:G:272:VAL:HG22	1.85	0.56
1:B:78:ASN:HD21	1:B:91:GLY:HA3	1.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HD21	1:C:106:TYR:HB2	1.87	0.56
1:D:39:ARG:NH1	1:D:149:PHE:CG	2.73	0.56
1:E:229:ILE:O	1:E:233:PRO:HD3	2.05	0.56
1:F:7:GLY:HA2	1:F:8:VAL:C	2.30	0.56
1:F:34:LEU:O	1:F:35:ASP:CG	2.48	0.56
1:F:68:LEU:HD21	1:F:154:ALA:HB2	1.87	0.56
1:G:30:TYR:H	1:G:136:ASN:HD21	1.54	0.56
1:G:39:ARG:HA	1:G:39:ARG:HE	1.65	0.56
1:G:110:THR:HG22	1:G:111:ALA:N	2.20	0.56
1:H:59:VAL:HG11	1:H:141:ILE:CG2	2.35	0.56
1:E:160:TYR:CE1	1:E:165:ARG:HG3	2.39	0.56
1:C:201:PRO:O	1:C:202:LEU:C	2.49	0.56
1:H:81:MET:HB3	1:H:288:SER:HB2	1.86	0.56
1:H:213:LEU:HD23	1:H:219:LEU:HD23	1.87	0.56
1:A:19:SER:H	1:A:20:GLY:CA	2.13	0.56
1:E:245:HIS:HE1	1:E:289:HIS:CD2	2.16	0.56
1:F:36:ALA:O	1:F:38:PHE:HB3	2.04	0.56
1:F:143:ARG:O	1:F:146:ASN:HB3	2.04	0.56
1:G:31:ARG:NH1	1:G:31:ARG:HG2	2.20	0.56
1:B:23:PHE:O	1:B:23:PHE:CD2	2.59	0.56
1:B:106:TYR:HA	1:B:120:VAL:HG11	1.88	0.56
1:D:44:ARG:HG2	1:D:45:TYR:CE2	2.40	0.56
1:E:160:TYR:CZ	1:E:165:ARG:HG3	2.40	0.56
1:B:122:ILE:HB	1:B:123:PRO:HA	1.87	0.56
1:H:67:GLY:C	1:H:69:GLU:H	2.14	0.56
1:C:87:THR:HG22	1:C:89:LEU:H	1.69	0.56
1:D:282:LYS:HZ3	1:D:301:GLY:HA3	1.71	0.56
1:G:2:GLY:HA3	1:G:11:ASP:HA	1.88	0.56
1:H:22:ARG:HB2	1:H:23:PHE:HA	1.88	0.56
1:H:91:GLY:O	1:H:94:VAL:CG2	2.52	0.56
1:A:147:SER:O	1:A:150:ASP:CG	2.49	0.55
1:A:159:TYR:HE1	1:A:224:LEU:HD23	1.71	0.55
1:D:2:GLY:HA3	1:D:9:TRP:CZ2	2.41	0.55
1:E:26:LYS:HD3	1:E:26:LYS:C	2.31	0.55
1:F:97:ASP:OD2	1:F:100:ASN:HB3	2.05	0.55
1:H:172:ASN:ND2	1:H:230:ARG:HE	2.04	0.55
1:A:192:GLN:O	1:A:196:GLU:HG3	2.06	0.55
1:A:299:PRO:O	1:A:301:GLY:N	2.39	0.55
1:D:172:ASN:HD21	1:D:227:ALA:HA	1.69	0.55
1:A:98:SER:O	1:A:99:ILE:HG13	2.05	0.55
1:A:271:ARG:HH11	1:A:271:ARG:HG2	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLN:HA	1:A:304:GLN:HE21	1.72	0.55
1:D:14:TYR:CD1	1:D:26:LYS:HE2	2.41	0.55
1:D:286:TYR:CZ	1:D:299:PRO:HG2	2.42	0.55
1:E:191:THR:HG22	1:E:194:ALA:H	1.71	0.55
1:G:167:GLU:CG	1:G:170:ARG:HH12	2.14	0.55
1:C:27:GLU:OE1	1:C:28:SER:HB3	2.06	0.55
1:C:298:VAL:O	1:D:192:GLN:NE2	2.39	0.55
1:D:87:THR:CG2	1:D:88:PHE:N	2.69	0.55
1:E:282:LYS:HZ2	1:E:301:GLY:HA3	1.68	0.55
1:F:79:ALA:HB2	1:F:280:HIS:CE1	2.41	0.55
1:A:284:HIS:O	1:A:288:SER:HB2	2.06	0.55
1:C:136:ASN:HD22	1:C:136:ASN:N	1.94	0.55
1:E:99:ILE:C	1:E:99:ILE:HD13	2.31	0.55
1:H:182:GLY:O	1:H:183:VAL:C	2.49	0.55
1:D:81:MET:HE3	1:D:86:TRP:CD2	2.42	0.55
1:E:16:THR:O	1:E:17:LYS:HB2	2.07	0.55
1:G:59:VAL:HG21	1:G:141:ILE:HG21	1.87	0.55
1:G:136:ASN:HD22	1:G:136:ASN:N	2.00	0.55
1:G:213:LEU:CD1	1:G:259:LEU:HD23	2.36	0.55
1:A:74:VAL:HG13	1:A:76:MET:HE3	1.89	0.55
1:A:199:PHE:O	1:A:202:LEU:HB3	2.07	0.55
1:A:282:LYS:HE2	1:A:301:GLY:CA	2.35	0.55
1:B:89:LEU:HB3	1:B:90:PRO:HD2	1.89	0.55
1:C:240:ALA:HB1	1:C:282:LYS:HD2	1.89	0.55
1:A:39:ARG:HD3	1:A:148:ALA:N	2.21	0.55
1:D:2:GLY:O	1:D:3:LEU:HD23	2.07	0.55
1:D:44:ARG:HD3	1:D:129:VAL:HG21	1.89	0.55
1:H:5:ILE:CG2	1:H:6:ASP:N	2.69	0.55
1:E:160:TYR:N	1:E:161:PRO:HD3	2.22	0.55
1:F:58:ARG:HD2	1:F:138:SER:OG	2.07	0.55
1:A:44:ARG:O	1:A:128:LYS:HG3	2.07	0.54
1:B:93:ASP:C	1:B:94:VAL:HG22	2.32	0.54
1:C:59:VAL:HA	1:C:142:ILE:HD11	1.88	0.54
1:D:241:ILE:CG1	1:D:282:LYS:HG2	2.38	0.54
1:G:312:GLN:HG2	1:G:313:SER:H	1.72	0.54
1:H:68:LEU:HD12	1:H:68:LEU:H	1.71	0.54
1:H:160:TYR:N	1:H:161:PRO:CD	2.70	0.54
1:H:162:ALA:HA	1:H:165:ARG:CD	2.37	0.54
1:A:170:ARG:HG3	1:A:170:ARG:NH1	2.20	0.54
1:C:245:HIS:NE2	1:C:289:HIS:HD2	2.05	0.54
1:C:282:LYS:HZ2	1:C:301:GLY:HA3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LEU:HD23	1:D:145:LEU:N	2.22	0.54
1:E:115:THR:O	1:E:116:TYR:C	2.50	0.54
1:F:78:ASN:HD21	1:F:91:GLY:HA3	1.72	0.54
1:H:63:ARG:O	1:H:65:LEU:N	2.35	0.54
1:D:270:GLU:O	1:D:271:ARG:CB	2.54	0.54
1:E:62:MET:HE2	1:E:142:ILE:HD12	1.88	0.54
1:G:44:ARG:HG3	1:G:129:VAL:HG23	1.90	0.54
1:H:30:TYR:H	1:H:136:ASN:HD21	1.55	0.54
1:H:57:HIS:CD2	1:H:237:ARG:HH22	2.25	0.54
1:B:76:MET:HB2	1:B:94:VAL:HB	1.89	0.54
1:C:13:TRP:HE1	1:E:13:TRP:HA	1.73	0.54
1:D:231:LEU:HG	1:D:231:LEU:O	2.05	0.54
1:C:299:PRO:HG3	1:D:247:LYS:HD3	1.90	0.54
1:D:47:LEU:HD22	1:D:48:TYR:N	2.22	0.54
1:H:164:PHE:HE1	1:H:221:GLY:HA3	1.72	0.54
1:H:268:SER:O	1:H:269:HIS:C	2.51	0.54
1:C:26:LYS:HB2	1:C:27:GLU:OE2	2.07	0.54
1:C:265:LYS:CA	1:C:310:THR:HG21	2.36	0.54
1:D:282:LYS:HZ2	1:D:301:GLY:HA3	1.73	0.54
1:E:13:TRP:HZ2	1:E:17:LYS:HZ2	1.55	0.54
1:H:256:TYR:HB3	1:H:259:LEU:HB2	1.90	0.54
1:H:282:LYS:NZ	1:H:301:GLY:CA	2.71	0.54
1:C:162:ALA:HA	1:C:165:ARG:CD	2.38	0.54
1:E:44:ARG:HG2	1:E:129:VAL:HG23	1.89	0.54
1:E:286:TYR:CZ	1:E:299:PRO:HG2	2.43	0.54
1:H:271:ARG:CG	1:H:271:ARG:NH1	2.58	0.54
1:A:160:TYR:N	1:A:161:PRO:HD3	2.22	0.54
1:C:19:SER:HB3	1:C:20:GLY:HA3	1.89	0.54
1:C:27:GLU:OE1	1:C:28:SER:N	2.41	0.54
1:H:299:PRO:C	1:H:301:GLY:N	2.66	0.54
1:A:39:ARG:NE	1:A:149:PHE:N	2.46	0.54
1:B:178:THR:O	1:B:202:LEU:HB2	2.08	0.54
1:C:167:GLU:HG3	1:C:170:ARG:HH11	1.73	0.54
1:D:150:ASP:O	1:D:152:VAL:N	2.39	0.54
1:E:37:GLY:CA	1:E:38:PHE:CD2	2.91	0.54
1:E:62:MET:HB2	1:E:142:ILE:CD1	2.37	0.54
1:E:66:LYS:HD2	1:E:146:ASN:HA	1.90	0.54
1:D:210:GLU:OE2	1:D:257:PRO:HG2	2.08	0.54
1:G:58:ARG:HD2	1:G:138:SER:OG	2.08	0.54
1:A:136:ASN:N	1:A:136:ASN:HD22	2.07	0.53
1:B:32:GLY:HA3	1:B:134:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TRP:CD1	1:D:126:TRP:C	2.85	0.53
1:D:159:TYR:HD1	1:D:224:LEU:O	1.92	0.53
1:E:208:TRP:O	1:E:209:LEU:C	2.50	0.53
1:F:256:TYR:O	1:F:260:SER:HB2	2.08	0.53
1:B:232:PHE:HB3	1:B:233:PRO:HD3	1.90	0.53
1:E:13:TRP:NE1	1:E:16:THR:HG22	2.23	0.53
1:G:210:GLU:OE1	1:G:256:TYR:HB3	2.08	0.53
1:A:39:ARG:NH2	1:A:149:PHE:N	2.47	0.53
1:F:30:TYR:O	1:F:135:ASN:HA	2.09	0.53
1:B:286:TYR:HB2	1:B:298:VAL:HG22	1.90	0.53
1:D:268:SER:HB2	1:D:309:LEU:HD22	1.89	0.53
1:E:160:TYR:N	1:E:161:PRO:CD	2.71	0.53
1:F:78:ASN:ND2	1:F:91:GLY:HA3	2.24	0.53
1:A:151:ASP:HB3	1:A:152:VAL:HG13	1.89	0.53
1:D:71:MET:HE1	1:D:153:GLY:HA3	1.90	0.53
1:E:150:ASP:CA	1:E:154:ALA:HB3	2.39	0.53
1:C:87:THR:CG2	1:C:89:LEU:HG	2.35	0.53
1:D:191:THR:O	1:D:192:GLN:C	2.50	0.53
1:G:312:GLN:HG2	1:G:313:SER:N	2.23	0.53
1:A:269:HIS:C	1:A:270:GLU:O	2.44	0.53
1:C:16:THR:HG22	1:C:18:SER:H	1.74	0.53
1:G:299:PRO:C	1:G:301:GLY:N	2.66	0.53
1:A:97:ASP:OD2	1:A:100:ASN:HB3	2.08	0.53
1:B:269:HIS:ND1	1:B:270:GLU:O	2.35	0.53
1:F:70:GLU:CD	1:F:70:GLU:H	2.16	0.53
1:G:31:ARG:NH1	1:G:140:GLU:OE2	2.41	0.53
1:A:39:ARG:CD	1:A:148:ALA:N	2.72	0.53
1:B:38:PHE:CB	1:B:39:ARG:O	2.52	0.53
1:B:93:ASP:CB	1:B:280:HIS:ND1	2.72	0.53
1:B:268:SER:CB	1:B:309:LEU:HG	2.39	0.53
1:C:251:ARG:NH2	2:C:401:HOH:O	2.19	0.53
1:H:66:LYS:C	1:H:68:LEU:HD12	2.34	0.53
1:H:97:ASP:O	1:H:101:GLY:HA2	2.09	0.53
1:E:210:GLU:OE2	1:E:258:ASN:HB2	2.08	0.53
1:H:226:GLU:O	1:H:230:ARG:HG3	2.08	0.53
1:B:44:ARG:NH1	1:B:45:TYR:OH	2.41	0.52
1:C:23:PHE:CD2	1:E:27:GLU:HB3	2.44	0.52
1:D:15:ASP:C	1:D:17:LYS:N	2.63	0.52
1:D:150:ASP:C	1:D:152:VAL:H	2.17	0.52
1:H:213:LEU:CD1	1:H:258:ASN:HB3	2.39	0.52
1:C:20:GLY:HA2	1:E:184:TYR:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ASP:O	1:E:36:ALA:C	2.52	0.52
1:E:172:ASN:HD21	1:E:227:ALA:HA	1.73	0.52
1:G:34:LEU:HD21	1:G:140:GLU:OE1	2.08	0.52
1:D:98:SER:O	1:D:100:ASN:N	2.42	0.52
1:D:136:ASN:ND2	1:D:136:ASN:O	2.42	0.52
1:E:142:ILE:HD13	1:E:142:ILE:O	2.10	0.52
1:G:213:LEU:CD2	1:G:219:LEU:HD23	2.34	0.52
1:C:25:ARG:CZ	1:C:29:GLN:HG2	2.40	0.52
1:F:60:LEU:HD21	1:F:76:MET:HE1	1.92	0.52
1:F:299:PRO:C	1:F:301:GLY:N	2.68	0.52
1:A:172:ASN:HD21	1:A:227:ALA:HA	1.75	0.52
1:C:23:PHE:HD1	1:C:23:PHE:O	1.93	0.52
1:D:44:ARG:HD3	1:D:129:VAL:CG2	2.38	0.52
1:D:66:LYS:HE3	1:D:146:ASN:HA	1.91	0.52
1:E:97:ASP:CB	1:E:102:ALA:HB3	2.39	0.52
1:H:81:MET:H	1:H:288:SER:HB3	1.74	0.52
1:A:35:ASP:O	1:A:36:ALA:C	2.52	0.52
1:A:282:LYS:CE	1:A:301:GLY:HA3	2.40	0.52
1:B:59:VAL:CG1	1:B:123:PRO:HG3	2.39	0.52
1:E:34:LEU:HD11	1:E:140:GLU:HB3	1.92	0.52
1:F:214:THR:HA	1:F:258:ASN:HD21	1.73	0.52
1:A:5:ILE:HG21	1:A:10:ARG:NH1	2.19	0.52
1:A:136:ASN:HD22	1:A:136:ASN:H	1.56	0.52
1:D:25:ARG:NH1	1:D:29:GLN:HG2	2.25	0.52
1:E:308:GLY:O	1:E:309:LEU:HG	2.10	0.52
1:G:238:PHE:CD1	1:G:253:ILE:HG12	2.44	0.52
1:H:63:ARG:C	1:H:65:LEU:H	2.18	0.52
1:H:81:MET:HB3	1:H:288:SER:CB	2.39	0.52
1:C:286:TYR:CE2	1:C:299:PRO:HD2	2.45	0.52
1:D:143:ARG:CG	1:D:143:ARG:NH1	2.54	0.52
1:H:97:ASP:HB3	1:H:102:ALA:H	1.75	0.52
1:B:94:VAL:HG12	1:B:95:VAL:HG12	1.92	0.52
1:B:231:LEU:HG	1:B:235:LEU:HD22	1.91	0.52
1:D:14:TYR:O	1:D:14:TYR:CG	2.63	0.52
1:D:230:ARG:O	1:D:233:PRO:HD2	2.10	0.52
1:H:4:LEU:HD12	1:H:116:TYR:CD2	2.45	0.52
1:H:266:LEU:O	1:H:272:VAL:HG21	2.09	0.52
1:D:269:HIS:CE1	1:D:271:ARG:HB2	2.46	0.52
1:E:71:MET:HE1	1:E:153:GLY:C	2.35	0.52
1:F:37:GLY:N	1:F:38:PHE:HB3	2.25	0.52
1:G:282:LYS:NZ	1:G:301:GLY:HA3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TYR:H	1:B:136:ASN:HD21	1.58	0.51
1:E:224:LEU:HD12	1:E:224:LEU:C	2.34	0.51
1:C:10:ARG:HG2	1:C:15:ASP:CG	2.34	0.51
1:D:135:ASN:HD21	1:D:140:GLU:HB2	1.74	0.51
1:F:59:VAL:HA	1:F:142:ILE:HD11	1.92	0.51
1:H:31:ARG:HG3	1:H:140:GLU:OE1	2.10	0.51
1:A:160:TYR:CE2	1:A:165:ARG:HD3	2.45	0.51
1:C:162:ALA:HA	1:C:165:ARG:HD2	1.92	0.51
1:G:203:PHE:CE1	1:G:250:LEU:HB3	2.46	0.51
1:H:47:LEU:HD22	1:H:48:TYR:N	2.25	0.51
1:C:179:LEU:HD12	1:C:202:LEU:HD21	1.92	0.51
1:E:214:THR:HG23	1:E:258:ASN:HD21	1.75	0.51
1:G:240:ALA:HA	1:G:302:PRO:HG2	1.92	0.51
1:H:56:ALA:CA	1:H:123:PRO:HD3	2.39	0.51
1:E:31:ARG:HH12	1:E:137:GLU:HG2	1.75	0.51
1:E:149:PHE:HB3	1:E:154:ALA:HB2	1.93	0.51
1:E:232:PHE:N	1:E:233:PRO:HD2	2.26	0.51
1:F:300:VAL:HG13	1:F:300:VAL:O	2.09	0.51
1:H:164:PHE:CE1	1:H:221:GLY:HA3	2.45	0.51
1:A:68:LEU:HD12	1:A:145:LEU:HD13	1.92	0.51
1:F:162:ALA:HA	1:F:165:ARG:NE	2.26	0.51
1:H:51:PHE:CE2	1:H:76:MET:HE3	2.45	0.51
1:D:269:HIS:CE1	1:D:270:GLU:O	2.63	0.51
1:F:47:LEU:HB3	1:F:74:VAL:HG12	1.92	0.51
1:F:163:GLU:HB2	1:F:164:PHE:CD1	2.45	0.51
1:G:176:TYR:CD1	1:G:176:TYR:C	2.88	0.51
1:A:161:PRO:HB2	1:A:164:PHE:HD1	1.76	0.51
1:C:44:ARG:HG3	1:C:129:VAL:HG23	1.93	0.51
1:D:176:TYR:C	1:D:176:TYR:CD2	2.89	0.51
1:E:31:ARG:NH1	1:E:137:GLU:HG2	2.25	0.51
1:E:202:LEU:HD12	1:E:203:PHE:N	2.25	0.51
1:F:7:GLY:HA2	1:F:8:VAL:CB	2.41	0.51
1:G:3:LEU:CD1	1:G:3:LEU:C	2.84	0.51
1:G:31:ARG:HG3	1:G:140:GLU:OE1	2.10	0.51
1:H:37:GLY:C	1:H:39:ARG:N	2.60	0.51
1:A:210:GLU:CD	1:A:258:ASN:HB2	2.35	0.51
1:B:191:THR:CG2	1:B:194:ALA:H	2.21	0.51
1:D:257:PRO:HG2	1:D:258:ASN:H	1.76	0.51
1:B:90:PRO:O	1:B:91:GLY:C	2.55	0.50
1:B:258:ASN:CG	1:B:261:ARG:HH21	2.19	0.50
1:C:37:GLY:HA2	1:C:38:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:LYS:HG2	1:F:299:PRO:HB3	1.93	0.50
1:H:137:GLU:HG3	1:H:139:SER:OG	2.10	0.50
1:A:2:GLY:HA3	1:A:9:TRP:CZ2	2.47	0.50
1:B:179:LEU:CD1	1:B:202:LEU:HD13	2.42	0.50
1:B:186:SER:OG	1:B:199:PHE:HB3	2.10	0.50
1:C:286:TYR:O	1:C:296:GLY:HA2	2.11	0.50
1:G:176:TYR:HE1	1:G:181:ASN:ND2	2.09	0.50
1:C:26:LYS:C	1:C:27:GLU:HG3	2.37	0.50
1:D:41:GLU:HA	1:D:152:VAL:HG11	1.94	0.50
1:G:205:THR:HG22	1:G:209:LEU:HD23	1.93	0.50
1:H:127:ASP:OD1	1:H:130:GLU:HG3	2.11	0.50
1:C:42:PRO:CG	1:C:152:VAL:HG11	2.37	0.50
1:D:149:PHE:O	1:D:149:PHE:CD2	2.64	0.50
1:E:68:LEU:HD12	1:E:68:LEU:H	1.76	0.50
1:F:37:GLY:C	1:F:39:ARG:N	2.69	0.50
1:H:178:THR:O	1:H:182:GLY:HA3	2.11	0.50
1:H:277:ASN:C	1:H:277:ASN:OD1	2.54	0.50
1:C:5:ILE:HG13	1:C:22:ARG:HD2	1.93	0.50
1:D:3:LEU:HD13	1:D:24:VAL:HG11	1.94	0.50
1:E:165:ARG:N	1:E:166:PRO:HD2	2.26	0.50
1:E:177:GLU:O	1:E:177:GLU:HG2	2.11	0.50
1:H:80:TYR:CE2	1:H:82:GLY:HA3	2.46	0.50
1:H:211:GLU:O	1:H:214:THR:HB	2.10	0.50
1:A:37:GLY:CA	1:A:38:PHE:CB	2.61	0.50
1:D:44:ARG:HG2	1:D:45:TYR:CZ	2.46	0.50
1:D:184:TYR:O	1:D:185:ARG:C	2.54	0.50
1:D:210:GLU:OE2	1:D:257:PRO:HD2	2.12	0.50
1:F:161:PRO:HB3	1:F:223:ARG:NH2	2.26	0.50
1:F:265:LYS:HB2	1:F:309:LEU:HD13	1.93	0.50
1:H:166:PRO:HG2	1:H:167:GLU:N	2.23	0.50
1:H:166:PRO:CG	1:H:167:GLU:H	2.20	0.50
1:H:232:PHE:O	1:H:236:VAL:HG12	2.12	0.50
1:C:63:ARG:HH11	1:C:63:ARG:CG	2.17	0.50
1:F:37:GLY:N	1:F:38:PHE:CB	2.75	0.50
1:H:22:ARG:HH11	1:H:23:PHE:HD2	1.60	0.50
1:H:282:LYS:HZ2	1:H:301:GLY:HA3	1.77	0.50
1:E:107:GLN:HA	1:E:110:THR:CG2	2.41	0.50
1:E:243:HIS:CD2	1:E:249:ASN:HA	2.47	0.50
1:F:78:ASN:HB2	1:F:87:THR:HG22	1.92	0.50
1:A:79:ALA:HB2	1:A:280:HIS:CE1	2.46	0.50
1:E:36:ALA:O	1:E:37:GLY:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ILE:HG13	1:E:220:VAL:HG11	1.94	0.50
1:H:44:ARG:HH11	1:H:129:VAL:HB	1.76	0.50
1:H:163:GLU:C	1:H:164:PHE:CD2	2.90	0.50
1:B:71:MET:HE1	1:B:153:GLY:CA	2.41	0.49
1:D:122:ILE:HB	1:D:123:PRO:CA	2.39	0.49
1:E:42:PRO:HA	1:E:71:MET:HB3	1.93	0.49
1:H:59:VAL:HG11	1:H:141:ILE:HG21	1.93	0.49
1:H:172:ASN:CB	1:H:230:ARG:HH21	2.24	0.49
1:D:269:HIS:CE1	1:D:271:ARG:CB	2.95	0.49
1:F:90:PRO:O	1:F:91:GLY:O	2.31	0.49
1:A:17:LYS:C	1:A:21:GLY:HA3	2.37	0.49
1:C:2:GLY:N	1:E:19:SER:CB	2.75	0.49
1:C:226:GLU:O	1:C:230:ARG:HG2	2.12	0.49
1:E:44:ARG:CG	1:E:129:VAL:HG23	2.41	0.49
1:E:208:TRP:O	1:E:211:GLU:N	2.46	0.49
1:G:24:VAL:HG23	1:H:26:LYS:HD3	1.94	0.49
1:H:231:LEU:HD11	1:H:235:LEU:CD2	2.42	0.49
1:C:16:THR:HG22	1:C:18:SER:N	2.27	0.49
1:C:272:VAL:O	1:C:275:THR:HG23	2.12	0.49
1:D:167:GLU:HG2	1:D:171:ILE:HD12	1.94	0.49
1:B:231:LEU:HG	1:B:235:LEU:CD2	2.43	0.49
1:D:34:LEU:O	1:D:36:ALA:N	2.46	0.49
1:E:150:ASP:HA	1:E:154:ALA:HB3	1.93	0.49
1:E:273:ALA:HB3	1:E:274:PRO:HD3	1.93	0.49
1:A:294:PRO:HG3	1:B:294:PRO:HG3	1.94	0.49
1:D:152:VAL:HG12	1:D:152:VAL:O	2.12	0.49
1:E:67:GLY:O	1:E:69:GLU:HG2	2.12	0.49
1:G:235:LEU:HB3	1:G:263:VAL:CG2	2.42	0.49
1:H:49:ALA:O	1:H:77:VAL:HG22	2.12	0.49
1:A:106:TYR:CA	1:A:120:VAL:HG11	2.42	0.49
1:B:190:THR:HG23	1:D:6:ASP:OD1	2.12	0.49
1:D:162:ALA:HB2	1:D:165:ARG:CZ	2.43	0.49
1:H:142:ILE:HD11	1:H:226:GLU:HB2	1.95	0.49
1:H:143:ARG:NH1	1:H:160:TYR:CZ	2.81	0.49
1:A:138:SER:O	1:A:139:SER:C	2.55	0.49
1:A:218:TRP:CZ3	1:A:224:LEU:HD13	2.48	0.49
1:C:106:TYR:CD1	1:C:106:TYR:C	2.91	0.49
1:D:66:LYS:C	1:D:68:LEU:H	2.20	0.49
1:G:109:TYR:CD1	1:G:120:VAL:HG13	2.47	0.49
1:A:178:THR:O	1:A:202:LEU:HD22	2.13	0.49
1:B:295:THR:OG1	1:B:297:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ARG:HD2	1:C:140:GLU:OE1	2.13	0.49
1:E:98:SER:O	1:E:99:ILE:HG22	2.13	0.49
1:F:160:TYR:CE1	1:F:165:ARG:HG2	2.48	0.49
1:H:271:ARG:HH11	1:H:271:ARG:CB	2.25	0.49
1:A:143:ARG:NH1	1:A:226:GLU:OE1	2.45	0.48
1:F:218:TRP:CZ2	1:F:265:LYS:HD3	2.48	0.48
1:H:20:GLY:HA3	1:H:22:ARG:N	2.20	0.48
1:H:63:ARG:HH11	1:H:63:ARG:CG	2.16	0.48
1:A:14:TYR:CG	1:A:14:TYR:O	2.67	0.48
1:C:37:GLY:CA	1:C:38:PHE:HB3	2.42	0.48
1:D:243:HIS:CD2	1:D:249:ASN:HA	2.48	0.48
1:F:273:ALA:N	1:F:274:PRO:HD2	2.28	0.48
1:B:33:GLY:O	1:B:34:LEU:HB2	2.12	0.48
1:C:42:PRO:HD3	1:C:152:VAL:HG21	1.95	0.48
1:C:136:ASN:H	1:C:136:ASN:ND2	2.06	0.48
1:E:97:ASP:OD2	1:E:102:ALA:HB3	2.13	0.48
1:F:220:VAL:CG1	1:F:221:GLY:N	2.74	0.48
1:G:237:ARG:HG3	1:G:237:ARG:HH11	1.78	0.48
1:C:25:ARG:O	1:C:27:GLU:N	2.45	0.48
1:F:42:PRO:HD3	1:F:152:VAL:CG1	2.44	0.48
1:A:31:ARG:NH1	1:A:140:GLU:OE2	2.46	0.48
1:D:66:LYS:HB2	1:D:68:LEU:HG	1.95	0.48
1:E:183:VAL:HG21	1:E:242:TYR:CE2	2.48	0.48
1:E:263:VAL:HG12	1:E:264:GLY:N	2.29	0.48
1:F:6:ASP:HA	1:F:115:THR:O	2.14	0.48
1:F:47:LEU:C	1:F:47:LEU:CD2	2.87	0.48
1:H:92:ASP:OD1	1:H:92:ASP:N	2.36	0.48
1:H:231:LEU:HD11	1:H:235:LEU:HD22	1.96	0.48
1:E:202:LEU:C	1:E:202:LEU:CD1	2.79	0.48
1:F:34:LEU:O	1:F:35:ASP:HB3	2.13	0.48
1:A:22:ARG:CG	1:A:22:ARG:NH1	2.58	0.48
1:A:238:PHE:CD1	1:A:253:ILE:HG12	2.48	0.48
1:E:98:SER:C	1:E:99:ILE:HG22	2.38	0.48
1:H:31:ARG:HD2	1:H:140:GLU:CD	2.39	0.48
1:H:44:ARG:O	1:H:128:LYS:HB2	2.13	0.48
1:H:57:HIS:O	1:H:61:ILE:HG12	2.13	0.48
1:H:306:LEU:HB3	1:H:307:PRO:CD	2.29	0.48
1:D:39:ARG:HB2	1:D:148:ALA:HB1	1.96	0.48
1:E:68:LEU:HD23	1:E:149:PHE:CD2	2.48	0.48
1:F:99:ILE:O	1:F:100:ASN:HB2	2.14	0.48
1:F:119:ARG:CG	1:F:119:ARG:NH1	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ARG:NE	1:G:39:ARG:CA	2.59	0.48
1:G:213:LEU:HD12	1:G:259:LEU:CD2	2.36	0.48
1:H:91:GLY:C	1:H:94:VAL:HG23	2.39	0.48
1:A:95:VAL:HA	1:A:96:PRO:HD3	1.63	0.48
1:E:191:THR:CG2	1:E:194:ALA:H	2.27	0.48
1:G:39:ARG:HE	1:G:40:GLY:CA	2.27	0.48
1:H:7:GLY:HA2	1:H:8:VAL:CB	2.44	0.48
1:C:19:SER:N	1:C:20:GLY:HA3	2.28	0.47
1:C:229:ILE:O	1:C:233:PRO:HD3	2.14	0.47
1:D:105:LEU:HD21	1:D:122:ILE:HG23	1.96	0.47
1:D:175:VAL:HG22	1:D:175:VAL:O	2.13	0.47
1:E:47:LEU:C	1:E:47:LEU:CD2	2.87	0.47
1:E:178:THR:O	1:E:182:GLY:HA3	2.14	0.47
1:F:269:HIS:CE1	1:F:270:GLU:O	2.66	0.47
1:D:167:GLU:O	1:D:168:ILE:C	2.57	0.47
1:E:229:ILE:O	1:E:233:PRO:CD	2.61	0.47
1:E:302:PRO:O	1:E:305:PRO:HD3	2.14	0.47
1:G:299:PRO:O	1:G:301:GLY:N	2.47	0.47
1:H:259:LEU:O	1:H:263:VAL:HG23	2.14	0.47
1:C:47:LEU:HD21	1:C:59:VAL:HG21	1.96	0.47
1:C:160:TYR:N	1:C:161:PRO:HD3	2.28	0.47
1:D:17:LYS:HG3	1:D:21:GLY:H	1.80	0.47
1:H:171:ILE:O	1:H:175:VAL:HG23	2.15	0.47
1:H:229:ILE:O	1:H:233:PRO:HD3	2.14	0.47
1:A:92:ASP:O	1:A:93:ASP:HB2	2.13	0.47
1:B:307:PRO:O	1:B:308:GLY:O	2.32	0.47
1:G:266:LEU:C	1:G:268:SER:H	2.22	0.47
1:H:46:HIS:HB2	1:H:128:LYS:HE3	1.96	0.47
1:A:270:GLU:O	1:A:271:ARG:CB	2.38	0.47
1:D:238:PHE:HA	1:D:242:TYR:HB2	1.97	0.47
1:H:151:ASP:C	1:H:153:GLY:H	2.22	0.47
1:B:309:LEU:HD22	1:B:310:THR:N	2.30	0.47
1:C:38:PHE:H	1:C:39:ARG:NH1	2.12	0.47
1:D:210:GLU:CD	1:D:258:ASN:HB2	2.39	0.47
1:F:243:HIS:CD2	1:F:249:ASN:HA	2.50	0.47
1:H:24:VAL:O	1:H:25:ARG:HB2	2.15	0.47
1:A:127:ASP:OD1	1:A:127:ASP:C	2.58	0.47
1:B:199:PHE:C	1:B:202:LEU:H	2.23	0.47
1:C:20:GLY:HA2	1:E:184:TYR:HB2	1.97	0.47
1:C:179:LEU:HA	1:C:202:LEU:CD2	2.44	0.47
1:D:87:THR:CG2	1:D:89:LEU:CG	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ARG:HG3	1:F:129:VAL:HG23	1.96	0.47
1:F:152:VAL:CG1	1:F:152:VAL:O	2.61	0.47
1:F:210:GLU:OE2	1:F:258:ASN:HB2	2.13	0.47
1:F:210:GLU:CD	1:F:258:ASN:HB2	2.38	0.47
1:G:30:TYR:O	1:G:135:ASN:HA	2.15	0.47
1:G:299:PRO:C	1:G:301:GLY:H	2.22	0.47
1:G:302:PRO:O	1:G:305:PRO:HG3	2.15	0.47
1:H:266:LEU:O	1:H:272:VAL:CG2	2.63	0.47
1:A:223:ARG:CB	1:A:223:ARG:NH1	2.62	0.47
1:D:4:LEU:HD12	1:D:116:TYR:CD2	2.50	0.47
1:D:61:ILE:O	1:D:62:MET:C	2.56	0.47
1:E:47:LEU:HD22	1:E:48:TYR:N	2.29	0.47
1:E:75:SER:C	1:E:76:MET:HG2	2.38	0.47
1:E:278:LEU:HD12	1:E:278:LEU:HA	1.66	0.47
1:F:167:GLU:O	1:F:171:ILE:HG13	2.14	0.47
1:H:44:ARG:O	1:H:44:ARG:HG3	2.13	0.47
1:C:61:ILE:CG2	1:C:65:LEU:HD22	2.45	0.47
1:D:78:ASN:OD1	1:D:79:ALA:N	2.47	0.47
1:E:97:ASP:HB3	1:E:102:ALA:HB3	1.96	0.47
1:F:33:GLY:O	1:F:34:LEU:HD22	2.14	0.47
1:G:37:GLY:HA2	1:G:38:PHE:HB3	1.97	0.47
1:H:30:TYR:O	1:H:135:ASN:HA	2.15	0.47
1:H:61:ILE:O	1:H:62:MET:C	2.58	0.47
1:B:89:LEU:C	1:B:91:GLY:N	2.71	0.46
1:C:23:PHE:HE2	1:E:27:GLU:HB3	1.80	0.46
1:C:25:ARG:NH1	1:C:29:GLN:HG2	2.29	0.46
1:C:33:GLY:O	1:C:34:LEU:CB	2.55	0.46
1:C:174:ARG:HD3	1:C:208:TRP:CE3	2.50	0.46
1:C:179:LEU:HD12	1:C:202:LEU:HD22	1.96	0.46
1:D:39:ARG:HB3	1:D:148:ALA:O	2.15	0.46
1:D:277:ASN:OD1	1:D:277:ASN:C	2.57	0.46
1:E:310:THR:HG22	1:E:311:LEU:N	2.30	0.46
1:G:8:VAL:CB	1:G:10:ARG:HH11	2.28	0.46
1:G:9:TRP:NE1	1:G:84:ASN:HA	2.30	0.46
1:G:134:LEU:O	1:G:134:LEU:HD12	2.15	0.46
1:G:295:THR:HB	1:G:297:ILE:HG12	1.96	0.46
1:H:165:ARG:N	1:H:166:PRO:CD	2.78	0.46
1:A:304:GLN:HE21	1:A:304:GLN:CA	2.27	0.46
1:B:69:GLU:H	1:B:69:GLU:HG2	1.59	0.46
1:B:79:ALA:HB2	1:B:280:HIS:NE2	2.30	0.46
1:B:147:SER:O	1:B:149:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASP:O	1:B:207:ASP:HB2	2.15	0.46
1:C:35:ASP:O	1:C:36:ALA:HB2	2.14	0.46
1:D:165:ARG:N	1:D:166:PRO:CD	2.77	0.46
1:G:47:LEU:C	1:G:47:LEU:CD2	2.88	0.46
1:G:137:GLU:HG3	1:G:140:GLU:HG3	1.97	0.46
1:H:126:TRP:CD1	1:H:126:TRP:C	2.93	0.46
1:D:75:SER:C	1:D:76:MET:HG2	2.39	0.46
1:F:210:GLU:OE1	1:F:256:TYR:HB3	2.16	0.46
1:G:38:PHE:O	1:G:39:ARG:CB	2.64	0.46
1:A:39:ARG:NH1	1:A:147:SER:CA	2.78	0.46
1:B:312:GLN:HG2	1:B:313:SER:N	2.22	0.46
1:D:37:GLY:HA2	1:D:38:PHE:CG	2.51	0.46
1:E:7:GLY:CA	1:E:8:VAL:CB	2.72	0.46
1:G:210:GLU:OE2	1:G:258:ASN:HB2	2.15	0.46
1:A:5:ILE:HD12	1:A:5:ILE:HA	1.81	0.46
1:B:218:TRP:CH2	1:B:265:LYS:HD3	2.50	0.46
1:D:19:SER:N	1:D:20:GLY:HA3	2.30	0.46
1:D:149:PHE:O	1:D:149:PHE:HD2	1.99	0.46
1:H:68:LEU:HD21	1:H:149:PHE:HD2	1.80	0.46
1:A:39:ARG:HD2	1:A:144:ILE:O	2.14	0.46
1:D:14:TYR:CE2	1:D:24:VAL:HB	2.50	0.46
1:D:78:ASN:HA	1:D:94:VAL:HG22	1.97	0.46
1:E:75:SER:HA	1:E:95:VAL:HG12	1.98	0.46
1:A:311:LEU:HD13	1:A:311:LEU:O	2.16	0.46
1:D:47:LEU:HD22	1:D:47:LEU:C	2.40	0.46
1:E:299:PRO:C	1:E:301:GLY:N	2.73	0.46
1:F:187:GLY:HA3	1:F:246:PHE:CD1	2.51	0.46
1:A:33:GLY:O	1:A:34:LEU:CB	2.60	0.46
1:C:17:LYS:O	1:C:18:SER:HB2	2.16	0.46
1:C:69:GLU:H	1:C:69:GLU:HG2	1.50	0.46
1:G:34:LEU:HD21	1:G:140:GLU:CD	2.41	0.46
1:G:171:ILE:O	1:G:174:ARG:N	2.40	0.46
1:H:37:GLY:HA2	1:H:39:ARG:N	2.30	0.46
1:H:57:HIS:CG	1:H:237:ARG:HH22	2.34	0.46
1:A:91:GLY:O	1:A:94:VAL:HG23	2.16	0.46
1:C:37:GLY:CA	1:C:38:PHE:CB	2.93	0.46
1:C:90:PRO:O	1:C:91:GLY:O	2.33	0.46
1:C:136:ASN:ND2	1:C:136:ASN:C	2.69	0.46
1:C:204:ASP:O	1:C:207:ASP:HB2	2.16	0.46
1:E:214:THR:HG23	1:E:258:ASN:ND2	2.30	0.46
1:G:92:ASP:C	1:G:94:VAL:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:271:ARG:NH1	1:H:271:ARG:CB	2.78	0.46
1:D:293:ASN:CG	1:D:293:ASN:O	2.59	0.46
1:G:160:TYR:CE2	1:G:165:ARG:HD3	2.51	0.46
1:A:179:LEU:HA	1:A:202:LEU:HD22	1.97	0.45
1:C:23:PHE:CD1	1:C:23:PHE:O	2.69	0.45
1:C:136:ASN:N	1:C:136:ASN:ND2	2.63	0.45
1:C:258:ASN:O	1:C:261:ARG:N	2.49	0.45
1:D:210:GLU:CD	1:D:257:PRO:HD2	2.41	0.45
1:E:36:ALA:O	1:E:37:GLY:C	2.59	0.45
1:F:7:GLY:CA	1:F:8:VAL:C	2.89	0.45
1:F:220:VAL:HG12	1:F:221:GLY:N	2.28	0.45
1:C:214:THR:C	1:C:216:ARG:H	2.24	0.45
1:C:224:LEU:HD12	1:C:224:LEU:C	2.41	0.45
1:D:167:GLU:OE1	1:D:220:VAL:HG22	2.16	0.45
1:G:245:HIS:CE1	1:G:289:HIS:HD2	2.30	0.45
1:H:151:ASP:O	1:H:153:GLY:N	2.47	0.45
1:H:232:PHE:N	1:H:233:PRO:HD2	2.31	0.45
1:A:37:GLY:CA	1:A:38:PHE:HD1	2.30	0.45
1:D:241:ILE:HG13	1:D:282:LYS:HG2	1.98	0.45
1:F:6:ASP:C	1:F:115:THR:O	2.59	0.45
1:F:37:GLY:CA	1:F:38:PHE:HB3	2.45	0.45
1:F:211:GLU:O	1:F:214:THR:HB	2.15	0.45
1:G:161:PRO:O	1:G:162:ALA:C	2.59	0.45
1:G:191:THR:HG23	1:G:194:ALA:N	2.15	0.45
1:H:163:GLU:O	1:H:164:PHE:HD2	2.00	0.45
1:C:44:ARG:HD3	1:C:45:TYR:CZ	2.52	0.45
1:C:47:LEU:HD11	1:C:59:VAL:CG2	2.46	0.45
1:C:105:LEU:HD12	1:C:105:LEU:HA	1.76	0.45
1:C:174:ARG:HD3	1:C:208:TRP:CZ3	2.51	0.45
1:C:232:PHE:N	1:C:233:PRO:CD	2.79	0.45
1:D:214:THR:CG2	1:D:215:GLY:N	2.65	0.45
1:E:66:LYS:C	1:E:68:LEU:H	2.22	0.45
1:E:97:ASP:OD2	1:E:102:ALA:CB	2.64	0.45
1:G:165:ARG:N	1:G:166:PRO:HD2	2.32	0.45
1:H:218:TRP:CZ3	1:H:224:LEU:HD13	2.52	0.45
1:C:5:ILE:HG22	1:C:6:ASP:H	1.78	0.45
1:D:120:VAL:HG12	1:D:120:VAL:O	2.17	0.45
1:E:44:ARG:HG3	1:E:129:VAL:CG2	2.46	0.45
1:G:231:LEU:HG	1:G:235:LEU:CD2	2.45	0.45
1:G:266:LEU:O	1:G:268:SER:N	2.50	0.45
1:B:160:TYR:CZ	1:B:165:ARG:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ARG:NH2	1:D:74:VAL:HG13	2.31	0.45
1:D:135:ASN:OD1	1:D:135:ASN:C	2.59	0.45
1:E:172:ASN:ND2	1:E:230:ARG:HD3	2.31	0.45
1:E:231:LEU:HG	1:E:235:LEU:HD22	1.98	0.45
1:G:200:TYR:C	1:G:202:LEU:N	2.72	0.45
1:A:12:ALA:O	1:A:13:TRP:O	2.34	0.45
1:A:249:ASN:OD1	1:B:301:GLY:CA	2.63	0.45
1:B:223:ARG:O	1:B:225:THR:HG23	2.17	0.45
1:C:59:VAL:HA	1:C:142:ILE:CD1	2.47	0.45
1:H:139:SER:C	1:H:142:ILE:HG22	2.42	0.45
1:A:63:ARG:NH2	1:A:74:VAL:HG23	2.32	0.45
1:C:235:LEU:HB3	1:C:263:VAL:HG21	1.98	0.45
1:D:14:TYR:CE1	1:D:26:LYS:HE2	2.52	0.45
1:D:161:PRO:HG3	1:D:223:ARG:NH2	2.31	0.45
1:G:143:ARG:HE	1:G:226:GLU:CD	2.24	0.45
1:A:5:ILE:CG2	1:A:10:ARG:NH1	2.77	0.45
1:A:13:TRP:HB2	1:A:15:ASP:HA	1.99	0.45
1:A:39:ARG:HH12	1:A:145:LEU:C	2.25	0.45
1:A:159:TYR:C	1:A:161:PRO:HD3	2.42	0.45
1:A:221:GLY:CA	2:A:401:HOH:O	2.21	0.45
1:C:241:ILE:HD13	1:C:285:TYR:HD1	1.81	0.45
1:D:204:ASP:O	1:D:207:ASP:HB2	2.17	0.45
1:E:57:HIS:NE2	1:E:275:THR:O	2.48	0.45
1:E:176:TYR:CD2	1:E:176:TYR:C	2.94	0.45
1:E:250:LEU:CD1	1:F:303:ALA:HB2	2.47	0.45
1:G:92:ASP:O	1:G:94:VAL:N	2.50	0.45
1:G:290:PRO:HD2	1:G:291:SER:H	1.82	0.45
1:H:98:SER:C	1:H:99:ILE:HG23	2.41	0.45
1:H:160:TYR:CZ	1:H:165:ARG:HG2	2.52	0.45
1:B:39:ARG:CZ	1:B:41:GLU:OE2	2.65	0.45
1:C:71:MET:HE1	1:C:153:GLY:HA3	1.98	0.45
1:D:33:GLY:HA3	1:D:144:ILE:HD11	1.98	0.45
1:D:142:ILE:HA	1:D:142:ILE:HD12	1.47	0.45
1:D:162:ALA:HA	1:D:165:ARG:CG	2.43	0.45
1:E:62:MET:HG2	1:E:142:ILE:HD13	1.98	0.45
1:E:281:ALA:O	1:E:282:LYS:C	2.59	0.45
1:F:33:GLY:O	1:F:34:LEU:CB	2.63	0.45
1:H:86:TRP:HB2	1:H:105:LEU:CD2	2.46	0.45
1:H:99:ILE:O	1:H:99:ILE:CG1	2.65	0.45
1:A:2:GLY:O	1:A:3:LEU:HD23	2.17	0.44
1:C:2:GLY:C	1:C:3:LEU:HD13	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:MET:H	1:C:95:VAL:HB	1.81	0.44
1:D:39:ARG:NH1	1:D:149:PHE:CB	2.79	0.44
1:E:51:PHE:HB2	1:E:280:HIS:CD2	2.52	0.44
1:F:142:ILE:HA	1:F:142:ILE:HD13	1.32	0.44
1:F:250:LEU:HD12	1:F:250:LEU:HA	1.63	0.44
1:F:269:HIS:C	1:F:269:HIS:HD1	2.25	0.44
1:G:270:GLU:O	1:G:271:ARG:CB	2.61	0.44
1:A:19:SER:HB3	1:F:3:LEU:HD21	1.99	0.44
1:B:93:ASP:O	1:B:94:VAL:CG1	2.64	0.44
1:B:152:VAL:O	1:B:152:VAL:HG13	2.15	0.44
1:B:210:GLU:OE1	1:B:259:LEU:HG	2.16	0.44
1:B:278:LEU:HD12	1:B:278:LEU:HA	1.59	0.44
1:D:71:MET:HB3	1:D:149:PHE:HZ	1.82	0.44
1:E:116:TYR:C	1:E:116:TYR:CD2	2.95	0.44
1:H:201:PRO:HA	1:H:204:ASP:HB2	2.00	0.44
1:B:5:ILE:CG2	1:B:6:ASP:N	2.81	0.44
1:B:232:PHE:N	1:B:233:PRO:CD	2.80	0.44
1:C:39:ARG:HB2	1:C:40:GLY:H	1.46	0.44
1:C:245:HIS:CD2	1:C:246:PHE:CE1	3.06	0.44
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.55	0.44
1:C:286:TYR:CD2	1:C:299:PRO:HD2	2.52	0.44
1:D:53:CYS:SG	1:D:55:TRP:HD1	2.41	0.44
1:D:66:LYS:O	1:D:68:LEU:N	2.51	0.44
1:F:38:PHE:C	1:F:40:GLY:N	2.71	0.44
1:G:39:ARG:HE	1:G:39:ARG:CA	2.24	0.44
1:G:171:ILE:O	1:G:172:ASN:C	2.61	0.44
1:G:286:TYR:CD2	1:G:299:PRO:HD2	2.52	0.44
1:A:5:ILE:CG2	1:A:6:ASP:N	2.79	0.44
1:B:266:LEU:HA	1:B:266:LEU:HD23	1.59	0.44
1:C:16:THR:C	1:C:18:SER:N	2.73	0.44
1:D:37:GLY:HA2	1:D:38:PHE:CD2	2.53	0.44
1:D:135:ASN:HD21	1:D:140:GLU:CB	2.31	0.44
1:E:30:TYR:O	1:E:135:ASN:HA	2.17	0.44
1:G:278:LEU:HD12	1:G:278:LEU:HA	1.85	0.44
1:A:176:TYR:HA	1:A:180:ASN:HB2	1.98	0.44
1:A:300:VAL:CB	1:B:199:PHE:HZ	2.30	0.44
1:B:48:TYR:HB2	1:B:124:ILE:HB	2.00	0.44
1:D:68:LEU:HD12	1:D:145:LEU:HD13	2.00	0.44
1:G:60:LEU:HD23	1:G:60:LEU:HA	1.55	0.44
1:H:7:GLY:CA	1:H:8:VAL:O	2.66	0.44
1:H:30:TYR:H	1:H:136:ASN:ND2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:GLN:O	1:H:192:GLN:HG3	2.16	0.44
1:H:278:LEU:HD12	1:H:278:LEU:HA	1.54	0.44
1:H:295:THR:OG1	1:H:297:ILE:HG13	2.17	0.44
1:A:79:ALA:HB2	1:A:280:HIS:NE2	2.33	0.44
1:A:214:THR:HA	1:A:258:ASN:ND2	2.33	0.44
1:C:258:ASN:O	1:C:259:LEU:C	2.61	0.44
1:C:290:PRO:C	1:C:292:VAL:H	2.25	0.44
1:D:269:HIS:HE1	1:D:271:ARG:CB	2.30	0.44
1:E:252:ARG:O	1:E:255:ASP:HB2	2.17	0.44
1:F:3:LEU:CD1	1:F:24:VAL:HG11	2.47	0.44
1:B:34:LEU:HD21	1:B:140:GLU:HG2	2.00	0.44
1:C:18:SER:O	1:C:19:SER:CB	2.64	0.44
1:C:147:SER:O	1:C:149:PHE:N	2.50	0.44
1:D:14:TYR:O	1:D:18:SER:HB3	2.18	0.44
1:D:61:ILE:HG21	1:D:229:ILE:HG23	2.00	0.44
1:F:122:ILE:HB	1:F:123:PRO:HA	2.00	0.44
1:G:219:LEU:HG	1:G:228:ASP:OD2	2.17	0.44
1:H:44:ARG:HH12	1:H:130:GLU:HG3	1.83	0.44
1:H:235:LEU:HA	1:H:235:LEU:HD12	1.71	0.44
1:B:3:LEU:HD12	1:B:24:VAL:HG11	1.99	0.44
1:D:53:CYS:HB3	1:D:56:ALA:HB3	1.99	0.44
1:E:218:TRP:CB	1:E:223:ARG:O	2.66	0.44
1:G:205:THR:O	1:G:209:LEU:HB2	2.18	0.44
1:H:68:LEU:HD21	1:H:149:PHE:CD2	2.53	0.44
1:A:37:GLY:CA	1:A:38:PHE:CD1	3.01	0.43
1:B:183:VAL:HG23	1:B:184:TYR:N	2.33	0.43
1:E:304:GLN:HA	1:E:305:PRO:HD2	1.69	0.43
1:G:5:ILE:O	1:G:6:ASP:CB	2.59	0.43
1:G:86:TRP:CH2	1:G:284:HIS:CD2	3.06	0.43
1:G:203:PHE:CZ	1:G:250:LEU:N	2.86	0.43
1:H:241:ILE:HG21	1:H:285:TYR:CD1	2.53	0.43
1:B:4:LEU:HD23	1:B:4:LEU:HA	1.72	0.43
1:B:63:ARG:NH2	1:B:72:ILE:O	2.42	0.43
1:C:168:ILE:CD1	1:C:225:THR:HB	2.48	0.43
1:D:39:ARG:CB	1:D:148:ALA:HB1	2.48	0.43
1:D:58:ARG:O	1:D:61:ILE:HB	2.18	0.43
1:G:80:TYR:CE2	1:G:82:GLY:HA3	2.52	0.43
1:B:104:TYR:HD2	1:B:106:TYR:CZ	2.36	0.43
1:C:38:PHE:C	1:C:39:ARG:O	2.61	0.43
1:D:4:LEU:HD23	1:D:4:LEU:HA	1.92	0.43
1:E:42:PRO:N	1:E:152:VAL:HG11	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:VAL:O	1:E:300:VAL:HG13	2.19	0.43
1:F:22:ARG:O	1:F:22:ARG:CG	2.63	0.43
1:H:231:LEU:CD1	1:H:235:LEU:HD22	2.49	0.43
1:A:99:ILE:O	1:A:99:ILE:CD1	2.61	0.43
1:B:172:ASN:HD21	1:B:227:ALA:HA	1.82	0.43
1:C:220:VAL:C	1:C:221:GLY:O	2.60	0.43
1:G:5:ILE:C	1:G:7:GLY:HA3	2.44	0.43
1:G:160:TYR:N	1:G:161:PRO:HD3	2.32	0.43
1:E:237:ARG:HG3	1:E:237:ARG:NH1	2.31	0.43
1:E:270:GLU:O	1:E:271:ARG:CB	2.48	0.43
1:G:220:VAL:C	1:G:221:GLY:O	2.60	0.43
1:H:36:ALA:C	1:H:38:PHE:HB3	2.42	0.43
1:C:87:THR:CG2	1:C:88:PHE:N	2.80	0.43
1:E:191:THR:HB	1:E:194:ALA:HB3	2.01	0.43
1:G:24:VAL:O	1:G:25:ARG:HG2	2.19	0.43
1:G:37:GLY:CA	1:G:38:PHE:CB	2.96	0.43
1:H:40:GLY:HA2	1:H:149:PHE:CE1	2.54	0.43
1:A:14:TYR:CD1	1:A:24:VAL:HB	2.53	0.43
1:A:17:LYS:HB3	1:F:291:SER:CB	2.48	0.43
1:A:26:LYS:HB3	1:A:119:ARG:HD2	1.99	0.43
1:C:161:PRO:O	1:C:165:ARG:HG3	2.19	0.43
1:D:5:ILE:HD12	1:D:117:THR:HG23	2.00	0.43
1:D:122:ILE:HD13	1:D:122:ILE:HG21	1.71	0.43
1:D:175:VAL:HG21	1:D:231:LEU:HB2	2.01	0.43
1:D:225:THR:HG23	1:D:228:ASP:OD1	2.19	0.43
1:E:94:VAL:HG12	1:E:95:VAL:N	2.33	0.43
1:G:99:ILE:HG22	1:G:100:ASN:N	2.33	0.43
1:G:282:LYS:NZ	1:G:301:GLY:CA	2.82	0.43
1:H:264:GLY:O	1:H:265:LYS:C	2.62	0.43
1:A:74:VAL:HG12	1:A:75:SER:N	2.33	0.43
1:A:304:GLN:HA	1:A:304:GLN:NE2	2.33	0.43
1:A:309:LEU:N	1:A:309:LEU:HD12	2.34	0.43
1:B:109:TYR:CD1	1:B:120:VAL:HG13	2.53	0.43
1:B:160:TYR:CE1	1:B:165:ARG:HG2	2.53	0.43
1:C:300:VAL:HG23	1:D:195:TYR:CE2	2.54	0.43
1:D:39:ARG:HD2	1:D:149:PHE:HA	1.98	0.43
1:D:65:LEU:HD21	1:D:224:LEU:HD21	2.01	0.43
1:E:46:HIS:CD2	1:E:99:ILE:HG21	2.53	0.43
1:G:38:PHE:O	1:G:39:ARG:HG2	2.18	0.43
1:G:88:PHE:O	1:G:89:LEU:C	2.59	0.43
1:G:162:ALA:O	1:G:163:GLU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:PHE:O	1:G:202:LEU:HB3	2.18	0.43
1:A:218:TRP:CE2	1:A:265:LYS:HE3	2.53	0.43
1:B:92:ASP:OD1	1:B:92:ASP:C	2.62	0.43
1:C:20:GLY:HA2	1:E:184:TYR:HB3	2.01	0.43
1:C:167:GLU:O	1:C:168:ILE:C	2.61	0.43
1:D:39:ARG:HH11	1:D:149:PHE:CB	2.30	0.43
1:G:66:LYS:NZ	1:G:146:ASN:O	2.51	0.43
1:G:251:ARG:HG3	1:G:256:TYR:HE2	1.82	0.43
1:G:273:ALA:N	1:G:274:PRO:CD	2.82	0.43
1:H:24:VAL:O	1:H:24:VAL:HG22	2.18	0.43
1:A:97:ASP:OD2	1:A:100:ASN:CB	2.67	0.43
1:C:183:VAL:HG11	1:C:242:TYR:CD2	2.54	0.43
1:D:105:LEU:CD2	1:D:122:ILE:HG23	2.49	0.43
1:F:235:LEU:HD23	1:F:263:VAL:HG23	2.01	0.43
1:F:299:PRO:O	1:F:301:GLY:N	2.51	0.43
1:A:98:SER:O	1:A:99:ILE:CG1	2.65	0.42
1:B:300:VAL:N	1:B:301:GLY:HA3	2.31	0.42
1:C:12:ALA:HB1	1:E:13:TRP:HE3	1.82	0.42
1:C:109:TYR:CE1	1:C:124:ILE:HD11	2.53	0.42
1:C:183:VAL:HG23	1:C:184:TYR:N	2.34	0.42
1:D:5:ILE:HD12	1:D:5:ILE:HA	1.43	0.42
1:D:269:HIS:HE1	1:D:271:ARG:HB2	1.83	0.42
1:G:217:GLU:HB3	1:G:265:LYS:NZ	2.34	0.42
1:H:183:VAL:O	1:H:186:SER:HB2	2.19	0.42
1:A:300:VAL:CB	1:B:199:PHE:CZ	2.97	0.42
1:B:241:ILE:HG21	1:B:285:TYR:CG	2.53	0.42
1:C:19:SER:HB3	1:C:20:GLY:CA	2.49	0.42
1:C:68:LEU:HD23	1:C:68:LEU:HA	1.56	0.42
1:C:164:PHE:O	1:C:165:ARG:C	2.60	0.42
1:D:37:GLY:CA	1:D:38:PHE:CB	2.83	0.42
1:D:176:TYR:CD2	1:D:177:GLU:N	2.87	0.42
1:E:80:TYR:CE2	1:E:82:GLY:HA3	2.53	0.42
1:F:38:PHE:O	1:F:38:PHE:CD1	2.64	0.42
1:F:232:PHE:O	1:F:233:PRO:C	2.62	0.42
1:G:125:LEU:HD12	1:G:125:LEU:HA	1.84	0.42
1:G:203:PHE:CZ	1:G:250:LEU:HB3	2.53	0.42
1:H:159:TYR:C	1:H:161:PRO:CD	2.92	0.42
1:H:294:PRO:O	1:H:295:THR:C	2.61	0.42
1:A:61:ILE:HG23	1:A:272:VAL:HG22	2.01	0.42
1:B:164:PHE:O	1:B:165:ARG:C	2.61	0.42
1:B:167:GLU:O	1:B:168:ILE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:LEU:O	1:E:180:ASN:C	2.61	0.42
1:G:5:ILE:O	1:G:7:GLY:CA	2.67	0.42
1:G:184:TYR:OH	1:G:285:TYR:OH	2.34	0.42
1:A:34:LEU:HA	1:A:34:LEU:HD12	1.80	0.42
1:A:39:ARG:NH1	1:A:147:SER:H	2.11	0.42
1:A:223:ARG:O	1:A:225:THR:HG23	2.19	0.42
1:B:136:ASN:HD22	1:B:136:ASN:N	2.07	0.42
1:C:219:LEU:HG	1:C:228:ASP:OD2	2.19	0.42
1:D:32:GLY:HA3	1:D:134:LEU:CD1	2.49	0.42
1:D:214:THR:HA	1:D:258:ASN:HD21	1.80	0.42
1:E:47:LEU:HD23	1:E:124:ILE:O	2.19	0.42
1:F:99:ILE:O	1:F:99:ILE:CG1	2.68	0.42
1:F:174:ARG:HD3	1:F:208:TRP:CZ3	2.54	0.42
1:H:35:ASP:O	1:H:38:PHE:CD1	2.73	0.42
1:H:304:GLN:HA	1:H:305:PRO:HD3	1.81	0.42
1:A:91:GLY:O	1:A:92:ASP:C	2.63	0.42
1:C:12:ALA:CB	1:E:13:TRP:CE3	3.02	0.42
1:C:16:THR:O	1:C:17:LYS:C	2.62	0.42
1:C:133:ILE:HG22	1:C:134:LEU:N	2.33	0.42
1:C:162:ALA:O	1:C:163:GLU:C	2.62	0.42
1:D:3:LEU:CD1	1:D:24:VAL:HG11	2.49	0.42
1:D:14:TYR:CD2	1:D:14:TYR:O	2.72	0.42
1:D:76:MET:N	1:D:95:VAL:HB	2.35	0.42
1:D:81:MET:CE	1:D:86:TRP:CE2	2.94	0.42
1:D:127:ASP:OD1	1:D:129:VAL:HB	2.19	0.42
1:F:31:ARG:HD2	1:F:140:GLU:OE1	2.19	0.42
1:G:6:ASP:HB2	1:G:7:GLY:HA2	2.02	0.42
1:G:242:TYR:HA	1:G:246:PHE:HB2	2.01	0.42
1:H:161:PRO:HG3	1:H:223:ARG:NH1	2.34	0.42
1:A:195:TYR:OH	1:B:300:VAL:HB	2.19	0.42
1:B:147:SER:C	1:B:149:PHE:H	2.28	0.42
1:C:160:TYR:N	1:C:161:PRO:CD	2.82	0.42
1:D:229:ILE:O	1:D:233:PRO:CD	2.67	0.42
1:E:168:ILE:HD11	1:E:225:THR:HB	2.00	0.42
1:A:159:TYR:CE1	1:A:224:LEU:HD23	2.53	0.42
1:A:286:TYR:CD1	1:A:299:PRO:HD3	2.54	0.42
1:B:75:SER:HA	1:B:95:VAL:HG22	2.02	0.42
1:C:210:GLU:CD	1:C:258:ASN:HB2	2.45	0.42
1:D:146:ASN:C	1:D:146:ASN:ND2	2.78	0.42
1:D:165:ARG:O	1:D:169:ASP:HB2	2.20	0.42
1:E:57:HIS:HB3	1:E:233:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HB3	1:F:291:SER:HB3	2.01	0.42
1:A:39:ARG:NH1	1:A:145:LEU:C	2.78	0.42
1:C:270:GLU:O	1:C:271:ARG:CB	2.54	0.42
1:E:44:ARG:CG	1:E:129:VAL:CG2	2.98	0.42
1:H:43:GLY:O	1:H:128:LYS:HD2	2.20	0.42
1:C:58:ARG:C	1:C:142:ILE:HD11	2.44	0.42
1:C:250:LEU:HD12	1:C:250:LEU:HA	1.70	0.42
1:C:300:VAL:HG23	1:D:195:TYR:HE2	1.85	0.42
1:D:37:GLY:CA	1:D:38:PHE:CD2	3.03	0.42
1:F:6:ASP:CA	1:F:115:THR:O	2.67	0.42
1:F:87:THR:CG2	1:F:88:PHE:N	2.81	0.42
1:A:143:ARG:HH12	1:A:226:GLU:CD	2.27	0.42
1:B:191:THR:O	1:B:192:GLN:C	2.59	0.42
1:C:59:VAL:O	1:C:60:LEU:C	2.63	0.42
1:C:273:ALA:N	1:C:274:PRO:CD	2.82	0.42
1:D:31:ARG:NH1	1:D:140:GLU:OE2	2.53	0.42
1:E:56:ALA:O	1:E:57:HIS:C	2.63	0.42
1:E:245:HIS:HB2	1:E:286:TYR:CZ	2.54	0.42
1:F:213:LEU:HD12	1:F:259:LEU:HD23	2.02	0.42
1:A:37:GLY:HA3	1:A:38:PHE:HD1	1.85	0.41
1:C:312:GLN:O	1:C:313:SER:HB3	2.20	0.41
1:F:7:GLY:CA	1:F:8:VAL:O	2.65	0.41
1:H:238:PHE:O	1:H:239:ASP:C	2.63	0.41
1:A:17:LYS:HD2	1:A:18:SER:HB3	2.00	0.41
1:C:5:ILE:HD12	1:C:5:ILE:HA	1.46	0.41
1:C:159:TYR:C	1:C:161:PRO:HD3	2.45	0.41
1:D:66:LYS:C	1:D:68:LEU:N	2.77	0.41
1:D:249:ASN:O	1:D:250:LEU:C	2.63	0.41
1:E:4:LEU:O	1:E:5:ILE:HD13	2.20	0.41
1:E:310:THR:HG22	1:E:311:LEU:H	1.85	0.41
1:C:5:ILE:O	1:C:117:THR:HG23	2.20	0.41
1:D:33:GLY:O	1:D:34:LEU:HB2	2.20	0.41
1:D:39:ARG:HD3	1:D:149:PHE:CD2	2.56	0.41
1:F:31:ARG:HA	1:F:135:ASN:ND2	2.35	0.41
1:F:37:GLY:CA	1:F:38:PHE:CB	2.98	0.41
1:G:47:LEU:HD22	1:G:48:TYR:C	2.45	0.41
1:H:59:VAL:O	1:H:60:LEU:C	2.63	0.41
1:H:188:PHE:O	1:H:189:ALA:C	2.64	0.41
1:A:44:ARG:NH1	1:A:127:ASP:OD2	2.53	0.41
1:B:6:ASP:O	1:B:115:THR:HA	2.19	0.41
1:B:78:ASN:OD1	1:B:79:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ALA:HB2	1:D:250:LEU:CD1	2.50	0.41
1:D:44:ARG:HH11	1:D:129:VAL:HB	1.86	0.41
1:E:44:ARG:HG3	1:E:129:VAL:HG21	2.02	0.41
1:F:49:ALA:HB3	1:F:76:MET:CE	2.51	0.41
1:F:86:TRP:CH2	1:F:284:HIS:CE1	3.08	0.41
1:H:23:PHE:H	1:H:24:VAL:HB	1.86	0.41
1:A:39:ARG:CZ	1:A:149:PHE:N	2.83	0.41
1:C:210:GLU:OE2	1:C:257:PRO:CD	2.56	0.41
1:D:126:TRP:CD1	1:D:126:TRP:O	2.73	0.41
1:E:135:ASN:OD1	1:E:141:ILE:HG13	2.19	0.41
1:E:218:TRP:NE1	1:E:265:LYS:NZ	2.69	0.41
1:E:218:TRP:HB2	1:E:223:ARG:O	2.21	0.41
1:G:195:TYR:CE1	1:G:199:PHE:HB2	2.56	0.41
1:H:175:VAL:HG12	1:H:180:ASN:OD1	2.20	0.41
1:B:172:ASN:HD22	1:B:172:ASN:HA	1.65	0.41
1:B:229:ILE:O	1:B:233:PRO:CD	2.69	0.41
1:C:25:ARG:O	1:C:26:LYS:C	2.63	0.41
1:C:139:SER:HB2	1:C:230:ARG:NH1	2.35	0.41
1:C:244:GLY:O	1:C:245:HIS:C	2.63	0.41
1:G:167:GLU:CG	1:G:170:ARG:NH1	2.67	0.41
1:H:32:GLY:HA3	1:H:134:LEU:HD12	2.02	0.41
1:H:72:ILE:HD11	1:H:149:PHE:HE2	1.86	0.41
1:H:93:ASP:OD2	1:H:93:ASP:N	2.53	0.41
1:H:199:PHE:O	1:H:202:LEU:HB3	2.20	0.41
1:H:262:LEU:HD12	1:H:262:LEU:O	2.20	0.41
1:H:282:LYS:HZ1	1:H:301:GLY:HA3	1.79	0.41
1:A:235:LEU:HA	1:A:235:LEU:HD12	1.84	0.41
1:B:89:LEU:CB	1:B:90:PRO:HD2	2.47	0.41
1:B:162:ALA:HA	1:B:165:ARG:CD	2.50	0.41
1:B:245:HIS:CE1	1:B:289:HIS:CD2	2.88	0.41
1:C:89:LEU:HB3	1:C:90:PRO:HD2	2.02	0.41
1:C:155:LEU:HA	1:C:155:LEU:HD23	1.83	0.41
1:F:38:PHE:C	1:F:38:PHE:CD1	2.98	0.41
1:F:297:ILE:H	1:F:297:ILE:HG12	1.74	0.41
1:A:17:LYS:HB3	1:F:291:SER:OG	2.20	0.41
1:A:269:HIS:ND1	1:A:270:GLU:O	2.47	0.41
1:B:179:LEU:O	1:B:180:ASN:C	2.64	0.41
1:C:142:ILE:HA	1:C:142:ILE:HD13	1.75	0.41
1:E:139:SER:O	1:E:142:ILE:HG22	2.20	0.41
1:G:220:VAL:HG12	1:G:221:GLY:N	2.35	0.41
1:G:282:LYS:HZ1	1:G:301:GLY:HA3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:GLY:N	1:H:94:VAL:HG21	2.36	0.41
1:A:300:VAL:O	1:A:300:VAL:HG13	2.20	0.41
1:B:87:THR:HG23	1:B:89:LEU:H	1.86	0.41
1:B:183:VAL:HG11	1:B:242:TYR:CD2	2.55	0.41
1:C:95:VAL:HA	1:C:96:PRO:HD3	1.91	0.41
1:C:265:LYS:HA	1:C:310:THR:CG2	2.45	0.41
1:D:4:LEU:HD12	1:D:116:TYR:HD2	1.86	0.41
1:D:11:ASP:O	1:D:11:ASP:CG	2.63	0.41
1:D:59:VAL:O	1:D:60:LEU:C	2.61	0.41
1:D:87:THR:HG22	1:D:88:PHE:N	2.36	0.41
1:D:262:LEU:O	1:D:263:VAL:C	2.64	0.41
1:E:68:LEU:N	1:E:68:LEU:CD1	2.82	0.41
1:F:95:VAL:HA	1:F:96:PRO:HD3	1.75	0.41
1:F:253:ILE:H	1:F:253:ILE:HG12	1.64	0.41
1:F:302:PRO:O	1:F:303:ALA:C	2.63	0.41
1:G:43:GLY:O	1:G:128:LYS:HD2	2.21	0.41
1:G:282:LYS:HZ1	1:G:301:GLY:CA	2.34	0.41
1:H:53:CYS:HA	1:H:54:PRO:HD3	1.89	0.41
1:H:246:PHE:O	1:H:248:CYS:N	2.54	0.41
1:A:17:LYS:CE	1:A:18:SER:OG	2.68	0.41
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.80	0.41
1:C:235:LEU:HB3	1:C:263:VAL:CG2	2.50	0.41
1:D:63:ARG:HH21	1:D:74:VAL:HG13	1.86	0.41
1:D:160:TYR:N	1:D:161:PRO:CD	2.84	0.41
1:D:245:HIS:HB2	1:D:286:TYR:CZ	2.55	0.41
1:E:17:LYS:CA	1:E:18:SER:CB	2.93	0.41
1:E:87:THR:CG2	1:E:89:LEU:HG	2.51	0.41
1:E:137:GLU:O	1:E:138:SER:C	2.64	0.41
1:F:278:LEU:HD12	1:F:278:LEU:HA	1.94	0.41
1:G:99:ILE:HG22	1:G:100:ASN:OD1	2.21	0.41
1:H:202:LEU:C	1:H:202:LEU:CD2	2.90	0.41
1:C:186:SER:HB3	1:C:198:ALA:HB3	2.02	0.40
1:E:306:LEU:HD12	1:E:306:LEU:HA	1.88	0.40
1:F:176:TYR:HA	1:F:180:ASN:HB2	2.04	0.40
1:G:75:SER:C	1:G:76:MET:HG2	2.46	0.40
1:H:282:LYS:HZ1	1:H:301:GLY:CA	2.34	0.40
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.90	0.40
1:B:273:ALA:N	1:B:274:PRO:CD	2.84	0.40
1:C:87:THR:N	2:C:402:HOH:O	2.54	0.40
1:F:87:THR:HG23	1:F:88:PHE:N	2.36	0.40
1:G:38:PHE:O	1:G:39:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:LEU:C	1:G:47:LEU:HD22	2.46	0.40
1:H:3:LEU:HD22	1:H:3:LEU:HA	1.61	0.40
1:H:71:MET:HE3	1:H:71:MET:HB2	1.94	0.40
1:B:104:TYR:O	1:B:105:LEU:C	2.62	0.40
1:C:89:LEU:HA	1:C:90:PRO:HD3	1.94	0.40
1:D:212:HIS:C	1:D:214:THR:H	2.29	0.40
1:E:143:ARG:O	1:E:146:ASN:HB3	2.21	0.40
1:H:59:VAL:C	1:H:61:ILE:N	2.78	0.40
1:H:257:PRO:O	1:H:258:ASN:C	2.64	0.40
1:H:307:PRO:HB2	1:H:308:GLY:H	1.71	0.40
1:A:281:ALA:O	1:A:282:LYS:C	2.64	0.40
1:B:306:LEU:HD13	1:B:306:LEU:N	2.36	0.40
1:C:4:LEU:HD12	1:C:116:TYR:HD2	1.87	0.40
1:C:312:GLN:O	1:C:313:SER:CB	2.69	0.40
1:D:125:LEU:HB2	1:D:141:ILE:HG12	2.04	0.40
1:D:269:HIS:CE1	1:D:271:ARG:HB3	2.57	0.40
1:E:41:GLU:HA	1:E:152:VAL:HG11	2.03	0.40
1:H:5:ILE:HA	1:H:5:ILE:HD12	1.55	0.40
1:H:160:TYR:CD2	1:H:165:ARG:NE	2.90	0.40
1:H:220:VAL:HG23	1:H:225:THR:HG21	2.04	0.40
1:H:246:PHE:O	1:H:247:LYS:C	2.64	0.40
1:A:185:ARG:O	1:A:189:ALA:HB2	2.21	0.40
1:A:300:VAL:CG2	1:B:199:PHE:HZ	2.34	0.40
1:D:68:LEU:HD22	1:D:149:PHE:CE1	2.56	0.40
1:E:235:LEU:HB3	1:E:263:VAL:CG2	2.51	0.40
1:E:307:PRO:CG	1:E:308:GLY:N	2.83	0.40
1:F:37:GLY:HA2	1:F:38:PHE:HB3	2.02	0.40
1:H:21:GLY:O	1:H:22:ARG:HB3	2.22	0.40
1:H:210:GLU:O	1:H:210:GLU:HG3	2.20	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	310/313 (99%)	263 (85%)	33 (11%)	14 (4%)	2	12
1	B	299/313 (96%)	252 (84%)	39 (13%)	8 (3%)	4	22
1	C	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1	5
1	D	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1	5
1	E	310/313 (99%)	247 (80%)	41 (13%)	22 (7%)	1	4
1	F	304/313 (97%)	262 (86%)	27 (9%)	15 (5%)	1	10
1	G	301/313 (96%)	241 (80%)	39 (13%)	21 (7%)	1	4
1	H	305/313 (97%)	213 (70%)	60 (20%)	32 (10%)	0	2
All	All	2449/2504 (98%)	1954 (80%)	343 (14%)	152 (6%)	1	6

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	TRP
1	A	36	ALA
1	A	38	PHE
1	A	147	SER
1	A	307	PRO
1	B	91	GLY
1	B	92	ASP
1	B	308	GLY
1	C	13	TRP
1	C	18	SER
1	C	19	SER
1	C	26	LYS
1	C	27	GLU
1	C	35	ASP
1	C	38	PHE
1	C	39	ARG
1	C	91	GLY
1	C	92	ASP
1	D	16	THR
1	D	35	ASP
1	D	38	PHE
1	D	98	SER
1	D	214	THR
1	D	271	ARG
1	E	18	SER
1	E	68	LEU
1	E	99	ILE

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Mol	Chain	Res	Type
1	E	148	ALA
1	E	150	ASP
1	E	307	PRO
1	E	312	GLN
1	F	36	ALA
1	F	90	PRO
1	F	91	GLY
1	F	100	ASN
1	F	116	TYR
1	F	152	VAL
1	G	6	ASP
1	G	36	ALA
1	G	38	PHE
1	G	39	ARG
1	G	176	TYR
1	G	307	PRO
1	G	309	LEU
1	H	38	PHE
1	H	68	LEU
1	H	96	PRO
1	H	152	VAL
1	H	219	LEU
1	H	238	PHE
1	H	247	LYS
1	H	257	PRO
1	H	303	ALA
1	A	18	SER
1	A	99	ILE
1	A	100	ASN
1	A	142	ILE
1	A	300	VAL
1	B	95	VAL
1	C	36	ALA
1	C	148	ALA
1	D	151	ASP
1	D	173	ALA
1	D	265	LYS
1	D	308	GLY
1	E	8	VAL
1	E	15	ASP
1	E	16	THR
1	E	37	GLY

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Mol	Chain	Res	Type
1	E	38	PHE
1	E	39	ARG
1	E	67	GLY
1	E	116	TYR
1	E	152	VAL
1	F	98	SER
1	F	271	ARG
1	G	93	ASP
1	H	26	LYS
1	H	35	ASP
1	H	61	ILE
1	H	64	ALA
1	H	111	ALA
1	H	155	LEU
1	H	269	HIS
1	H	276	ILE
1	H	297	ILE
1	H	300	VAL
1	A	151	ASP
1	B	299	PRO
1	C	34	LEU
1	C	100	ASN
1	D	148	ALA
1	D	269	HIS
1	E	17	LYS
1	E	271	ARG
1	F	35	ASP
1	G	5	ILE
1	G	83	GLU
1	G	311	LEU
1	H	8	VAL
1	H	13	TRP
1	H	63	ARG
1	H	268	SER
1	A	39	ARG
1	A	271	ARG
1	B	90	PRO
1	C	8	VAL
1	D	96	PRO
1	D	238	PHE
1	D	257	PRO
1	D	309	LEU

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Mol	Chain	Res	Type
1	E	209	LEU
1	E	219	LEU
1	E	269	HIS
1	F	21	GLY
1	F	138	SER
1	F	300	VAL
1	G	163	GLU
1	G	219	LEU
1	G	267	ALA
1	G	300	VAL
1	H	99	ILE
1	H	154	ALA
1	H	285	TYR
1	H	307	PRO
1	H	309	LEU
1	C	12	ALA
1	C	245	HIS
1	D	8	VAL
1	D	150	ASP
1	F	8	VAL
1	G	8	VAL
1	G	271	ARG
1	H	156	PRO
1	A	312	GLN
1	B	8	VAL
1	C	152	VAL
1	D	67	GLY
1	G	25	ARG
1	G	101	GLY
1	G	290	PRO
1	H	34	LEU
1	H	259	LEU
1	D	156	PRO
1	H	37	GLY
1	B	32	GLY
1	C	90	PRO
1	E	101	GLY
1	G	306	LEU
1	C	21	GLY
1	F	99	ILE
1	F	307	PRO

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	258/260 (99%)	219 (85%)	39 (15%)	3	14
1	B	250/260 (96%)	211 (84%)	39 (16%)	2	13
1	C	256/260 (98%)	216 (84%)	40 (16%)	2	13
1	D	255/260 (98%)	212 (83%)	43 (17%)	2	11
1	E	254/260 (98%)	212 (84%)	42 (16%)	2	12
1	F	252/260 (97%)	214 (85%)	38 (15%)	3	14
1	G	250/260 (96%)	213 (85%)	37 (15%)	3	15
1	H	249/260 (96%)	207 (83%)	42 (17%)	2	11
All	All	2024/2080 (97%)	1704 (84%)	320 (16%)	2	13

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	10	ARG
1	A	13	TRP
1	A	14	TYR
1	A	22	ARG
1	A	34	LEU
1	A	35	ASP
1	A	44	ARG
1	A	47	LEU
1	A	59	VAL
1	A	65	LEU
1	A	69	GLU
1	A	70	GLU
1	A	87	THR
1	A	90	PRO
1	A	110	THR
1	A	122	ILE
1	A	136	ASN
1	A	138	SER

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Mol	Chain	Res	Type
1	A	142	ILE
1	A	143	ARG
1	A	145	LEU
1	A	146	ASN
1	A	175	VAL
1	A	190	THR
1	A	202	LEU
1	A	214	THR
1	A	222	ASP
1	A	223	ARG
1	A	228	ASP
1	A	235	LEU
1	A	251	ARG
1	A	278	LEU
1	A	282	LYS
1	A	291	SER
1	A	300	VAL
1	A	304	GLN
1	A	309	LEU
1	A	311	LEU
1	B	5	ILE
1	B	6	ASP
1	B	10	ARG
1	B	28	SER
1	B	34	LEU
1	B	38	PHE
1	B	39	ARG
1	B	41	GLU
1	B	47	LEU
1	B	59	VAL
1	B	69	GLU
1	B	70	GLU
1	B	73	SER
1	B	74	VAL
1	B	83	GLU
1	B	94	VAL
1	B	95	VAL
1	B	110	THR
1	B	125	LEU
1	B	136	ASN
1	B	138	SER
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	147	SER
1	B	152	VAL
1	B	167	GLU
1	B	172	ASN
1	B	175	VAL
1	B	190	THR
1	B	199	PHE
1	B	202	LEU
1	B	222	ASP
1	B	223	ARG
1	B	235	LEU
1	B	278	LEU
1	B	295	THR
1	B	300	VAL
1	B	304	GLN
1	B	306	LEU
1	B	309	LEU
1	C	3	LEU
1	C	5	ILE
1	C	16	THR
1	C	17	LYS
1	C	18	SER
1	C	22	ARG
1	C	23	PHE
1	C	25	ARG
1	C	27	GLU
1	C	34	LEU
1	C	38	PHE
1	C	39	ARG
1	C	47	LEU
1	C	59	VAL
1	C	63	ARG
1	C	65	LEU
1	C	69	GLU
1	C	71	MET
1	C	87	THR
1	C	92	ASP
1	C	94	VAL
1	C	100	ASN
1	C	110	THR
1	C	115	THR
1	C	122	ILE

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Mol	Chain	Res	Type
1	C	130	GLU
1	C	136	ASN
1	C	145	LEU
1	C	211	GLU
1	C	223	ARG
1	C	231	LEU
1	C	235	LEU
1	C	247	LYS
1	C	275	THR
1	C	278	LEU
1	C	291	SER
1	C	292	VAL
1	C	297	ILE
1	C	306	LEU
1	C	309	LEU
1	D	3	LEU
1	D	5	ILE
1	D	14	TYR
1	D	17	LYS
1	D	18	SER
1	D	34	LEU
1	D	39	ARG
1	D	41	GLU
1	D	44	ARG
1	D	47	LEU
1	D	59	VAL
1	D	60	LEU
1	D	63	ARG
1	D	69	GLU
1	D	87	THR
1	D	99	ILE
1	D	110	THR
1	D	135	ASN
1	D	136	ASN
1	D	142	ILE
1	D	143	ARG
1	D	145	LEU
1	D	146	ASN
1	D	155	LEU
1	D	171	ILE
1	D	193	GLU
1	D	202	LEU

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Mol	Chain	Res	Type
1	D	213	LEU
1	D	219	LEU
1	D	225	THR
1	D	229	ILE
1	D	231	LEU
1	D	234	THR
1	D	259	LEU
1	D	260	SER
1	D	271	ARG
1	D	278	LEU
1	D	279	ARG
1	D	291	SER
1	D	295	THR
1	D	297	ILE
1	D	306	LEU
1	D	311	LEU
1	E	14	TYR
1	E	15	ASP
1	E	17	LYS
1	E	25	ARG
1	E	26	LYS
1	E	28	SER
1	E	31	ARG
1	E	39	ARG
1	E	44	ARG
1	E	47	LEU
1	E	57	HIS
1	E	59	VAL
1	E	61	ILE
1	E	65	LEU
1	E	68	LEU
1	E	70	GLU
1	E	74	VAL
1	E	87	THR
1	E	92	ASP
1	E	99	ILE
1	E	110	THR
1	E	119	ARG
1	E	121	THR
1	E	122	ILE
1	E	142	ILE
1	E	147	SER

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Mol	Chain	Res	Type
1	E	161	PRO
1	E	197	GLU
1	E	202	LEU
1	E	211	GLU
1	E	214	THR
1	E	220	VAL
1	E	224	LEU
1	E	235	LEU
1	E	251	ARG
1	E	263	VAL
1	E	270	GLU
1	E	278	LEU
1	E	295	THR
1	E	300	VAL
1	E	304	GLN
1	E	306	LEU
1	F	11	ASP
1	F	22	ARG
1	F	26	LYS
1	F	27	GLU
1	F	34	LEU
1	F	35	ASP
1	F	47	LEU
1	F	53	CYS
1	F	59	VAL
1	F	69	GLU
1	F	70	GLU
1	F	87	THR
1	F	90	PRO
1	F	98	SER
1	F	99	ILE
1	F	100	ASN
1	F	110	THR
1	F	117	THR
1	F	119	ARG
1	F	122	ILE
1	F	136	ASN
1	F	142	ILE
1	F	147	SER
1	F	152	VAL
1	F	193	GLU
1	F	214	THR

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Mol	Chain	Res	Type
1	F	216	ARG
1	F	222	ASP
1	F	223	ARG
1	F	224	LEU
1	F	235	LEU
1	F	236	VAL
1	F	251	ARG
1	F	260	SER
1	F	278	LEU
1	F	279	ARG
1	F	282	LYS
1	F	300	VAL
1	G	3	LEU
1	G	5	ILE
1	G	22	ARG
1	G	23	PHE
1	G	24	VAL
1	G	31	ARG
1	G	34	LEU
1	G	38	PHE
1	G	39	ARG
1	G	47	LEU
1	G	53	CYS
1	G	59	VAL
1	G	87	THR
1	G	93	ASP
1	G	100	ASN
1	G	108	VAL
1	G	110	THR
1	G	115	THR
1	G	136	ASN
1	G	144	ILE
1	G	145	LEU
1	G	147	SER
1	G	181	ASN
1	G	183	VAL
1	G	186	SER
1	G	190	THR
1	G	206	LEU
1	G	209	LEU
1	G	211	GLU
1	G	216	ARG

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Mol	Chain	Res	Type
1	G	222	ASP
1	G	226	GLU
1	G	234	THR
1	G	235	LEU
1	G	278	LEU
1	G	291	SER
1	G	300	VAL
1	H	3	LEU
1	H	5	ILE
1	H	29	GLN
1	H	35	ASP
1	H	44	ARG
1	H	47	LEU
1	H	63	ARG
1	H	69	GLU
1	H	70	GLU
1	H	81	MET
1	H	92	ASP
1	H	93	ASP
1	H	99	ILE
1	H	107	GLN
1	H	110	THR
1	H	119	ARG
1	H	120	VAL
1	H	132	ARG
1	H	136	ASN
1	H	142	ILE
1	H	144	ILE
1	H	145	LEU
1	H	149	PHE
1	H	152	VAL
1	H	170	ARG
1	H	172	ASN
1	H	181	ASN
1	H	191	THR
1	H	197	GLU
1	H	205	THR
1	H	211	GLU
1	H	223	ARG
1	H	234	THR
1	H	235	LEU
1	H	265	LYS

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Mol	Chain	Res	Type
1	H	271	ARG
1	H	277	ASN
1	H	278	LEU
1	H	288	SER
1	H	291	SER
1	H	295	THR
1	H	304	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	136	ASN
1	A	172	ASN
1	A	212	HIS
1	A	243	HIS
1	A	245	HIS
1	A	289	HIS
1	A	304	GLN
1	B	84	ASN
1	B	136	ASN
1	B	172	ASN
1	B	181	ASN
1	B	245	HIS
1	B	289	HIS
1	B	312	GLN
1	C	84	ASN
1	C	136	ASN
1	C	172	ASN
1	C	289	HIS
1	C	304	GLN
1	C	312	GLN
1	D	29	GLN
1	D	136	ASN
1	D	172	ASN
1	D	243	HIS
1	D	245	HIS
1	D	280	HIS
1	D	289	HIS
1	D	293	ASN
1	E	29	GLN
1	E	172	ASN

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Mol	Chain	Res	Type
1	E	180	ASN
1	E	243	HIS
1	E	245	HIS
1	E	289	HIS
1	E	304	GLN
1	F	100	ASN
1	F	136	ASN
1	F	172	ASN
1	F	180	ASN
1	F	181	ASN
1	F	245	HIS
1	F	289	HIS
1	G	29	GLN
1	G	136	ASN
1	G	172	ASN
1	G	180	ASN
1	G	181	ASN
1	G	212	HIS
1	G	245	HIS
1	G	289	HIS
1	G	304	GLN
1	H	29	GLN
1	H	57	HIS
1	H	100	ASN
1	H	136	ASN
1	H	172	ASN
1	H	245	HIS
1	H	249	ASN
1	H	280	HIS
1	H	289	HIS
1	H	304	GLN
1	H	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	312/313 (99%)	-0.59	14 (4%)	38	20	15, 25, 76, 137	0
1	B	303/313 (96%)	-0.35	8 (2%)	57	34	20, 38, 68, 147	0
1	C	312/313 (99%)	-0.31	14 (4%)	38	20	21, 36, 90, 132	0
1	D	312/313 (99%)	-0.15	14 (4%)	38	20	26, 45, 94, 153	0
1	E	312/313 (99%)	-0.19	14 (4%)	38	20	19, 41, 87, 146	0
1	F	308/313 (98%)	-0.51	10 (3%)	50	29	17, 29, 78, 139	0
1	G	305/313 (97%)	-0.11	13 (4%)	40	21	32, 49, 86, 154	0
1	H	309/313 (98%)	0.23	16 (5%)	33	17	36, 63, 99, 164	0
All	All	2473/2504 (98%)	-0.25	103 (4%)	40	22	15, 41, 88, 164	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	13	TRP	8.7
1	H	15	ASP	8.3
1	B	11	ASP	7.3
1	H	309	LEU	6.8
1	G	311	LEU	6.6
1	E	311	LEU	6.2
1	F	16	THR	6.2
1	F	310	THR	5.8
1	C	311	LEU	5.8
1	A	311	LEU	5.8
1	B	310	THR	5.5
1	G	310	THR	5.5
1	H	311	LEU	5.2
1	C	309	LEU	5.1
1	E	18	SER	5.0
1	C	308	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	309	LEU	5.0
1	E	20	GLY	4.9
1	H	310	THR	4.9
1	B	308	GLY	4.8
1	G	312	GLN	4.7
1	D	16	THR	4.5
1	G	21	GLY	4.4
1	D	310	THR	4.4
1	F	307	PRO	4.4
1	B	309	LEU	4.3
1	A	308	GLY	4.2
1	F	311	LEU	4.0
1	A	309	LEU	4.0
1	H	19	SER	4.0
1	G	12	ALA	3.9
1	D	311	LEU	3.9
1	E	19	SER	3.8
1	A	313	SER	3.8
1	G	309	LEU	3.7
1	D	308	GLY	3.6
1	A	14	TYR	3.6
1	C	14	TYR	3.6
1	D	15	ASP	3.6
1	C	13	TRP	3.5
1	D	17	LYS	3.5
1	C	92	ASP	3.4
1	H	13	TRP	3.4
1	F	11	ASP	3.4
1	G	6	ASP	3.4
1	F	17	LYS	3.4
1	F	309	LEU	3.3
1	C	11	ASP	3.3
1	E	14	TYR	3.2
1	B	311	LEU	3.2
1	E	309	LEU	3.2
1	A	310	THR	3.2
1	C	12	ALA	3.2
1	D	13	TRP	3.2
1	E	13	TRP	3.2
1	G	308	GLY	3.2
1	D	307	PRO	3.1
1	A	12	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	313	SER	3.1
1	F	23	PHE	3.0
1	G	307	PRO	3.0
1	D	14	TYR	3.0
1	A	16	THR	3.0
1	H	36	ALA	2.9
1	E	38	PHE	2.9
1	E	17	LYS	2.9
1	B	21	GLY	2.9
1	D	18	SER	2.8
1	E	12	ALA	2.8
1	C	18	SER	2.8
1	H	23	PHE	2.7
1	H	14	TYR	2.7
1	H	12	ALA	2.6
1	A	312	GLN	2.6
1	B	38	PHE	2.5
1	A	18	SER	2.5
1	H	26	LYS	2.5
1	H	21	GLY	2.5
1	A	13	TRP	2.5
1	A	38	PHE	2.5
1	H	20	GLY	2.4
1	G	23	PHE	2.4
1	F	19	SER	2.4
1	G	313	SER	2.4
1	C	16	THR	2.3
1	C	310	THR	2.3
1	E	308	GLY	2.3
1	G	22	ARG	2.3
1	D	21	GLY	2.3
1	C	17	LYS	2.3
1	F	308	GLY	2.2
1	B	23	PHE	2.2
1	H	313	SER	2.2
1	A	307	PRO	2.2
1	E	310	THR	2.1
1	A	15	ASP	2.1
1	E	15	ASP	2.1
1	D	312	GLN	2.1
1	E	21	GLY	2.1
1	C	307	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	307	PRO	2.0
1	C	23	PHE	2.0
1	H	38	PHE	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.