



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:10 AM UTC

PDB ID : 4LQL / pdb_00004lql
Title : Crystal structure of L-arabinose isomerase from Lactobacillus fermentum CGMCC2921
Authors : Xu, Z.
Deposited on : 2013-07-19
Resolution : 3.23 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

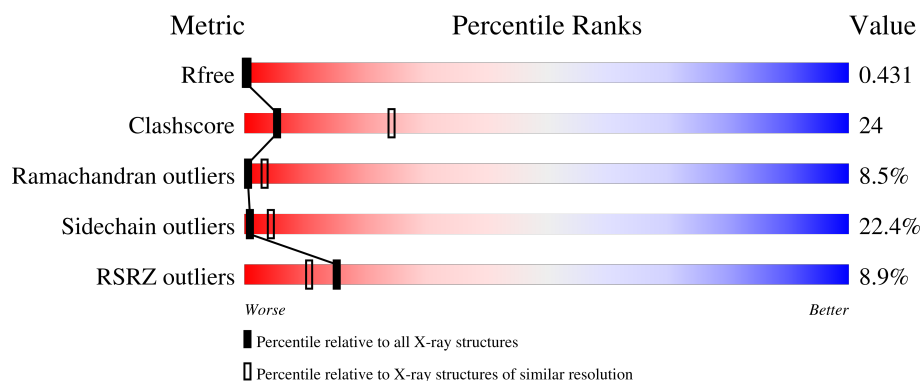
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	474	8% 51% 38% 10%
1	B	474	6% 51% 37% 11%
1	C	474	9% 57% 34% 7%
1	D	474	12% 57% 34% 9%
1	E	474	9% 50% 40% 10%

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Mol	Chain	Length	Quality of chain
1	F	474	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: 10% (red), 50% (green), 41% (yellow), and 9% (orange). The segments are labeled with their respective percentages.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18516 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.

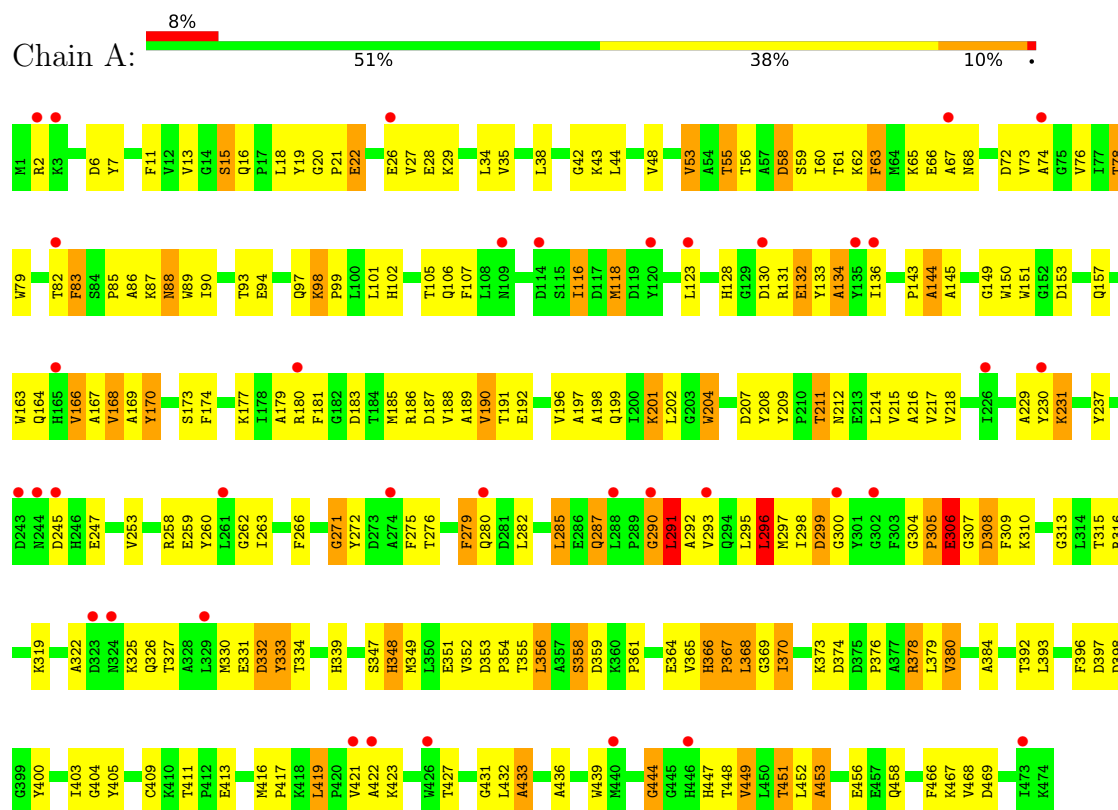
- Molecule 1 is a protein called L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3111	1999	538	566	8			
1	B	474	Total	C	N	O	S	0	0	0
			3130	2013	539	570	8			
1	C	474	Total	C	N	O	S	0	0	0
			3017	1936	517	556	8			
1	D	474	Total	C	N	O	S	0	0	0
			3111	1999	538	566	8			
1	E	474	Total	C	N	O	S	0	0	0
			3130	2013	539	570	8			
1	F	474	Total	C	N	O	S	0	0	0
			3017	1936	517	556	8			

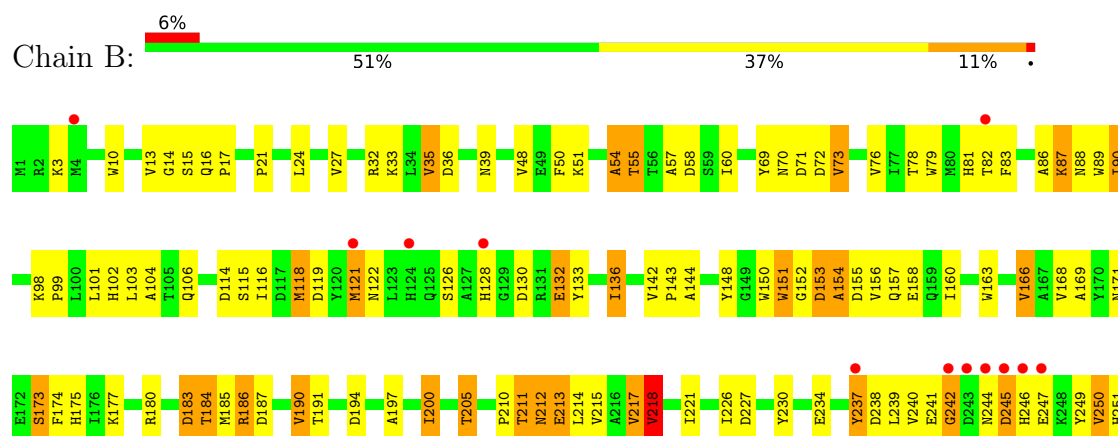
3 Residue-property plots

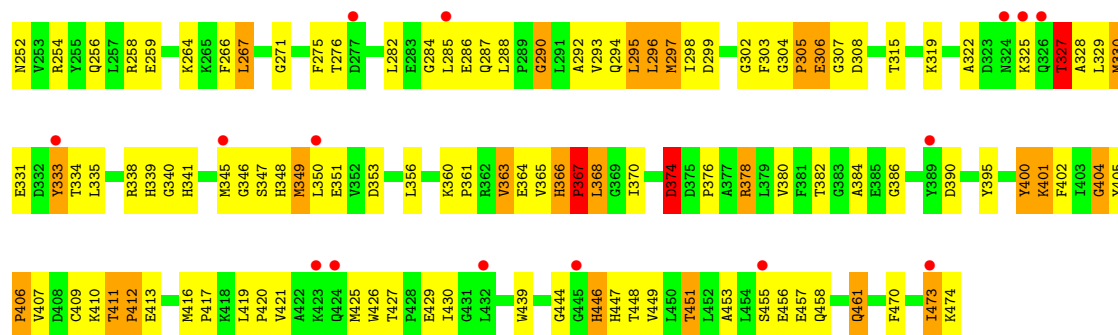
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L-arabinose isomerase

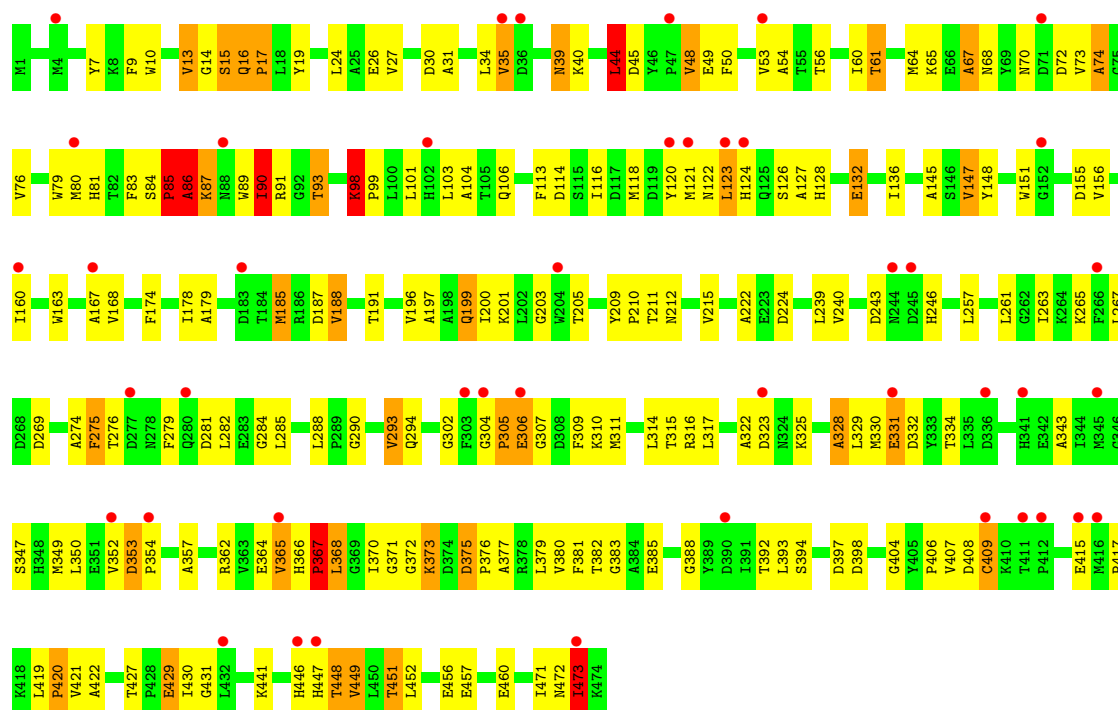


- Molecule 1: L-arabinose isomerase

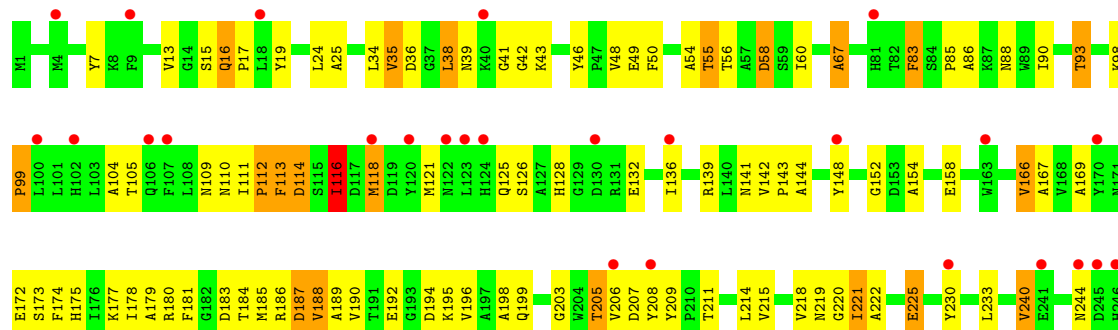


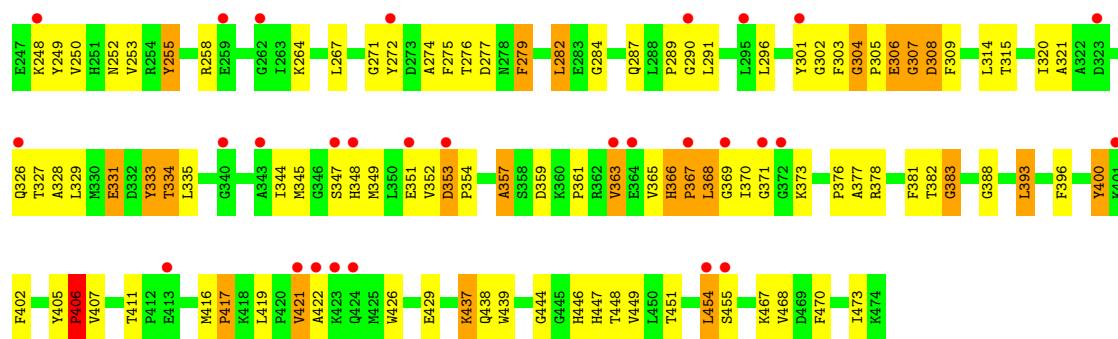


• Molecule 1: L-arabinose isomerase

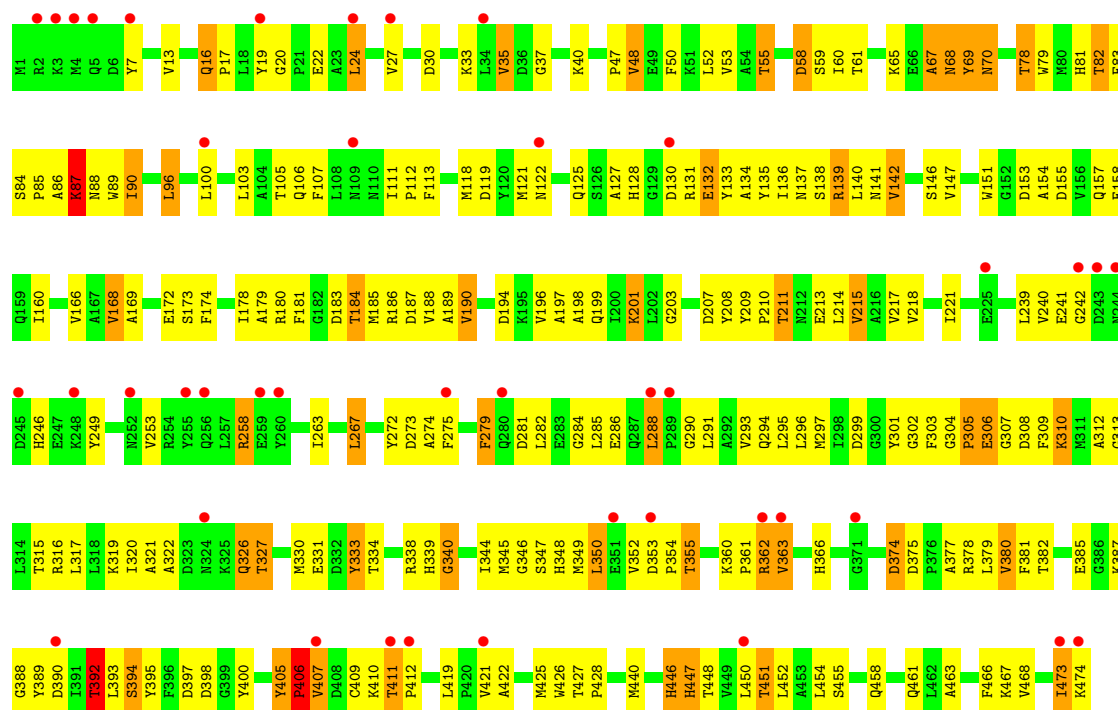


• Molecule 1: L-arabinose isomerase

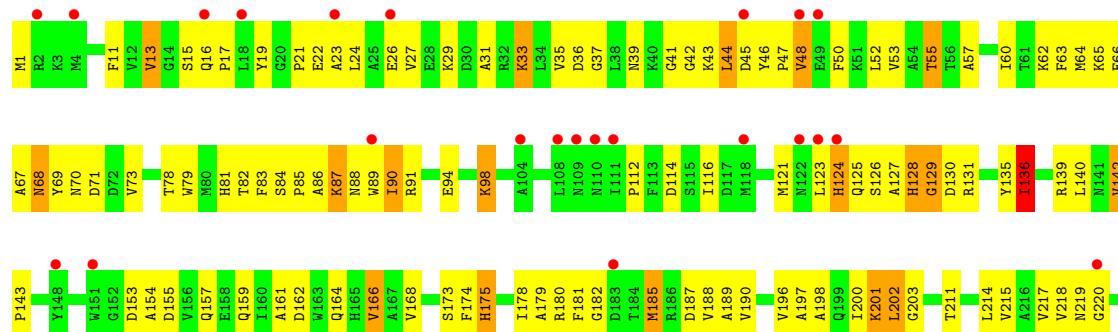


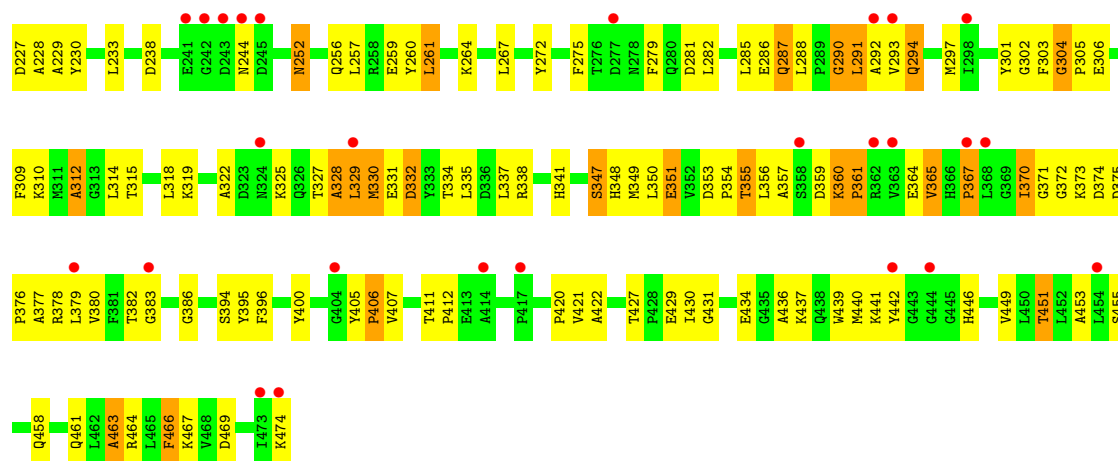


• Molecule 1: L-arabinose isomerase



• Molecule 1: L-arabinose isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.20Å 184.83Å 186.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.85 – 3.23 44.85 – 3.23	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.85-3.23) 99.1 (44.85-3.23)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.314 , 0.432 0.316 , 0.431	Depositor DCC
R_{free} test set	2404 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 135.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18516	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.79	0/3156	1.34	40/4270 (0.9%)
1	B	0.86	0/3176	1.26	25/4293 (0.6%)
1	C	0.71	0/3060	1.24	28/4151 (0.7%)
1	D	0.69	0/3156	1.20	27/4270 (0.6%)
1	E	0.67	0/3176	1.22	24/4293 (0.6%)
1	F	0.77	2/3060 (0.1%)	1.27	33/4151 (0.8%)
All	All	0.75	2/18784 (0.0%)	1.25	177/25428 (0.7%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	175	HIS	CD2-NE2	-7.37	1.29	1.37
1	F	175	HIS	CG-CD2	7.29	1.43	1.35

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	GLY	CA-C-N	16.28	140.19	119.84
1	F	304	GLY	C-N-CA	16.28	140.19	119.84
1	D	16	GLN	CA-C-N	13.54	136.76	119.84
1	D	16	GLN	C-N-CA	13.54	136.76	119.84
1	E	304	GLY	CA-C-N	12.78	135.81	119.84
1	E	304	GLY	C-N-CA	12.78	135.81	119.84
1	A	174	PHE	N-CA-C	-11.18	99.63	113.38
1	C	16	GLN	CA-C-N	11.02	133.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	GLN	C-N-CA	11.02	133.61	119.84
1	B	411	THR	CA-C-N	10.63	133.12	119.84
1	B	411	THR	C-N-CA	10.63	133.12	119.84
1	A	427	THR	CA-C-N	10.56	133.05	119.84
1	A	427	THR	C-N-CA	10.56	133.05	119.84
1	D	304	GLY	CA-C-N	10.49	132.95	119.84
1	D	304	GLY	C-N-CA	10.49	132.95	119.84
1	E	142	VAL	CA-C-N	9.86	132.16	119.84
1	E	142	VAL	C-N-CA	9.86	132.16	119.84
1	D	366	HIS	CA-C-N	9.72	132.00	119.84
1	D	366	HIS	C-N-CA	9.72	132.00	119.84
1	A	149	GLY	N-CA-C	9.56	121.74	112.08
1	E	16	GLN	CA-C-N	9.54	131.76	119.84
1	E	16	GLN	C-N-CA	9.54	131.76	119.84
1	C	304	GLY	CA-C-N	9.53	131.75	119.84
1	C	304	GLY	C-N-CA	9.53	131.75	119.84
1	E	90	ILE	N-CA-C	9.31	119.33	110.30
1	E	405	TYR	CA-C-N	9.16	131.29	119.84
1	E	405	TYR	C-N-CA	9.16	131.29	119.84
1	F	463	ALA	N-CA-C	-9.07	100.96	111.03
1	A	94	GLU	N-CA-C	-8.98	100.65	111.69
1	A	253	VAL	N-CA-C	-8.55	105.58	113.71
1	C	98	LYS	CA-C-N	8.38	128.90	119.93
1	C	98	LYS	C-N-CA	8.38	128.90	119.93
1	A	295	LEU	N-CA-C	-8.36	103.12	112.57
1	B	200	ILE	N-CA-C	-7.97	104.10	111.67
1	A	304	GLY	CA-C-N	7.95	129.77	119.84
1	A	304	GLY	C-N-CA	7.95	129.77	119.84
1	D	240	VAL	N-CA-C	7.93	118.81	108.35
1	F	466	PHE	N-CA-C	-7.87	103.82	113.50
1	B	130	ASP	N-CA-C	-7.85	102.67	111.07
1	D	225	GLU	N-CA-C	-7.56	102.71	112.23
1	D	353	ASP	N-CA-C	7.34	118.59	109.57
1	A	466	PHE	N-CA-C	-7.16	104.55	113.28
1	F	427	THR	CA-C-N	6.98	128.57	119.84
1	F	427	THR	C-N-CA	6.98	128.57	119.84
1	C	87	LYS	N-CA-C	-6.97	103.69	111.28
1	E	258	ARG	N-CA-C	-6.94	104.78	113.18
1	B	330	MET	N-CA-C	6.86	119.57	108.32
1	C	452	LEU	N-CA-C	-6.86	105.45	113.88
1	C	209	TYR	CA-C-N	6.81	129.65	120.79
1	C	209	TYR	C-N-CA	6.81	129.65	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	GLY	N-CA-C	-6.79	104.39	115.46
1	C	328	ALA	N-CA-C	6.75	117.15	108.24
1	A	366	HIS	CA-C-N	6.68	128.19	119.84
1	A	366	HIS	C-N-CA	6.68	128.19	119.84
1	E	52	LEU	N-CA-C	6.62	118.88	110.33
1	E	394	SER	N-CA-C	6.59	118.96	107.49
1	B	3	LYS	N-CA-C	-6.58	104.14	111.71
1	C	353	ASP	CA-C-N	6.57	126.25	119.82
1	C	353	ASP	C-N-CA	6.57	126.25	119.82
1	A	168	VAL	N-CA-C	-6.56	104.15	113.07
1	C	427	THR	CA-C-N	6.54	128.02	119.84
1	C	427	THR	C-N-CA	6.54	128.02	119.84
1	F	386	GLY	N-CA-C	6.48	119.18	110.43
1	C	394	SER	N-CA-C	6.44	120.20	109.95
1	D	255	TYR	N-CA-C	-6.42	105.35	113.43
1	F	140	LEU	N-CA-C	-6.42	105.03	112.92
1	B	190	VAL	CB-CA-C	-6.36	102.77	112.05
1	A	291	LEU	N-CA-C	-6.33	105.45	113.43
1	A	188	VAL	N-CA-C	6.30	117.56	108.48
1	F	405	TYR	CA-C-N	6.26	126.03	119.76
1	F	405	TYR	C-N-CA	6.26	126.03	119.76
1	F	360	LYS	CA-C-N	6.25	127.65	119.84
1	F	360	LYS	C-N-CA	6.25	127.65	119.84
1	E	411	THR	CA-C-N	6.24	127.10	120.11
1	E	411	THR	C-N-CA	6.24	127.10	120.11
1	D	321	ALA	N-CA-C	-6.24	102.95	111.56
1	B	251	HIS	N-CA-C	-6.23	105.16	112.89
1	B	144	ALA	N-CA-C	6.22	117.91	110.19
1	A	208	TYR	N-CA-C	6.21	118.53	108.41
1	F	396	PHE	N-CA-C	6.17	118.43	110.65
1	A	28	GLU	N-CA-C	-6.16	105.25	112.89
1	B	54	ALA	N-CA-C	6.16	118.72	108.20
1	F	351	GLU	N-CA-C	6.14	119.35	108.24
1	E	330	MET	N-CA-C	6.14	119.28	107.44
1	C	343	ALA	N-CA-C	6.13	116.33	108.24
1	A	167	ALA	N-CA-C	-6.12	106.41	114.31
1	E	288	LEU	CA-C-N	6.10	126.12	119.90
1	E	288	LEU	C-N-CA	6.10	126.12	119.90
1	A	468	VAL	N-CA-C	-6.08	106.84	112.43
1	E	20	GLY	CA-C-N	6.05	125.93	119.28
1	E	20	GLY	C-N-CA	6.05	125.93	119.28
1	A	7	TYR	N-CA-C	6.04	119.36	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	TYR	N-CA-C	-6.03	104.34	111.03
1	A	392	THR	N-CA-C	6.03	116.04	108.45
1	B	410	LYS	N-CA-C	5.99	117.30	108.86
1	F	48	VAL	N-CA-C	5.97	116.54	108.17
1	B	404	GLY	N-CA-C	5.96	127.31	113.18
1	D	195	LYS	N-CA-C	-5.96	106.55	113.88
1	D	67	ALA	N-CA-C	-5.95	105.51	112.89
1	E	392	THR	N-CA-C	5.89	117.59	109.29
1	E	296	LEU	N-CA-C	-5.88	106.74	114.04
1	C	366	HIS	CA-C-N	5.88	127.19	119.84
1	C	366	HIS	C-N-CA	5.88	127.19	119.84
1	B	116	ILE	N-CA-C	5.87	115.80	106.88
1	C	188	VAL	N-CA-C	5.85	116.73	108.36
1	F	52	LEU	N-CA-C	5.84	119.29	110.64
1	B	234	GLU	N-CA-C	-5.83	105.66	112.89
1	E	48	VAL	N-CA-C	5.73	116.30	110.05
1	A	134	ALA	N-CA-C	5.73	117.52	111.28
1	F	202	LEU	N-CA-C	-5.71	104.86	113.89
1	C	67	ALA	N-CA-C	-5.71	105.65	113.30
1	F	302	GLY	N-CA-C	5.71	120.88	110.95
1	A	296	LEU	N-CA-C	-5.70	106.97	114.04
1	C	473	ILE	N-CA-C	5.70	121.19	109.34
1	A	98	LYS	CA-C-N	-5.70	112.56	120.25
1	A	98	LYS	C-N-CA	-5.70	112.56	120.25
1	B	98	LYS	CA-C-N	5.68	126.94	119.84
1	B	98	LYS	C-N-CA	5.68	126.94	119.84
1	A	214	LEU	N-CA-C	-5.65	106.39	113.28
1	D	405	TYR	CA-C-N	5.64	126.89	119.84
1	D	405	TYR	C-N-CA	5.64	126.89	119.84
1	A	280	GLN	N-CA-C	-5.63	105.09	112.41
1	F	469	ASP	N-CA-C	5.60	118.66	107.62
1	F	142	VAL	CA-C-N	5.59	126.83	119.84
1	F	142	VAL	C-N-CA	5.59	126.83	119.84
1	E	189	ALA	N-CA-C	5.58	120.08	112.04
1	A	116	ILE	N-CA-C	5.55	115.68	108.35
1	A	130	ASP	N-CA-C	-5.55	106.34	113.23
1	A	452	LEU	N-CA-C	-5.55	106.58	113.19
1	B	366	HIS	CA-C-N	5.50	126.72	119.84
1	B	366	HIS	C-N-CA	5.50	126.72	119.84
1	F	189	ALA	N-CA-C	5.50	119.71	111.96
1	B	430	ILE	CB-CA-C	-5.49	102.28	111.29
1	F	175	HIS	CB-CA-C	-5.44	100.34	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	GLY	N-CA-C	5.40	118.59	111.03
1	F	357	ALA	N-CA-C	5.38	115.65	108.38
1	A	396	PHE	N-CA-C	5.38	118.92	111.55
1	E	130	ASP	N-CA-C	-5.37	106.60	112.72
1	D	142	VAL	CA-C-N	5.32	126.49	119.84
1	D	142	VAL	C-N-CA	5.32	126.49	119.84
1	D	320	ILE	N-CA-C	-5.31	107.80	112.90
1	C	275	PHE	N-CA-C	5.30	117.03	109.14
1	A	98	LYS	N-CA-C	5.29	117.50	109.41
1	F	294	GLN	N-CA-C	-5.28	106.78	114.12
1	A	369	GLY	N-CA-C	-5.24	107.83	114.16
1	C	86	ALA	N-CA-C	5.23	121.94	110.80
1	A	88	ASN	N-CA-C	-5.23	106.95	113.38
1	B	173	SER	N-CA-C	-5.21	105.68	111.36
1	D	388	GLY	N-CA-C	5.20	118.66	110.91
1	F	87	LYS	N-CA-C	-5.18	106.66	112.87
1	D	46	TYR	CA-C-N	-5.17	114.59	119.76
1	D	46	TYR	C-N-CA	-5.17	114.59	119.76
1	D	426	TRP	N-CA-C	5.17	116.70	108.79
1	C	84	SER	CA-C-N	5.17	126.30	119.84
1	C	84	SER	C-N-CA	5.17	126.30	119.84
1	A	333	TYR	N-CA-C	5.16	119.63	113.23
1	A	144	ALA	N-CA-C	5.15	121.78	110.80
1	B	297	MET	N-CA-C	-5.14	105.76	111.36
1	F	411	THR	CA-C-N	5.12	126.24	119.84
1	F	411	THR	C-N-CA	5.12	126.24	119.84
1	F	328	ALA	N-CA-C	5.11	116.60	108.79
1	D	331	GLU	N-CA-C	-5.10	102.61	109.95
1	D	363	VAL	N-CA-C	5.10	116.53	109.29
1	A	313	GLY	N-CA-C	5.09	120.32	114.16
1	F	136	ILE	N-CA-C	5.09	119.22	111.89
1	A	58	ASP	N-CA-C	-5.08	106.25	112.90
1	A	187	ASP	N-CA-C	5.07	118.59	111.74
1	F	261	LEU	N-CA-C	-5.06	105.95	112.68
1	F	256	GLN	N-CA-C	-5.06	105.90	113.89
1	B	427	THR	CA-C-N	5.05	126.15	119.84
1	B	427	THR	C-N-CA	5.05	126.15	119.84
1	D	400	TYR	N-CA-C	5.04	117.90	110.59
1	C	329	LEU	N-CA-C	5.02	117.42	109.24
1	B	205	THR	N-CA-C	5.01	116.56	108.34
1	D	43	LYS	N-CA-C	-5.01	104.32	111.24
1	D	205	THR	N-CA-C	5.00	115.57	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	291	LEU	N-CA-C	-5.00	106.02	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3111	0	2557	138	0
1	B	3130	0	2581	154	0
1	C	3017	0	2377	130	0
1	D	3111	0	2557	129	0
1	E	3130	0	2581	161	0
1	F	3017	0	2377	161	0
All	All	18516	0	15030	804	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 24.

All (804) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:GLN:HE21	1:C:352:VAL:H	1.20	0.89
1:A:439:TRP:NE1	1:A:444:GLY:O	2.07	0.88
1:A:308:ASP:OD2	1:A:447:HIS:ND1	2.07	0.87
1:A:85:PRO:HB3	1:C:188:VAL:HG22	1.58	0.86
1:A:192:GLU:O	1:A:310:LYS:NZ	2.09	0.85
1:C:305:PRO:O	1:C:307:GLY:N	2.11	0.82
1:F:331:GLU:OE2	1:F:348:HIS:NE2	2.12	0.82
1:F:35:VAL:O	1:F:39:ASN:ND2	2.14	0.80
1:C:322:ALA:HB1	1:C:325:LYS:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:VAL:O	1:F:98:LYS:NZ	2.17	0.77
1:E:338:ARG:O	1:E:340:GLY:N	2.18	0.77
1:B:194:ASP:HB3	1:B:197:ALA:HB3	1.66	0.77
1:B:416:MET:HB3	1:B:419:LEU:HB3	1.65	0.77
1:F:463:ALA:O	1:F:466:PHE:N	2.18	0.77
1:B:183:ASP:OD1	1:B:184:THR:N	2.16	0.77
1:A:285:LEU:O	1:A:373:LYS:NZ	2.15	0.76
1:D:331:GLU:HG3	1:D:447:HIS:HD2	1.51	0.76
1:D:308:ASP:OD2	1:D:447:HIS:ND1	2.17	0.76
1:A:183:ASP:OD2	1:E:180:ARG:NH2	2.19	0.76
1:A:331:GLU:OE2	1:A:348:HIS:NE2	2.19	0.76
1:E:282:LEU:HD11	1:E:288:LEU:HD13	1.68	0.75
1:E:331:GLU:OE2	1:E:348:HIS:NE2	2.20	0.75
1:B:406:PRO:HB2	1:B:474:LYS:HB2	1.69	0.74
1:C:67:ALA:HB1	1:C:73:VAL:HG11	1.70	0.74
1:A:199:GLN:NE2	1:F:87:LYS:O	2.20	0.74
1:C:106:GLN:NE2	1:C:124:HIS:O	2.20	0.73
1:E:361:PRO:O	1:E:363:VAL:N	2.20	0.73
1:E:409:CYS:HB2	1:E:426:TRP:HB3	1.70	0.73
1:F:458:GLN:HA	1:F:461:GLN:HE21	1.53	0.73
1:E:319:LYS:NZ	1:E:327:THR:O	2.21	0.73
1:D:166:VAL:O	1:D:169:ALA:N	2.22	0.73
1:E:86:ALA:O	1:E:89:TRP:N	2.20	0.72
1:F:463:ALA:O	1:F:467:LYS:N	2.19	0.72
1:B:455:SER:O	1:B:457:GLU:N	2.22	0.72
1:E:253:VAL:HG22	1:E:377:ALA:HB2	1.71	0.72
1:E:446:HIS:HB3	1:F:128:HIS:HB3	1.71	0.72
1:F:364:GLU:HA	1:F:377:ALA:HA	1.71	0.72
1:B:78:THR:O	1:B:103:LEU:N	2.19	0.72
1:C:288:LEU:HD21	1:C:349:MET:HE3	1.70	0.72
1:A:451:THR:O	1:A:451:THR:OG1	2.08	0.71
1:C:64:MET:O	1:C:68:ASN:ND2	2.23	0.71
1:C:73:VAL:O	1:C:98:LYS:NZ	2.23	0.71
1:B:405:TYR:HA	1:B:473:ILE:O	1.91	0.71
1:E:137:ASN:O	1:E:139:ARG:N	2.25	0.70
1:D:357:ALA:HA	1:D:383:GLY:HA2	1.73	0.70
1:B:347:SER:OG	1:B:348:HIS:N	2.24	0.70
1:E:166:VAL:HG11	1:E:461:GLN:HB2	1.74	0.70
1:A:15:SER:O	1:A:55:THR:HA	1.92	0.70
1:B:256:GLN:HA	1:B:259:GLU:HB2	1.73	0.70
1:A:305:PRO:O	1:A:307:GLY:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:MET:HB3	1:F:353:ASP:CG	2.17	0.69
1:A:364:GLU:O	1:A:378:ARG:NH1	2.24	0.69
1:B:446:HIS:H	1:B:446:HIS:CD2	2.07	0.69
1:E:446:HIS:HE1	1:F:83:PHE:CZ	2.10	0.69
1:A:61:THR:O	1:A:65:LYS:HB2	1.94	0.68
1:B:221:ILE:O	1:B:258:ARG:NH2	2.26	0.68
1:A:131:ARG:NH1	1:C:332:ASP:OD1	2.26	0.68
1:B:104:ALA:HB3	1:B:148:TYR:HA	1.76	0.67
1:C:448:THR:OG1	1:C:449:VAL:N	2.27	0.66
1:B:87:LYS:HE3	1:E:199:GLN:OE1	1.96	0.66
1:A:319:LYS:NZ	1:A:327:THR:O	2.28	0.66
1:D:282:LEU:HB2	1:D:373:LYS:HE3	1.78	0.66
1:D:378:ARG:HG3	1:D:421:VAL:HG13	1.76	0.66
1:A:332:ASP:O	1:B:128:HIS:HB3	1.95	0.66
1:A:73:VAL:O	1:A:98:LYS:HE2	1.94	0.66
1:B:16:GLN:HA	1:B:55:THR:HG22	1.77	0.66
1:D:54:ALA:HB1	1:D:60:ILE:HG12	1.76	0.66
1:B:345:MET:HA	1:B:425:MET:HA	1.79	0.65
1:F:125:GLN:OE1	1:F:128:HIS:NE2	2.28	0.65
1:B:227:ASP:HA	1:B:230:TYR:HB3	1.78	0.65
1:E:294:GLN:HE21	1:E:352:VAL:H	1.44	0.65
1:E:137:ASN:C	1:E:139:ARG:H	2.04	0.65
1:B:306:GLU:OE2	1:B:447:HIS:NE2	2.24	0.65
1:E:347:SER:OG	1:E:348:HIS:N	2.29	0.65
1:A:347:SER:OG	1:A:348:HIS:N	2.27	0.65
1:C:116:ILE:HG13	1:C:120:TYR:HB3	1.79	0.64
1:A:6:ASP:O	1:A:72:ASP:HB3	1.98	0.64
1:E:133:TYR:O	1:E:136:ILE:HG22	1.97	0.64
1:C:90:ILE:O	1:C:93:THR:N	2.31	0.64
1:A:118:MET:SD	1:A:118:MET:N	2.67	0.64
1:E:313:GLY:O	1:E:317:LEU:N	2.28	0.64
1:D:331:GLU:OE2	1:D:447:HIS:NE2	2.31	0.64
1:F:128:HIS:CD2	1:F:129:GLY:H	2.15	0.63
1:E:446:HIS:O	1:E:448:THR:N	2.30	0.63
1:A:199:GLN:HE22	1:F:87:LYS:HB3	1.63	0.63
1:D:306:GLU:C	1:D:308:ASP:H	2.07	0.63
1:A:358:SER:OG	1:A:359:ASP:N	2.26	0.63
1:A:376:PRO:O	1:A:378:ARG:NH2	2.30	0.63
1:F:309:PHE:HA	1:F:312:ALA:HB3	1.80	0.63
1:D:348:HIS:ND1	1:D:351:GLU:OE2	2.32	0.63
1:E:344:ILE:O	1:E:426:TRP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:LEU:HB3	1:E:378:ARG:HA	1.81	0.63
1:E:79:TRP:NE1	1:E:105:THR:O	2.32	0.63
1:C:26:GLU:O	1:C:30:ASP:N	2.30	0.63
1:F:37:GLY:O	1:F:41:GLY:N	2.29	0.63
1:B:27:VAL:HG12	1:B:81:HIS:CD2	2.34	0.62
1:F:62:LYS:HA	1:F:65:LYS:HB2	1.81	0.62
1:B:366:HIS:O	1:B:368:LEU:N	2.32	0.62
1:F:297:MET:SD	1:F:353:ASP:HB2	2.38	0.62
1:D:35:VAL:HG21	1:D:50:PHE:HB2	1.80	0.62
1:B:173:SER:C	1:B:175:HIS:H	2.07	0.62
1:D:279:PHE:HD2	1:D:279:PHE:H	1.47	0.62
1:F:35:VAL:HG21	1:F:50:PHE:HB2	1.81	0.62
1:F:121:MET:O	1:F:125:GLN:NE2	2.31	0.62
1:F:173:SER:C	1:F:175:HIS:H	2.05	0.62
1:B:338:ARG:O	1:B:340:GLY:N	2.33	0.62
1:C:14:GLY:HA2	1:C:54:ALA:HB3	1.81	0.62
1:D:118:MET:HE1	1:F:370:ILE:HD11	1.82	0.62
1:D:190:VAL:HG23	1:E:132:GLU:OE2	1.98	0.62
1:D:314:LEU:HD13	1:D:393:LEU:HD13	1.81	0.62
1:C:199:GLN:CD	1:D:90:ILE:HG13	2.25	0.62
1:E:305:PRO:O	1:E:307:GLY:N	2.28	0.62
1:D:173:SER:C	1:D:175:HIS:H	2.08	0.62
1:A:431:GLY:O	1:A:433:ALA:N	2.31	0.61
1:A:403:ILE:O	1:A:405:TYR:N	2.33	0.61
1:B:305:PRO:O	1:B:307:GLY:N	2.30	0.61
1:A:331:GLU:OE2	1:A:447:HIS:NE2	2.34	0.61
1:B:163:TRP:O	1:B:166:VAL:N	2.30	0.61
1:F:291:LEU:HA	1:F:294:GLN:OE1	2.01	0.61
1:A:166:VAL:HG11	1:A:458:GLN:O	2.01	0.61
1:C:457:GLU:HA	1:C:460:GLU:HB2	1.83	0.61
1:C:364:GLU:HA	1:C:377:ALA:HA	1.82	0.61
1:F:267:LEU:O	1:F:272:TYR:N	2.33	0.61
1:B:86:ALA:O	1:B:88:ASN:N	2.34	0.60
1:B:368:LEU:HD23	1:B:370:ILE:O	2.00	0.60
1:B:249:TYR:O	1:B:252:ASN:ND2	2.27	0.60
1:D:132:GLU:OE2	1:F:190:VAL:N	2.21	0.60
1:E:187:ASP:O	1:F:85:PRO:HB3	2.01	0.60
1:F:395:TYR:HB2	1:F:400:TYR:CE1	2.35	0.60
1:A:189:ALA:HB2	1:B:86:ALA:HB3	1.82	0.60
1:B:322:ALA:HB1	1:B:325:LYS:HB2	1.83	0.60
1:C:265:LYS:O	1:C:269:ASP:N	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HA	1:A:299:ASP:HB2	1.84	0.60
1:C:282:LEU:HD22	1:C:285:LEU:HD12	1.82	0.60
1:B:86:ALA:O	1:B:89:TRP:N	2.27	0.60
1:E:127:ALA:O	1:E:131:ARG:NH1	2.34	0.60
1:B:14:GLY:O	1:B:15:SER:OG	2.20	0.59
1:B:333:TYR:H	1:B:346:GLY:HA2	1.66	0.59
1:D:36:ASP:HA	1:D:39:ASN:ND2	2.17	0.59
1:E:35:VAL:HG21	1:E:50:PHE:HB2	1.84	0.59
1:B:333:TYR:CE1	1:C:121:MET:HE3	2.37	0.59
1:E:344:ILE:N	1:E:426:TRP:O	2.24	0.59
1:F:291:LEU:HB2	1:F:378:ARG:HA	1.85	0.59
1:A:128:HIS:ND1	1:C:332:ASP:O	2.35	0.59
1:E:140:LEU:O	1:E:142:VAL:N	2.35	0.59
1:B:186:ARG:HD3	1:D:208:TYR:O	2.03	0.59
1:C:179:ALA:H	1:C:275:PHE:HA	1.67	0.59
1:D:13:VAL:O	1:D:54:ALA:N	2.34	0.59
1:D:334:THR:O	1:D:345:MET:N	2.25	0.59
1:E:125:GLN:HB2	1:E:128:HIS:HE1	1.68	0.59
1:C:263:ILE:O	1:C:267:LEU:N	2.21	0.58
1:B:153:ASP:O	1:B:156:VAL:N	2.36	0.58
1:D:180:ARG:HD2	1:D:206:VAL:CG1	2.32	0.58
1:D:184:THR:HA	1:D:307:GLY:HA3	1.86	0.58
1:C:27:VAL:HG13	1:C:123:LEU:HD11	1.84	0.58
1:F:322:ALA:HA	1:F:325:LYS:HB2	1.84	0.58
1:A:34:LEU:O	1:A:38:LEU:HG	2.02	0.58
1:D:58:ASP:OD2	1:D:58:ASP:N	2.35	0.58
1:E:361:PRO:HD2	1:E:380:VAL:O	2.03	0.58
1:C:185:MET:HE2	1:C:306:GLU:HG2	1.84	0.58
1:E:390:ASP:O	1:E:405:TYR:N	2.36	0.58
1:A:333:TYR:HE1	1:A:348:HIS:HA	1.67	0.58
1:C:90:ILE:HG22	1:C:91:ARG:N	2.18	0.58
1:B:180:ARG:NH2	1:D:183:ASP:OD2	2.36	0.58
1:D:222:ALA:HB3	1:D:225:GLU:HB2	1.86	0.58
1:A:101:LEU:HD22	1:A:163:TRP:CE3	2.39	0.58
1:B:245:ASP:O	1:B:246:HIS:ND1	2.36	0.58
1:A:347:SER:HB3	1:A:423:LYS:HB3	1.85	0.57
1:E:390:ASP:HB3	1:E:405:TYR:HB2	1.85	0.57
1:E:111:ILE:O	1:E:113:PHE:N	2.38	0.57
1:F:406:PRO:HB2	1:F:474:LYS:HA	1.84	0.57
1:A:86:ALA:HA	1:A:89:TRP:HD1	1.69	0.57
1:B:15:SER:OG	1:B:82:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:TRP:NE1	1:B:444:GLY:O	2.37	0.57
1:C:311:MET:HA	1:C:314:LEU:HB3	1.87	0.57
1:A:164:GLN:O	1:A:168:VAL:HG23	2.03	0.57
1:D:296:LEU:O	1:D:301:TYR:HB2	2.04	0.57
1:C:281:ASP:O	1:C:282:LEU:HD23	2.05	0.57
1:B:334:THR:OG1	1:B:335:LEU:N	2.38	0.57
1:D:16:GLN:HB3	1:D:19:TYR:CZ	2.40	0.57
1:F:420:PRO:HG2	1:F:421:VAL:HG23	1.84	0.57
1:A:150:TRP:HB3	1:A:153:ASP:HB2	1.87	0.57
1:D:407:VAL:HA	1:D:429:GLU:HB2	1.86	0.57
1:F:125:GLN:HB2	1:F:128:HIS:HE2	1.69	0.57
1:B:356:LEU:O	1:B:384:ALA:N	2.38	0.57
1:C:39:ASN:OD1	1:C:39:ASN:N	2.35	0.57
1:F:166:VAL:HG11	1:F:461:GLN:HB2	1.86	0.57
1:E:96:LEU:HD21	1:E:100:LEU:HD13	1.87	0.56
1:E:378:ARG:HG2	1:E:379:LEU:O	2.05	0.56
1:C:330:MET:O	1:C:448:THR:HG23	2.05	0.56
1:E:82:THR:OG1	1:E:83:PHE:N	2.34	0.56
1:E:360:LYS:HA	1:E:381:PHE:HB3	1.86	0.56
1:F:310:LYS:O	1:F:314:LEU:HB2	2.06	0.56
1:C:15:SER:OG	1:C:16:GLN:N	2.39	0.56
1:E:172:GLU:C	1:E:174:PHE:H	2.11	0.56
1:F:304:GLY:HA3	1:F:312:ALA:HB2	1.86	0.56
1:D:178:ILE:O	1:D:207:ASP:N	2.37	0.56
1:B:214:LEU:HD23	1:B:285:LEU:HD21	1.87	0.56
1:F:84:SER:OG	1:F:89:TRP:NE1	2.37	0.56
1:E:275:PHE:CE1	1:E:303:PHE:HB2	2.40	0.56
1:B:240:VAL:O	1:B:242:GLY:N	2.39	0.56
1:B:14:GLY:HA2	1:B:54:ALA:HB3	1.88	0.56
1:B:361:PRO:HD2	1:B:380:VAL:O	2.06	0.56
1:E:33:LYS:O	1:E:37:GLY:N	2.26	0.56
1:A:275:PHE:CE1	1:A:296:LEU:HD13	2.41	0.55
1:F:13:VAL:HA	1:F:79:TRP:O	2.05	0.55
1:B:194:ASP:N	1:B:400:TYR:OH	2.33	0.55
1:C:328:ALA:HB1	1:C:353:ASP:HB3	1.86	0.55
1:E:7:TYR:HD2	1:E:168:VAL:HG22	1.71	0.55
1:C:35:VAL:HG11	1:C:50:PHE:HB2	1.88	0.55
1:D:180:ARG:N	1:D:207:ASP:O	2.36	0.55
1:E:303:PHE:CZ	1:E:305:PRO:HA	2.41	0.55
1:F:70:ASN:O	1:F:73:VAL:HG12	2.06	0.55
1:C:239:LEU:HB3	1:C:243:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ALA:HB3	1:D:148:TYR:CG	2.42	0.55
1:D:34:LEU:O	1:D:38:LEU:HB2	2.06	0.55
1:D:219:ASN:O	1:D:258:ARG:NH1	2.40	0.55
1:E:86:ALA:N	1:E:132:GLU:OE1	2.28	0.55
1:E:333:TYR:H	1:E:346:GLY:HA2	1.72	0.55
1:E:172:GLU:O	1:E:174:PHE:N	2.40	0.55
1:F:197:ALA:O	1:F:201:LYS:HB2	2.05	0.55
1:C:34:LEU:HA	1:C:151:TRP:CZ3	2.42	0.54
1:C:210:PRO:O	1:C:212:ASN:N	2.40	0.54
1:F:185:MET:HE2	1:F:306:GLU:HB3	1.88	0.54
1:A:86:ALA:O	1:A:89:TRP:N	2.29	0.54
1:F:185:MET:HE2	1:F:306:GLU:CB	2.37	0.54
1:A:16:GLN:HG2	1:A:18:LEU:H	1.71	0.54
1:B:305:PRO:C	1:B:307:GLY:H	2.15	0.54
1:C:371:GLY:O	1:C:373:LYS:N	2.39	0.54
1:B:420:PRO:HD2	1:B:421:VAL:HG23	1.89	0.54
1:C:275:PHE:HZ	1:C:293:VAL:HG13	1.70	0.54
1:E:291:LEU:O	1:E:295:LEU:N	2.39	0.54
1:C:118:MET:O	1:C:122:ASN:N	2.41	0.54
1:F:287:GLN:HG3	1:F:376:PRO:HB3	1.90	0.54
1:E:294:GLN:HG2	1:E:354:PRO:HD3	1.89	0.54
1:B:294:GLN:HA	1:B:297:MET:HE3	1.89	0.53
1:D:179:ALA:HB2	1:D:272:TYR:CG	2.43	0.53
1:F:429:GLU:C	1:F:431:GLY:H	2.15	0.53
1:B:10:TRP:CE2	1:B:51:LYS:HE3	2.42	0.53
1:B:10:TRP:CZ2	1:B:51:LYS:HE3	2.44	0.53
1:B:296:LEU:HA	1:B:299:ASP:HB2	1.90	0.53
1:E:463:ALA:O	1:E:467:LYS:N	2.40	0.53
1:F:257:LEU:C	1:F:259:GLU:H	2.16	0.53
1:F:288:LEU:HD23	1:F:350:LEU:HD12	1.89	0.53
1:A:322:ALA:HB1	1:A:325:LYS:HB2	1.90	0.53
1:F:218:VAL:C	1:F:220:GLY:H	2.17	0.53
1:F:436:ALA:HA	1:F:439:TRP:HB3	1.90	0.53
1:A:128:HIS:HB3	1:C:332:ASP:HB3	1.90	0.53
1:C:331:GLU:OE2	1:C:447:HIS:NE2	2.36	0.53
1:E:187:ASP:C	1:F:87:LYS:HG3	2.33	0.53
1:E:392:THR:OG1	1:E:393:LEU:N	2.39	0.53
1:B:70:ASN:O	1:B:72:ASP:N	2.42	0.53
1:C:14:GLY:HA3	1:C:80:MET:HA	1.90	0.53
1:D:186:ARG:C	1:D:188:VAL:H	2.17	0.53
1:F:173:SER:O	1:F:175:HIS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:PHE:O	1:B:470:PHE:HA	2.09	0.53
1:A:218:VAL:HG13	1:A:258:ARG:O	2.09	0.53
1:B:276:THR:HG22	1:B:304:GLY:O	2.09	0.53
1:C:197:ALA:HB2	1:D:139:ARG:HH21	1.72	0.53
1:D:177:LYS:NZ	1:D:271:GLY:HA3	2.23	0.53
1:A:322:ALA:HB1	1:A:325:LYS:CB	2.38	0.53
1:E:194:ASP:HB3	1:E:197:ALA:HB3	1.90	0.53
1:E:267:LEU:HD12	1:E:301:TYR:CD2	2.44	0.53
1:E:385:GLU:HA	1:E:410:LYS:HA	1.90	0.53
1:F:331:GLU:HG3	1:F:446:HIS:O	2.08	0.53
1:F:353:ASP:O	1:F:355:THR:N	2.41	0.53
1:C:199:GLN:OE1	1:D:90:ILE:HG13	2.10	0.52
1:F:81:HIS:CE1	1:F:124:HIS:H	2.27	0.52
1:A:86:ALA:O	1:A:88:ASN:N	2.42	0.52
1:B:10:TRP:CD2	1:B:51:LYS:HG3	2.43	0.52
1:C:9:PHE:C	1:C:10:TRP:HD1	2.17	0.52
1:C:81:HIS:O	1:C:126:SER:OG	2.19	0.52
1:D:186:ARG:O	1:D:188:VAL:N	2.42	0.52
1:A:181:PHE:HE2	1:A:266:PHE:HE2	1.56	0.52
1:B:451:THR:C	1:B:453:ALA:H	2.17	0.52
1:C:196:VAL:O	1:C:200:ILE:HG13	2.10	0.52
1:D:329:LEU:HA	1:D:449:VAL:HA	1.92	0.52
1:B:190:VAL:HG23	1:B:191:THR:HG23	1.92	0.52
1:C:7:TYR:HB3	1:C:74:ALA:HB2	1.92	0.52
1:E:302:GLY:HA3	1:E:316:ARG:HB2	1.91	0.52
1:B:303:PHE:CZ	1:B:305:PRO:HA	2.45	0.52
1:E:154:ALA:HA	1:E:157:GLN:HB2	1.92	0.52
1:D:112:PRO:O	1:D:114:ASP:N	2.40	0.52
1:D:274:ALA:HA	1:D:302:GLY:O	2.09	0.52
1:D:368:LEU:HD22	1:D:376:PRO:HG3	1.91	0.52
1:A:436:ALA:O	1:A:439:TRP:N	2.40	0.52
1:B:169:ALA:C	1:B:171:ASN:H	2.16	0.52
1:A:275:PHE:CZ	1:A:293:VAL:HG22	2.45	0.52
1:A:291:LEU:HG	1:A:379:LEU:HB2	1.91	0.52
1:D:333:TYR:HD1	1:D:347:SER:O	1.92	0.52
1:E:446:HIS:CE1	1:F:83:PHE:CZ	2.96	0.52
1:A:105:THR:OG1	1:A:106:GLN:N	2.43	0.51
1:A:180:ARG:HG2	1:A:276:THR:OG1	2.10	0.51
1:D:85:PRO:HB3	1:F:187:ASP:O	2.09	0.51
1:D:189:ALA:HB2	1:E:87:LYS:H	1.74	0.51
1:D:219:ASN:O	1:D:221:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:LYS:C	1:D:439:TRP:H	2.18	0.51
1:E:194:ASP:O	1:E:400:TYR:OH	2.28	0.51
1:C:156:VAL:O	1:C:160:ILE:HG13	2.10	0.51
1:E:174:PHE:HA	1:E:203:GLY:HA3	1.91	0.51
1:B:87:LYS:HA	1:B:90:ILE:HG13	1.91	0.51
1:B:328:ALA:O	1:B:449:VAL:HG13	2.10	0.51
1:E:302:GLY:CA	1:E:316:ARG:HB2	2.40	0.51
1:A:133:TYR:O	1:A:136:ILE:HG22	2.11	0.51
1:F:252:ASN:ND2	1:F:287:GLN:OE1	2.43	0.51
1:B:330:MET:O	1:B:448:THR:N	2.36	0.51
1:D:128:HIS:HB3	1:F:332:ASP:O	2.11	0.51
1:E:293:VAL:HG12	1:E:297:MET:HG3	1.91	0.51
1:A:86:ALA:C	1:A:88:ASN:H	2.19	0.51
1:C:257:LEU:O	1:C:261:LEU:HD12	2.10	0.51
1:F:41:GLY:O	1:F:43:LYS:N	2.42	0.51
1:A:326:GLN:HB3	1:A:355:THR:O	2.11	0.51
1:B:197:ALA:HA	1:B:200:ILE:HD12	1.93	0.51
1:E:198:ALA:HB2	1:E:400:TYR:OH	2.11	0.51
1:C:19:TYR:OH	1:C:83:PHE:O	2.23	0.51
1:D:177:LYS:HE3	1:D:271:GLY:O	2.11	0.51
1:F:164:GLN:O	1:F:168:VAL:HG23	2.11	0.51
1:F:315:THR:O	1:F:319:LYS:N	2.43	0.51
1:A:34:LEU:HA	1:A:151:TRP:CE3	2.45	0.51
1:A:26:GLU:HA	1:A:29:LYS:HB3	1.93	0.50
1:F:329:LEU:O	1:F:330:MET:HE2	2.10	0.50
1:B:276:THR:HG21	1:B:307:GLY:O	2.11	0.50
1:D:439:TRP:NE1	1:E:131:ARG:HE	2.09	0.50
1:E:58:ASP:OD1	1:E:58:ASP:N	2.42	0.50
1:F:15:SER:OG	1:F:16:GLN:N	2.44	0.50
1:A:16:GLN:HB3	1:A:19:TYR:CE1	2.46	0.50
1:B:33:LYS:HA	1:B:36:ASP:HB2	1.93	0.50
1:D:172:GLU:O	1:D:175:HIS:HB2	2.11	0.50
1:D:181:PHE:HA	1:D:209:TYR:O	2.10	0.50
1:E:183:ASP:OD1	1:E:184:THR:N	2.29	0.50
1:F:395:TYR:HB2	1:F:400:TYR:HE1	1.76	0.50
1:C:178:ILE:HA	1:C:274:ALA:O	2.11	0.50
1:C:54:ALA:HB1	1:C:60:ILE:HD11	1.94	0.50
1:E:293:VAL:O	1:E:297:MET:N	2.45	0.50
1:A:128:HIS:HB2	1:C:446:HIS:HB2	1.93	0.50
1:A:285:LEU:HD22	1:A:287:GLN:O	2.12	0.50
1:B:10:TRP:CD2	1:B:73:VAL:HG11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:LYS:NZ	1:E:467:LYS:O	2.40	0.50
1:E:319:LYS:O	1:E:322:ALA:N	2.33	0.50
1:F:57:ALA:HB2	1:F:88:ASN:CG	2.37	0.50
1:A:259:GLU:O	1:A:263:ILE:N	2.44	0.50
1:B:446:HIS:HB3	1:C:128:HIS:HB2	1.93	0.50
1:C:16:GLN:HB3	1:C:19:TYR:CZ	2.47	0.50
1:E:24:LEU:O	1:E:27:VAL:HG22	2.11	0.50
1:E:60:ILE:HD13	1:E:89:TRP:CG	2.47	0.50
1:E:211:THR:O	1:E:215:VAL:HG23	2.12	0.50
1:A:131:ARG:O	1:A:134:ALA:HB3	2.11	0.49
1:A:153:ASP:O	1:A:157:GLN:HB2	2.12	0.49
1:C:197:ALA:HB2	1:D:139:ARG:NH2	2.27	0.49
1:D:417:PRO:HG2	1:E:113:PHE:O	2.12	0.49
1:C:331:GLU:HG3	1:C:447:HIS:CD2	2.48	0.49
1:F:294:GLN:HB3	1:F:354:PRO:HD3	1.94	0.49
1:F:451:THR:C	1:F:453:ALA:H	2.20	0.49
1:A:74:ALA:O	1:A:99:PRO:HD2	2.12	0.49
1:A:245:ASP:C	1:A:247:GLU:H	2.20	0.49
1:B:378:ARG:HD3	1:B:420:PRO:O	2.12	0.49
1:D:214:LEU:O	1:D:218:VAL:HG23	2.12	0.49
1:D:331:GLU:HG3	1:D:447:HIS:CD2	2.40	0.49
1:F:159:GLN:HA	1:F:162:ASP:HB3	1.94	0.49
1:A:79:TRP:NE1	1:A:105:THR:O	2.46	0.49
1:B:446:HIS:CB	1:C:128:HIS:HB2	2.41	0.49
1:C:240:VAL:HG12	1:C:243:ASP:CG	2.38	0.49
1:C:385:GLU:HA	1:C:409:CYS:HB2	1.94	0.49
1:F:214:LEU:O	1:F:214:LEU:HG	2.13	0.49
1:A:20:GLY:O	1:A:22:GLU:N	2.45	0.49
1:D:67:ALA:O	1:D:98:LYS:NZ	2.43	0.49
1:C:352:VAL:HG21	1:C:422:ALA:O	2.13	0.49
1:D:111:ILE:O	1:D:113:PHE:N	2.45	0.49
1:F:26:GLU:HB2	1:F:123:LEU:HD11	1.94	0.49
1:F:429:GLU:O	1:F:431:GLY:N	2.44	0.49
1:C:31:ALA:O	1:C:34:LEU:N	2.45	0.49
1:E:137:ASN:C	1:E:139:ARG:N	2.71	0.49
1:F:33:LYS:O	1:F:37:GLY:N	2.46	0.49
1:A:151:TRP:H	1:A:151:TRP:CD1	2.31	0.49
1:B:87:LYS:HB3	1:E:199:GLN:HE22	1.78	0.49
1:E:67:ALA:O	1:E:69:TYR:N	2.46	0.49
1:F:19:TYR:HB3	1:F:23:ALA:HB3	1.95	0.49
1:F:21:PRO:HA	1:F:24:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:HIS:HD2	1:F:129:GLY:H	1.57	0.49
1:A:287:GLN:NE2	1:A:376:PRO:HB3	2.27	0.49
1:B:374:ASP:OD1	1:B:374:ASP:N	2.43	0.49
1:C:362:ARG:HA	1:C:379:LEU:HD23	1.95	0.49
1:D:190:VAL:C	1:D:192:GLU:H	2.21	0.49
1:F:198:ALA:O	1:F:202:LEU:HB2	2.13	0.48
1:F:290:GLY:O	1:F:293:VAL:HG22	2.13	0.48
1:B:118:MET:O	1:B:122:ASN:ND2	2.46	0.48
1:B:287:GLN:CD	1:B:376:PRO:HA	2.39	0.48
1:F:238:ASP:HB2	1:F:361:PRO:HB3	1.94	0.48
1:B:87:LYS:O	1:E:199:GLN:NE2	2.46	0.48
1:B:90:ILE:HD12	1:E:199:GLN:CD	2.38	0.48
1:D:166:VAL:O	1:D:167:ALA:C	2.55	0.48
1:C:404:GLY:N	1:C:471:ILE:O	2.46	0.48
1:A:279:PHE:CD1	1:A:370:ILE:HG23	2.48	0.48
1:A:271:GLY:O	1:A:272:TYR:CG	2.66	0.48
1:B:212:ASN:O	1:B:215:VAL:N	2.47	0.48
1:D:206:VAL:HG21	1:D:309:PHE:CG	2.48	0.48
1:E:61:THR:O	1:E:65:LYS:HB2	2.14	0.48
1:E:169:ALA:HA	1:E:172:GLU:HB2	1.95	0.48
1:E:179:ALA:HA	1:E:207:ASP:O	2.13	0.48
1:E:389:TYR:O	1:E:450:LEU:HA	2.14	0.48
1:A:356:LEU:O	1:A:384:ALA:HB2	2.14	0.48
1:B:21:PRO:HA	1:B:24:LEU:HD12	1.96	0.48
1:B:169:ALA:C	1:B:171:ASN:N	2.70	0.48
1:C:65:LYS:HA	1:C:68:ASN:HD22	1.79	0.48
1:E:151:TRP:H	1:E:151:TRP:CD1	2.30	0.48
1:F:201:LYS:NZ	1:F:467:LYS:O	2.47	0.48
1:F:294:GLN:NE2	1:F:379:LEU:HB2	2.29	0.48
1:D:306:GLU:O	1:D:308:ASP:N	2.47	0.48
1:E:214:LEU:O	1:E:217:VAL:N	2.47	0.48
1:F:455:SER:OG	1:F:458:GLN:HB2	2.14	0.48
1:B:101:LEU:HD23	1:B:102:HIS:N	2.30	0.47
1:B:405:TYR:HB3	1:B:439:TRP:CE3	2.49	0.47
1:C:70:ASN:CG	1:C:72:ASP:H	2.21	0.47
1:E:306:GLU:CD	1:E:348:HIS:HE1	2.21	0.47
1:E:405:TYR:HA	1:E:473:ILE:O	2.13	0.47
1:A:180:ARG:HD2	1:A:309:PHE:HB2	1.96	0.47
1:D:291:LEU:HB2	1:D:377:ALA:O	2.14	0.47
1:E:67:ALA:O	1:E:68:ASN:C	2.57	0.47
1:B:400:TYR:O	1:B:401:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ALA:C	1:C:224:ASP:H	2.21	0.47
1:E:190:VAL:HG12	1:F:135:TYR:HB2	1.96	0.47
1:F:128:HIS:O	1:F:131:ARG:N	2.47	0.47
1:B:177:LYS:HD3	1:B:271:GLY:O	2.14	0.47
1:B:221:ILE:HG21	1:B:258:ARG:HB2	1.96	0.47
1:B:390:ASP:O	1:B:404:GLY:HA2	2.14	0.47
1:D:109:ASN:C	1:F:337:LEU:HB2	2.39	0.47
1:D:359:ASP:HB2	1:D:361:PRO:HD3	1.95	0.47
1:F:267:LEU:HD21	1:F:275:PHE:HB3	1.97	0.47
1:F:309:PHE:HA	1:F:312:ALA:CB	2.44	0.47
1:A:179:ALA:HA	1:A:207:ASP:O	2.15	0.47
1:A:352:VAL:HG21	1:A:422:ALA:O	2.15	0.47
1:B:106:GLN:O	1:B:151:TRP:HD1	1.98	0.47
1:B:329:LEU:HA	1:B:449:VAL:HA	1.95	0.47
1:C:79:TRP:CD1	1:C:80:MET:N	2.83	0.47
1:D:348:HIS:H	1:D:352:VAL:HG22	1.78	0.47
1:A:229:ALA:C	1:A:231:LYS:H	2.23	0.47
1:B:69:TYR:CD2	1:E:69:TYR:HB2	2.50	0.47
1:B:331:GLU:OE2	1:B:447:HIS:CD2	2.68	0.47
1:B:406:PRO:CB	1:B:474:LYS:HB2	2.43	0.47
1:D:83:PHE:HE1	1:D:132:GLU:HG3	1.79	0.47
1:D:177:LYS:HZ2	1:D:271:GLY:HA3	1.80	0.47
1:E:279:PHE:C	1:E:281:ASP:H	2.20	0.47
1:F:173:SER:C	1:F:175:HIS:N	2.69	0.47
1:F:328:ALA:HB1	1:F:353:ASP:HB3	1.95	0.47
1:B:295:LEU:O	1:B:298:ILE:N	2.40	0.47
1:D:189:ALA:HB3	1:E:86:ALA:HB3	1.97	0.47
1:D:446:HIS:HB3	1:E:128:HIS:HB2	1.97	0.47
1:F:91:ARG:HA	1:F:94:GLU:HB2	1.96	0.47
1:F:318:LEU:O	1:F:327:THR:HG21	2.14	0.47
1:F:332:ASP:OD1	1:F:332:ASP:N	2.42	0.47
1:A:90:ILE:HG12	1:A:136:ILE:HD11	1.97	0.47
1:A:90:ILE:HG21	1:F:200:ILE:HG12	1.96	0.47
1:A:212:ASN:O	1:A:215:VAL:HB	2.15	0.47
1:B:226:ILE:O	1:B:230:TYR:N	2.48	0.47
1:C:65:LYS:HA	1:C:68:ASN:ND2	2.30	0.47
1:C:103:LEU:HA	1:C:147:VAL:HG23	1.97	0.47
1:C:388:GLY:HA3	1:C:451:THR:O	2.15	0.47
1:C:429:GLU:O	1:C:431:GLY:N	2.43	0.47
1:D:215:VAL:HG21	1:D:284:GLY:HA3	1.97	0.47
1:D:416:MET:HA	1:D:419:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:O	1:B:158:GLU:N	2.48	0.47
1:B:429:GLU:HB3	1:B:474:LYS:CG	2.45	0.47
1:F:86:ALA:C	1:F:88:ASN:N	2.71	0.47
1:A:198:ALA:O	1:A:202:LEU:HB2	2.15	0.46
1:D:255:TYR:HB2	1:D:287:GLN:NE2	2.30	0.46
1:F:348:HIS:ND1	1:F:351:GLU:OE1	2.48	0.46
1:C:104:ALA:HB3	1:C:148:TYR:CG	2.50	0.46
1:E:294:GLN:HA	1:E:297:MET:HB2	1.96	0.46
1:E:419:LEU:C	1:E:421:VAL:H	2.24	0.46
1:A:198:ALA:HB2	1:A:400:TYR:OH	2.15	0.46
1:C:101:LEU:HD12	1:C:145:ALA:O	2.15	0.46
1:A:297:MET:SD	1:A:353:ASP:HB2	2.55	0.46
1:C:279:PHE:CD1	1:C:279:PHE:C	2.93	0.46
1:D:179:ALA:HA	1:D:207:ASP:O	2.15	0.46
1:D:185:MET:HE2	1:D:306:GLU:CG	2.46	0.46
1:E:16:GLN:HA	1:E:55:THR:HG22	1.96	0.46
1:E:221:ILE:HB	1:E:258:ARG:NH2	2.30	0.46
1:F:17:PRO:HA	1:F:24:LEU:HD21	1.96	0.46
1:A:353:ASP:HA	1:A:354:PRO:HD3	1.79	0.46
1:D:230:TYR:HA	1:D:233:LEU:HB2	1.96	0.46
1:A:260:TYR:HB2	1:A:292:ALA:HA	1.98	0.46
1:A:315:THR:O	1:A:319:LYS:HG3	2.15	0.46
1:B:136:ILE:HD12	1:B:136:ILE:HA	1.64	0.46
1:F:64:MET:O	1:F:68:ASN:ND2	2.48	0.46
1:A:60:ILE:O	1:A:63:PHE:HB2	2.15	0.46
1:C:179:ALA:O	1:C:276:THR:N	2.47	0.46
1:D:249:TYR:HB3	1:D:252:ASN:HB2	1.98	0.46
1:A:275:PHE:HE1	1:A:296:LEU:HD13	1.81	0.46
1:B:338:ARG:O	1:B:341:HIS:N	2.48	0.46
1:C:240:VAL:H	1:C:243:ASP:HB2	1.81	0.46
1:E:69:TYR:HB3	1:E:70:ASN:H	1.65	0.46
1:E:134:ALA:O	1:E:137:ASN:N	2.46	0.46
1:E:353:ASP:C	1:E:355:THR:H	2.24	0.46
1:F:44:LEU:HA	1:F:161:ALA:CB	2.46	0.46
1:F:86:ALA:C	1:F:88:ASN:H	2.22	0.46
1:F:86:ALA:HA	1:F:89:TRP:HD1	1.81	0.46
1:B:173:SER:O	1:B:175:HIS:N	2.44	0.46
1:E:7:TYR:CD2	1:E:168:VAL:HG22	2.51	0.46
1:E:374:ASP:OD1	1:E:374:ASP:N	2.48	0.46
1:A:368:LEU:HD23	1:A:370:ILE:HB	1.98	0.46
1:D:35:VAL:HG11	1:D:49:GLU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PHE:CE2	1:F:185:MET:HE1	2.51	0.46
1:D:173:SER:C	1:D:175:HIS:N	2.74	0.46
1:E:198:ALA:HB2	1:E:400:TYR:CZ	2.50	0.46
1:A:177:LYS:HB2	1:A:272:TYR:HA	1.98	0.45
1:D:113:PHE:HA	1:D:116:ILE:CD1	2.45	0.45
1:E:331:GLU:HG3	1:E:446:HIS:HB2	1.96	0.45
1:F:153:ASP:OD1	1:F:155:ASP:N	2.49	0.45
1:A:298:ILE:C	1:A:300:GLY:H	2.24	0.45
1:F:347:SER:HB3	1:F:422:ALA:O	2.16	0.45
1:A:101:LEU:HD13	1:A:163:TRP:CG	2.51	0.45
1:D:185:MET:HE2	1:D:306:GLU:CD	2.42	0.45
1:E:395:TYR:O	1:F:139:ARG:NH1	2.49	0.45
1:F:55:THR:O	1:F:55:THR:OG1	2.34	0.45
1:F:121:MET:C	1:F:123:LEU:H	2.23	0.45
1:F:328:ALA:CB	1:F:353:ASP:HB3	2.47	0.45
1:B:70:ASN:C	1:B:72:ASP:N	2.75	0.45
1:D:277:ASP:HB2	1:D:303:PHE:HE1	1.80	0.45
1:E:455:SER:O	1:E:458:GLN:N	2.49	0.45
1:B:256:GLN:O	1:B:292:ALA:HB2	2.15	0.45
1:B:282:LEU:HD11	1:B:288:LEU:HD13	1.98	0.45
1:D:252:ASN:O	1:D:287:GLN:NE2	2.49	0.45
1:F:350:LEU:HD21	1:F:376:PRO:HG2	1.99	0.45
1:B:173:SER:C	1:B:175:HIS:N	2.75	0.45
1:D:353:ASP:HA	1:D:354:PRO:HD3	1.83	0.45
1:A:56:THR:OG1	1:A:59:SER:N	2.41	0.45
1:A:361:PRO:HB2	1:A:380:VAL:HG13	1.98	0.45
1:B:32:ARG:O	1:B:35:VAL:HB	2.17	0.45
1:B:319:LYS:HA	1:B:327:THR:HG21	1.98	0.45
1:D:287:GLN:HA	1:D:373:LYS:HB3	1.99	0.45
1:E:294:GLN:HB3	1:E:354:PRO:HG3	1.98	0.45
1:E:309:PHE:O	1:E:312:ALA:HB3	2.16	0.45
1:F:294:GLN:HE22	1:F:379:LEU:H	1.65	0.45
1:F:421:VAL:HG12	1:F:422:ALA:N	2.32	0.45
1:A:347:SER:HB2	1:A:352:VAL:HG21	1.98	0.45
1:A:416:MET:HB2	1:A:419:LEU:HD22	1.99	0.45
1:B:187:ASP:HA	1:C:87:LYS:HD2	1.98	0.45
1:C:90:ILE:HG21	1:D:199:GLN:HG2	1.98	0.45
1:D:214:LEU:O	1:D:214:LEU:HG	2.17	0.45
1:E:172:GLU:C	1:E:174:PHE:N	2.75	0.45
1:E:274:ALA:HA	1:E:302:GLY:O	2.17	0.45
1:F:153:ASP:OD1	1:F:154:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:GLY:O	1:E:249:TYR:HB2	2.16	0.45
1:F:69:TYR:O	1:F:71:ASP:N	2.50	0.45
1:C:215:VAL:HG21	1:C:284:GLY:HA3	1.99	0.45
1:A:169:ALA:O	1:A:170:TYR:C	2.60	0.44
1:A:327:THR:HG23	1:A:451:THR:CB	2.48	0.44
1:B:244:ASN:HB2	1:B:247:GLU:CB	2.47	0.44
1:C:13:VAL:HG13	1:C:53:VAL:HA	1.98	0.44
1:C:185:MET:HE2	1:C:306:GLU:CG	2.47	0.44
1:E:333:TYR:HB2	1:E:347:SER:H	1.82	0.44
1:B:153:ASP:O	1:B:157:GLN:N	2.44	0.44
1:C:10:TRP:CD1	1:C:49:GLU:HB2	2.52	0.44
1:C:472:ASN:C	1:C:473:ILE:HG13	2.41	0.44
1:E:188:VAL:HG22	1:F:85:PRO:HG3	1.98	0.44
1:F:22:GLU:C	1:F:24:LEU:H	2.25	0.44
1:A:85:PRO:HB2	1:C:187:ASP:O	2.17	0.44
1:A:86:ALA:C	1:A:88:ASN:N	2.75	0.44
1:B:119:ASP:HA	1:B:122:ASN:HD21	1.82	0.44
1:D:277:ASP:HB2	1:D:303:PHE:CE1	2.52	0.44
1:E:125:GLN:HB2	1:E:128:HIS:CE1	2.52	0.44
1:E:333:TYR:CE2	1:F:128:HIS:HE1	2.35	0.44
1:E:406:PRO:HB2	1:E:474:LYS:HA	1.98	0.44
1:E:446:HIS:N	1:E:446:HIS:CD2	2.84	0.44
1:F:260:TYR:HB2	1:F:292:ALA:HA	1.99	0.44
1:A:199:GLN:NE2	1:F:90:ILE:HD12	2.32	0.44
1:C:309:PHE:CG	1:C:310:LYS:N	2.85	0.44
1:E:178:ILE:HA	1:E:274:ALA:O	2.18	0.44
1:F:125:GLN:HB2	1:F:128:HIS:NE2	2.32	0.44
1:F:297:MET:HE2	1:F:303:PHE:CD2	2.53	0.44
1:F:356:LEU:O	1:F:383:GLY:HA2	2.17	0.44
1:A:290:GLY:HA2	1:A:351:GLU:HG3	2.00	0.44
1:B:395:TYR:HA	1:B:400:TYR:HA	2.00	0.44
1:F:287:GLN:NE2	1:F:376:PRO:HA	2.32	0.44
1:B:119:ASP:HA	1:B:122:ASN:ND2	2.33	0.44
1:B:331:GLU:OE2	1:B:447:HIS:NE2	2.51	0.44
1:D:90:ILE:O	1:D:93:THR:N	2.51	0.44
1:D:110:ASN:HA	1:F:337:LEU:H	1.83	0.44
1:A:245:ASP:O	1:A:247:GLU:N	2.50	0.44
1:E:319:LYS:O	1:E:321:ALA:N	2.51	0.44
1:E:345:MET:HA	1:E:425:MET:HA	2.00	0.44
1:E:349:MET:O	1:E:350:LEU:HD23	2.18	0.44
1:A:378:ARG:HE	1:A:378:ARG:HB3	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:TYR:HD2	1:B:333:TYR:HA	1.76	0.44
1:B:451:THR:O	1:B:451:THR:OG1	2.30	0.44
1:B:458:GLN:HA	1:B:461:GLN:HE21	1.83	0.44
1:E:147:VAL:HG21	1:E:160:ILE:HD13	1.99	0.44
1:F:126:SER:C	1:F:128:HIS:H	2.26	0.44
1:A:183:ASP:HB3	1:E:208:TYR:CG	2.52	0.44
1:C:79:TRP:CZ2	1:C:106:GLN:HA	2.53	0.44
1:C:352:VAL:O	1:C:381:PHE:HZ	2.01	0.44
1:A:179:ALA:HB1	1:A:209:TYR:CG	2.53	0.43
1:C:34:LEU:HA	1:C:151:TRP:CE3	2.53	0.43
1:D:83:PHE:HB2	1:D:128:HIS:CE1	2.53	0.43
1:D:105:THR:O	1:D:126:SER:OG	2.19	0.43
1:E:215:VAL:HG22	1:E:285:LEU:HG	1.99	0.43
1:F:128:HIS:O	1:F:130:ASP:N	2.51	0.43
1:F:349:MET:SD	1:F:370:ILE:HD12	2.57	0.43
1:B:237:TYR:HB3	1:B:360:LYS:O	2.18	0.43
1:B:264:LYS:HB3	1:B:264:LYS:HE2	1.69	0.43
1:C:60:ILE:HG21	1:C:89:TRP:CE3	2.53	0.43
1:C:61:THR:O	1:C:65:LYS:HB3	2.17	0.43
1:C:86:ALA:HB2	1:C:132:GLU:HG3	1.99	0.43
1:C:179:ALA:HB3	1:C:275:PHE:HB2	1.99	0.43
1:C:354:PRO:HA	1:C:381:PHE:CZ	2.53	0.43
1:D:15:SER:O	1:D:55:THR:HA	2.18	0.43
1:A:330:MET:HE2	1:A:330:MET:HB2	1.93	0.43
1:B:60:ILE:HD13	1:B:89:TRP:CD2	2.53	0.43
1:B:215:VAL:HG11	1:B:284:GLY:HA3	2.00	0.43
1:C:35:VAL:HG21	1:C:50:PHE:HB2	2.01	0.43
1:D:154:ALA:O	1:D:158:GLU:HB2	2.18	0.43
1:D:267:LEU:HD21	1:D:275:PHE:HB3	2.01	0.43
1:D:335:LEU:HB3	1:D:344:ILE:HA	2.00	0.43
1:F:436:ALA:O	1:F:440:MET:HB2	2.17	0.43
1:A:173:SER:O	1:A:204:TRP:N	2.51	0.43
1:B:240:VAL:HG11	1:B:363:VAL:HG13	2.00	0.43
1:B:386:GLY:O	1:B:409:CYS:N	2.50	0.43
1:C:375:ASP:HA	1:C:376:PRO:HD3	1.79	0.43
1:E:451:THR:O	1:E:451:THR:OG1	2.37	0.43
1:E:83:PHE:CE1	1:E:132:GLU:HG3	2.54	0.43
1:F:230:TYR:C	1:F:233:LEU:H	2.27	0.43
1:F:370:ILE:O	1:F:372:GLY:N	2.51	0.43
1:A:201:LYS:HB3	1:A:202:LEU:H	1.60	0.43
1:B:254:ARG:O	1:B:258:ARG:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:HG11	1:B:351:GLU:HG2	2.00	0.43
1:C:163:TRP:O	1:C:167:ALA:N	2.48	0.43
1:D:83:PHE:HZ	1:F:188:VAL:HG11	1.84	0.43
1:D:439:TRP:CD1	1:E:131:ARG:HE	2.37	0.43
1:D:446:HIS:O	1:D:448:THR:HG22	2.19	0.43
1:E:187:ASP:HB3	1:F:87:LYS:HB2	2.00	0.43
1:E:463:ALA:O	1:E:466:PHE:N	2.51	0.43
1:F:264:LYS:HG3	1:F:301:TYR:HE1	1.82	0.43
1:B:186:ARG:HE	1:B:186:ARG:HB2	1.36	0.43
1:B:366:HIS:O	1:B:367:PRO:C	2.61	0.43
1:C:294:GLN:NE2	1:C:350:LEU:O	2.52	0.43
1:C:415:GLU:O	1:C:417:PRO:HD3	2.18	0.43
1:D:406:PRO:O	1:D:429:GLU:HB3	2.19	0.43
1:E:272:TYR:O	1:E:274:ALA:N	2.52	0.43
1:A:199:GLN:HE21	1:F:90:ILE:HD12	1.83	0.43
1:B:118:MET:HE1	1:B:121:MET:SD	2.59	0.43
1:B:407:VAL:HG11	1:B:426:TRP:CD1	2.54	0.43
1:D:24:LEU:HD23	1:D:24:LEU:HA	1.89	0.43
1:F:27:VAL:HG12	1:F:81:HIS:ND1	2.34	0.43
1:F:44:LEU:HA	1:F:161:ALA:HB1	2.00	0.43
1:F:434:GLU:O	1:F:437:LYS:HB2	2.19	0.43
1:A:128:HIS:HB2	1:C:446:HIS:CB	2.48	0.43
1:A:186:ARG:HH11	1:E:209:TYR:HA	1.84	0.43
1:A:237:TYR:CE2	1:A:379:LEU:HD11	2.54	0.43
1:F:294:GLN:HB3	1:F:354:PRO:CD	2.49	0.43
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.62	0.43
1:B:70:ASN:C	1:B:72:ASP:H	2.27	0.43
1:B:290:GLY:HA3	1:B:350:LEU:HD13	2.01	0.43
1:E:19:TYR:OH	1:E:125:GLN:OE1	2.33	0.43
1:E:90:ILE:HD11	1:E:136:ILE:HD11	2.01	0.43
1:F:26:GLU:O	1:F:29:LYS:HB2	2.18	0.43
1:A:325:LYS:HB3	1:A:453:ALA:HB1	2.01	0.42
1:A:448:THR:HB	1:A:449:VAL:H	1.65	0.42
1:C:274:ALA:HA	1:C:302:GLY:O	2.18	0.42
1:E:306:GLU:CD	1:E:348:HIS:CE1	2.96	0.42
1:E:333:TYR:N	1:E:346:GLY:HA2	2.33	0.42
1:F:364:GLU:HA	1:F:377:ALA:CA	2.45	0.42
1:A:189:ALA:CB	1:B:86:ALA:HB3	2.47	0.42
1:C:331:GLU:HG3	1:C:447:HIS:HD2	1.84	0.42
1:C:353:ASP:HA	1:C:354:PRO:HD2	1.77	0.42
1:D:264:LYS:HB2	1:D:296:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:HA	1:E:30:ASP:HB2	2.02	0.42
1:E:84:SER:HA	1:E:85:PRO:HD3	1.73	0.42
1:B:190:VAL:HG22	1:C:132:GLU:OE2	2.18	0.42
1:B:213:GLU:O	1:B:217:VAL:HG23	2.18	0.42
1:C:352:VAL:HG11	1:C:422:ALA:HB3	2.01	0.42
1:D:369:GLY:O	1:D:371:GLY:N	2.51	0.42
1:E:136:ILE:HD12	1:E:136:ILE:HA	1.69	0.42
1:E:218:VAL:O	1:E:258:ARG:NE	2.28	0.42
1:E:263:ILE:O	1:E:267:LEU:N	2.37	0.42
1:F:329:LEU:O	1:F:330:MET:HB2	2.19	0.42
1:D:198:ALA:HB2	1:D:400:TYR:OH	2.20	0.42
1:E:305:PRO:C	1:E:307:GLY:H	2.23	0.42
1:E:310:LYS:HE3	1:E:310:LYS:HB2	1.60	0.42
1:F:31:ALA:HB1	1:F:50:PHE:CG	2.54	0.42
1:A:439:TRP:CD1	1:A:439:TRP:O	2.73	0.42
1:B:446:HIS:CD2	1:B:446:HIS:N	2.82	0.42
1:D:306:GLU:C	1:D:308:ASP:N	2.75	0.42
1:E:387:LYS:HB3	1:E:388:GLY:H	1.70	0.42
1:F:33:LYS:HA	1:F:36:ASP:HB2	2.00	0.42
1:F:282:LEU:HD21	1:F:288:LEU:HD12	2.01	0.42
1:A:331:GLU:OE2	1:A:447:HIS:CD2	2.73	0.42
1:C:35:VAL:HG21	1:C:50:PHE:CG	2.54	0.42
1:D:128:HIS:HB2	1:F:446:HIS:HB2	2.02	0.42
1:E:327:THR:HA	1:E:451:THR:HA	2.01	0.42
1:F:180:ARG:O	1:F:182:GLY:N	2.53	0.42
1:C:357:ALA:HB2	1:C:381:PHE:CD1	2.55	0.42
1:F:11:PHE:CD1	1:F:35:VAL:HG22	2.54	0.42
1:F:291:LEU:HD12	1:F:379:LEU:HG	2.02	0.42
1:C:99:PRO:C	1:C:163:TRP:HZ2	2.28	0.42
1:C:368:LEU:HD22	1:C:370:ILE:HG13	2.01	0.42
1:E:421:VAL:HG12	1:E:422:ALA:H	1.85	0.42
1:F:257:LEU:O	1:F:261:LEU:HD12	2.20	0.42
1:A:78:THR:O	1:A:102:HIS:HA	2.19	0.42
1:A:330:MET:O	1:A:448:THR:OG1	2.36	0.42
1:B:217:VAL:HB	1:B:218:VAL:H	1.66	0.42
1:C:31:ALA:O	1:C:35:VAL:N	2.48	0.42
1:D:419:LEU:HG	1:D:421:VAL:O	2.20	0.42
1:A:66:GLU:C	1:A:68:ASN:H	2.28	0.42
1:B:180:ARG:CZ	1:B:183:ASP:HA	2.50	0.42
1:B:413:GLU:HB2	1:C:113:PHE:CG	2.54	0.42
1:C:174:PHE:HA	1:C:203:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:PRO:O	1:D:116:ILE:HG12	2.20	0.42
1:D:187:ASP:CB	1:E:85:PRO:HB2	2.50	0.42
1:D:402:PHE:O	1:D:470:PHE:HA	2.20	0.42
1:E:381:PHE:HB2	1:E:382:THR:H	1.69	0.42
1:F:60:ILE:HD12	1:F:88:ASN:O	2.19	0.42
1:F:126:SER:C	1:F:128:HIS:N	2.77	0.42
1:A:82:THR:OG1	1:A:83:PHE:N	2.43	0.41
1:E:106:GLN:HG2	1:E:107:PHE:H	1.84	0.41
1:A:16:GLN:CA	1:A:55:THR:HG22	2.50	0.41
1:B:154:ALA:O	1:B:158:GLU:HB2	2.20	0.41
1:D:279:PHE:CD2	1:D:279:PHE:N	2.88	0.41
1:E:210:PRO:O	1:E:213:GLU:HB2	2.20	0.41
1:F:230:TYR:O	1:F:233:LEU:N	2.52	0.41
1:F:334:THR:HG22	1:F:335:LEU:N	2.35	0.41
1:A:86:ALA:N	1:A:132:GLU:OE1	2.47	0.41
1:A:191:THR:HB	1:A:308:ASP:HA	2.02	0.41
1:A:325:LYS:HB3	1:A:453:ALA:CB	2.51	0.41
1:A:349:MET:SD	1:A:370:ILE:HG21	2.61	0.41
1:B:197:ALA:HA	1:B:200:ILE:CD1	2.50	0.41
1:D:185:MET:HB2	1:D:306:GLU:HB3	2.02	0.41
1:D:451:THR:OG1	1:D:454:LEU:HD12	2.20	0.41
1:E:78:THR:O	1:E:103:LEU:N	2.43	0.41
1:F:179:ALA:H	1:F:272:TYR:HB3	1.85	0.41
1:F:227:ASP:C	1:F:229:ALA:H	2.28	0.41
1:F:293:VAL:HG21	1:F:351:GLU:HG2	2.01	0.41
1:A:85:PRO:HA	1:A:132:GLU:OE1	2.21	0.41
1:A:279:PHE:CE2	1:A:306:GLU:HG2	2.55	0.41
1:B:60:ILE:HG21	1:B:89:TRP:CE3	2.55	0.41
1:C:9:PHE:O	1:C:48:VAL:HA	2.21	0.41
1:C:15:SER:H	1:C:54:ALA:HB3	1.85	0.41
1:C:39:ASN:ND2	1:C:48:VAL:H	2.18	0.41
1:A:68:ASN:ND2	1:A:97:GLN:HB2	2.34	0.41
1:B:150:TRP:O	1:B:152:GLY:N	2.53	0.41
1:C:24:LEU:HA	1:C:27:VAL:HG22	2.03	0.41
1:C:275:PHE:CZ	1:C:293:VAL:HG13	2.53	0.41
1:D:86:ALA:C	1:D:88:ASN:H	2.28	0.41
1:D:381:PHE:H	1:D:422:ALA:HB2	1.85	0.41
1:D:396:PHE:HA	1:E:139:ARG:NE	2.36	0.41
1:F:375:ASP:HA	1:F:376:PRO:HD3	1.85	0.41
1:B:287:GLN:OE1	1:B:376:PRO:HA	2.21	0.41
1:C:419:LEU:HD12	1:C:420:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLY:O	1:D:42:GLY:C	2.63	0.41
1:D:83:PHE:H	1:D:125:GLN:HG3	1.85	0.41
1:D:276:THR:HG22	1:D:304:GLY:O	2.21	0.41
1:E:239:LEU:HA	1:E:362:ARG:HB3	2.01	0.41
1:E:375:ASP:OD2	1:E:375:ASP:N	2.53	0.41
1:F:62:LYS:O	1:F:66:GLU:HB2	2.21	0.41
1:F:367:PRO:HA	1:F:375:ASP:HB3	2.02	0.41
1:A:215:VAL:C	1:A:217:VAL:H	2.27	0.41
1:A:259:GLU:O	1:A:262:GLY:N	2.52	0.41
1:D:437:LYS:O	1:D:439:TRP:N	2.54	0.41
1:E:308:ASP:OD2	1:E:447:HIS:ND1	2.52	0.41
1:F:338:ARG:HB3	1:F:341:HIS:H	1.85	0.41
1:A:11:PHE:HZ	1:A:79:TRP:HE3	1.68	0.41
1:A:128:HIS:HB3	1:C:332:ASP:O	2.21	0.41
1:B:187:ASP:O	1:C:85:PRO:HB3	2.19	0.41
1:B:297:MET:SD	1:B:353:ASP:HB2	2.61	0.41
1:B:305:PRO:C	1:B:307:GLY:N	2.79	0.41
1:C:27:VAL:HG12	1:C:81:HIS:ND1	2.36	0.41
1:D:253:VAL:C	1:D:255:TYR:H	2.28	0.41
1:E:86:ALA:O	1:E:88:ASN:N	2.54	0.41
1:E:155:ASP:O	1:E:158:GLU:HB3	2.20	0.41
1:E:306:GLU:OE2	1:E:447:HIS:NE2	2.54	0.41
1:F:136:ILE:HD12	1:F:136:ILE:HA	1.89	0.41
1:F:297:MET:HE2	1:F:303:PHE:HB3	2.02	0.41
1:A:190:VAL:HG23	1:B:132:GLU:HG2	2.03	0.41
1:B:150:TRP:C	1:B:152:GLY:H	2.29	0.41
1:C:30:ASP:O	1:C:34:LEU:N	2.54	0.41
1:E:134:ALA:O	1:E:135:TYR:C	2.63	0.40
1:F:279:PHE:C	1:F:281:ASP:H	2.28	0.40
1:A:6:ASP:HB2	1:A:72:ASP:CG	2.46	0.40
1:A:59:SER:O	1:A:63:PHE:CG	2.74	0.40
1:B:237:TYR:O	1:B:239:LEU:N	2.55	0.40
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.85	0.40
1:B:153:ASP:O	1:B:154:ALA:C	2.64	0.40
1:B:183:ASP:HB2	1:D:183:ASP:CG	2.46	0.40
1:C:44:LEU:HB3	1:C:45:ASP:H	1.62	0.40
1:C:367:PRO:HA	1:C:375:ASP:HA	2.03	0.40
1:D:331:GLU:OE2	1:D:447:HIS:CD2	2.74	0.40
1:D:396:PHE:HA	1:E:139:ARG:HE	1.86	0.40
1:E:326:GLN:HB2	1:E:452:LEU:HB2	2.02	0.40
1:F:348:HIS:O	1:F:421:VAL:HG11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD12	1:A:145:ALA:HB3	2.03	0.40
1:B:86:ALA:C	1:B:88:ASN:N	2.80	0.40
1:B:210:PRO:O	1:B:211:THR:C	2.64	0.40
1:B:275:PHE:N	1:B:302:GLY:O	2.51	0.40
1:C:10:TRP:CD1	1:C:10:TRP:N	2.90	0.40
1:C:126:SER:O	1:C:128:HIS:N	2.54	0.40
1:F:26:GLU:HB3	1:F:123:LEU:HD21	2.04	0.40
1:B:39:ASN:HD21	1:B:48:VAL:CB	2.35	0.40
1:B:79:TRP:NE1	1:B:126:SER:OG	2.55	0.40
1:B:155:ASP:HA	1:B:158:GLU:HB3	2.03	0.40
1:B:266:PHE:O	1:B:267:LEU:C	2.64	0.40
1:C:215:VAL:HG22	1:C:285:LEU:HD23	2.03	0.40
1:C:429:GLU:C	1:C:431:GLY:H	2.28	0.40
1:D:54:ALA:CB	1:D:60:ILE:HG12	2.49	0.40
1:E:352:VAL:O	1:E:381:PHE:HZ	2.04	0.40
1:F:429:GLU:C	1:F:431:GLY:N	2.80	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	472/474 (100%)	336 (71%)	89 (19%)	47 (10%)	0	2
1	B	472/474 (100%)	345 (73%)	86 (18%)	41 (9%)	0	3
1	C	472/474 (100%)	360 (76%)	80 (17%)	32 (7%)	1	6
1	D	472/474 (100%)	348 (74%)	84 (18%)	40 (8%)	0	3
1	E	472/474 (100%)	325 (69%)	108 (23%)	39 (8%)	0	4
1	F	472/474 (100%)	323 (68%)	107 (23%)	42 (9%)	0	3
All	All	2832/2844 (100%)	2037 (72%)	554 (20%)	241 (8%)	0	3

All (241) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	305	PRO
1	A	306	GLU
1	A	356	LEU
1	A	367	PRO
1	A	404	GLY
1	A	453	ALA
1	B	50	PHE
1	B	183	ASP
1	B	212	ASN
1	B	217	VAL
1	B	218	VAL
1	B	241	GLU
1	B	339	HIS
1	B	349	MET
1	B	367	PRO
1	B	412	PRO
1	B	456	GLU
1	C	40	LYS
1	C	85	PRO
1	C	211	THR
1	C	305	PRO
1	C	306	GLU
1	C	317	LEU
1	C	331	GLU
1	C	347	SER
1	C	372	GLY
1	C	373	LYS
1	D	17	PRO
1	D	113	PHE
1	D	116	ILE
1	D	141	ASN
1	D	248	LYS
1	D	305	PRO
1	D	308	ASP
1	D	367	PRO
1	D	467	LYS
1	E	68	ASN
1	E	141	ASN
1	E	273	ASP
1	E	299	ASP
1	E	305	PRO

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Mol	Chain	Res	Type
1	E	339	HIS
1	E	362	ARG
1	E	366	HIS
1	E	380	VAL
1	E	427	THR
1	E	428	PRO
1	E	447	HIS
1	F	42	GLY
1	F	45	ASP
1	F	47	PRO
1	F	157	GLN
1	F	286	GLU
1	F	305	PRO
1	F	365	VAL
1	F	430	ILE
1	A	53	VAL
1	A	87	LYS
1	A	107	PHE
1	A	123	LEU
1	A	144	ALA
1	A	170	TYR
1	A	196	VAL
1	A	216	ALA
1	A	231	LYS
1	A	271	GLY
1	A	299	ASP
1	A	374	ASP
1	A	432	LEU
1	A	444	GLY
1	B	71	ASP
1	B	83	PHE
1	B	87	LYS
1	B	90	ILE
1	B	151	TRP
1	B	213	GLU
1	B	238	ASP
1	B	296	LEU
1	B	305	PRO
1	B	306	GLU
1	B	308	ASP
1	B	401	LYS
1	B	417	PRO

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Mol	Chain	Res	Type
1	C	44	LEU
1	C	90	ILE
1	C	127	ALA
1	C	316	ARG
1	D	25	ALA
1	D	35	VAL
1	D	144	ALA
1	D	174	PHE
1	D	187	ASP
1	D	220	GLY
1	D	244	ASN
1	D	307	GLY
1	D	328	ALA
1	D	383	GLY
1	D	417	PRO
1	D	444	GLY
1	E	81	HIS
1	E	82	THR
1	E	87	LYS
1	E	138	SER
1	E	173	SER
1	E	241	GLU
1	E	286	GLU
1	E	320	ILE
1	E	327	THR
1	F	44	LEU
1	F	68	ASN
1	F	129	GLY
1	F	178	ILE
1	F	196	VAL
1	F	203	GLY
1	F	244	ASN
1	F	360	LYS
1	F	371	GLY
1	F	464	ARG
1	A	83	PHE
1	A	197	ALA
1	A	230	TYR
1	A	316	ARG
1	A	370	ILE
1	A	397	ASP
1	A	433	ALA

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Mol	Chain	Res	Type
1	A	456	GLU
1	B	242	GLY
1	B	286	GLU
1	B	364	GLU
1	B	374	ASP
1	C	74	ALA
1	C	86	ALA
1	C	155	ASP
1	C	323	ASP
1	C	398	ASP
1	C	430	ILE
1	D	114	ASP
1	D	366	HIS
1	D	437	LYS
1	D	438	GLN
1	E	40	LYS
1	E	70	ASN
1	E	112	PRO
1	E	290	GLY
1	E	306	GLU
1	E	334	THR
1	E	397	ASP
1	E	406	PRO
1	E	440	MET
1	F	67	ALA
1	F	174	PHE
1	F	219	ASN
1	F	359	ASP
1	F	373	LYS
1	F	412	PRO
1	F	442	TYR
1	A	2	ARG
1	A	62	LYS
1	A	67	ALA
1	A	204	TRP
1	A	211	THR
1	A	279	PHE
1	A	290	GLY
1	A	308	ASP
1	A	365	VAL
1	A	417	PRO
1	A	467	LYS

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Mol	Chain	Res	Type
1	A	469	ASP
1	B	154	ALA
1	B	174	PHE
1	B	267	LEU
1	B	400	TYR
1	C	17	PRO
1	C	365	VAL
1	C	456	GLU
1	D	83	PHE
1	D	152	GLY
1	D	203	GLY
1	D	357	ALA
1	D	365	VAL
1	E	67	ALA
1	E	186	ARG
1	F	112	PRO
1	F	124	HIS
1	F	127	ALA
1	F	312	ALA
1	F	330	MET
1	F	361	PRO
1	F	441	LYS
1	A	21	PRO
1	A	43	LYS
1	A	339	HIS
1	A	413	GLU
1	B	57	ALA
1	B	245	ASP
1	B	295	LEU
1	B	327	THR
1	C	191	THR
1	C	397	ASP
1	C	429	GLU
1	C	441	LYS
1	D	112	PRO
1	D	290	GLY
1	D	306	GLU
1	D	406	PRO
1	E	47	PRO
1	E	69	TYR
1	F	33	LYS
1	F	46	TYR

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Mol	Chain	Res	Type
1	F	181	PHE
1	A	22	GLU
1	A	366	HIS
1	B	250	VAL
1	C	420	PRO
1	D	194	ASP
1	E	215	VAL
1	E	284	GLY
1	F	63	PHE
1	F	143	PRO
1	F	228	ALA
1	F	329	LEU
1	C	35	VAL
1	C	473	ILE
1	D	143	PRO
1	D	370	ILE
1	F	90	ILE
1	F	290	GLY
1	B	99	PRO
1	B	290	GLY
1	D	99	PRO
1	D	289	PRO
1	E	35	VAL
1	E	340	GLY
1	B	35	VAL
1	C	367	PRO
1	D	166	VAL
1	F	367	PRO
1	B	143	PRO
1	E	407	VAL
1	C	290	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/393 (49%)	153 (79%)	41 (21%)	1	5
1	B	199/393 (51%)	156 (78%)	43 (22%)	1	5
1	C	173/393 (44%)	129 (75%)	44 (25%)	0	3
1	D	194/393 (49%)	155 (80%)	39 (20%)	1	6
1	E	199/393 (51%)	147 (74%)	52 (26%)	0	2
1	F	173/393 (44%)	138 (80%)	35 (20%)	1	6
All	All	1132/2358 (48%)	878 (78%)	254 (22%)	1	4

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	15	SER
1	A	27	VAL
1	A	35	VAL
1	A	44	LEU
1	A	48	VAL
1	A	53	VAL
1	A	55	THR
1	A	58	ASP
1	A	76	VAL
1	A	78	THR
1	A	93	THR
1	A	116	ILE
1	A	118	MET
1	A	132	GLU
1	A	166	VAL
1	A	185	MET
1	A	190	VAL
1	A	201	LYS
1	A	211	THR
1	A	282	LEU
1	A	285	LEU
1	A	287	GLN
1	A	291	LEU
1	A	296	LEU
1	A	306	GLU
1	A	332	ASP

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Mol	Chain	Res	Type
1	A	334	THR
1	A	348	HIS
1	A	358	SER
1	A	367	PRO
1	A	368	LEU
1	A	378	ARG
1	A	380	VAL
1	A	398	ASP
1	A	409	CYS
1	A	411	THR
1	A	419	LEU
1	A	421	VAL
1	A	449	VAL
1	A	451	THR
1	B	13	VAL
1	B	17	PRO
1	B	55	THR
1	B	58	ASP
1	B	73	VAL
1	B	76	VAL
1	B	114	ASP
1	B	115	SER
1	B	118	MET
1	B	121	MET
1	B	132	GLU
1	B	136	ILE
1	B	142	VAL
1	B	153	ASP
1	B	160	ILE
1	B	166	VAL
1	B	168	VAL
1	B	184	THR
1	B	185	MET
1	B	186	ARG
1	B	205	THR
1	B	211	THR
1	B	218	VAL
1	B	237	TYR
1	B	250	VAL
1	B	315	THR
1	B	327	THR
1	B	333	TYR

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Mol	Chain	Res	Type
1	B	349	MET
1	B	363	VAL
1	B	365	VAL
1	B	367	PRO
1	B	368	LEU
1	B	374	ASP
1	B	378	ARG
1	B	382	THR
1	B	406	PRO
1	B	411	THR
1	B	412	PRO
1	B	446	HIS
1	B	451	THR
1	B	461	GLN
1	B	473	ILE
1	C	13	VAL
1	C	15	SER
1	C	17	PRO
1	C	39	ASN
1	C	44	LEU
1	C	48	VAL
1	C	56	THR
1	C	61	THR
1	C	76	VAL
1	C	85	PRO
1	C	90	ILE
1	C	93	THR
1	C	98	LYS
1	C	114	ASP
1	C	123	LEU
1	C	132	GLU
1	C	136	ILE
1	C	147	VAL
1	C	168	VAL
1	C	185	MET
1	C	199	GLN
1	C	201	LYS
1	C	205	THR
1	C	246	HIS
1	C	293	VAL
1	C	315	THR
1	C	334	THR

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Mol	Chain	Res	Type
1	C	365	VAL
1	C	367	PRO
1	C	368	LEU
1	C	375	ASP
1	C	380	VAL
1	C	382	THR
1	C	392	THR
1	C	393	LEU
1	C	406	PRO
1	C	407	VAL
1	C	408	ASP
1	C	409	CYS
1	C	421	VAL
1	C	448	THR
1	C	449	VAL
1	C	451	THR
1	C	473	ILE
1	D	7	TYR
1	D	38	LEU
1	D	48	VAL
1	D	55	THR
1	D	56	THR
1	D	58	ASP
1	D	93	THR
1	D	99	PRO
1	D	116	ILE
1	D	118	MET
1	D	121	MET
1	D	136	ILE
1	D	188	VAL
1	D	196	VAL
1	D	205	THR
1	D	211	THR
1	D	221	ILE
1	D	240	VAL
1	D	250	VAL
1	D	279	PHE
1	D	282	LEU
1	D	315	THR
1	D	326	GLN
1	D	327	THR
1	D	333	TYR

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Mol	Chain	Res	Type
1	D	334	THR
1	D	349	MET
1	D	363	VAL
1	D	367	PRO
1	D	368	LEU
1	D	382	THR
1	D	393	LEU
1	D	406	PRO
1	D	411	THR
1	D	421	VAL
1	D	454	LEU
1	D	455	SER
1	D	468	VAL
1	D	473	ILE
1	E	13	VAL
1	E	17	PRO
1	E	22	GLU
1	E	24	LEU
1	E	48	VAL
1	E	53	VAL
1	E	55	THR
1	E	58	ASP
1	E	59	SER
1	E	78	THR
1	E	87	LYS
1	E	96	LEU
1	E	118	MET
1	E	119	ASP
1	E	121	MET
1	E	122	ASN
1	E	132	GLU
1	E	139	ARG
1	E	146	SER
1	E	153	ASP
1	E	168	VAL
1	E	181	PHE
1	E	184	THR
1	E	185	MET
1	E	190	VAL
1	E	196	VAL
1	E	201	LYS
1	E	211	THR

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Mol	Chain	Res	Type
1	E	240	VAL
1	E	246	HIS
1	E	267	LEU
1	E	279	PHE
1	E	310	LYS
1	E	315	THR
1	E	326	GLN
1	E	333	TYR
1	E	350	LEU
1	E	355	THR
1	E	363	VAL
1	E	374	ASP
1	E	392	THR
1	E	394	SER
1	E	398	ASP
1	E	406	PRO
1	E	407	VAL
1	E	411	THR
1	E	412	PRO
1	E	446	HIS
1	E	451	THR
1	E	454	LEU
1	E	468	VAL
1	E	473	ILE
1	F	1	MET
1	F	13	VAL
1	F	48	VAL
1	F	53	VAL
1	F	55	THR
1	F	78	THR
1	F	82	THR
1	F	98	LYS
1	F	114	ASP
1	F	116	ILE
1	F	128	HIS
1	F	136	ILE
1	F	142	VAL
1	F	166	VAL
1	F	185	MET
1	F	201	LYS
1	F	211	THR
1	F	215	VAL

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Mol	Chain	Res	Type
1	F	217	VAL
1	F	252	ASN
1	F	285	LEU
1	F	287	GLN
1	F	332	ASP
1	F	347	SER
1	F	355	THR
1	F	365	VAL
1	F	370	ILE
1	F	374	ASP
1	F	380	VAL
1	F	382	THR
1	F	394	SER
1	F	406	PRO
1	F	407	VAL
1	F	449	VAL
1	F	451	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	106	GLN
1	A	199	GLN
1	A	287	GLN
1	B	461	GLN
1	C	16	GLN
1	C	68	ASN
1	D	81	HIS
1	D	199	GLN
1	D	219	ASN
1	E	68	ASN
1	E	446	HIS
1	F	81	HIS
1	F	106	GLN
1	F	252	ASN
1	F	287	GLN
1	F	461	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	474/474 (100%)	0.64	37 (7%)	19 13	29, 72, 143, 172	0
1	B	474/474 (100%)	0.50	27 (5%)	29 19	27, 57, 115, 221	0
1	C	474/474 (100%)	0.74	44 (9%)	14 10	35, 81, 134, 191	0
1	D	474/474 (100%)	0.82	55 (11%)	9 7	32, 83, 148, 204	0
1	E	474/474 (100%)	0.83	42 (8%)	15 11	33, 89, 151, 246	0
1	F	474/474 (100%)	0.75	49 (10%)	12 8	35, 78, 135, 165	0
All	All	2844/2844 (100%)	0.71	254 (8%)	15 11	27, 77, 140, 246	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ASN	9.6
1	E	3	LYS	6.8
1	B	243	ASP	6.4
1	F	474	LYS	5.2
1	F	49	GLU	5.2
1	A	261	LEU	5.1
1	B	242	GLY	5.0
1	D	422	ALA	4.9
1	D	423	LYS	4.6
1	D	244	ASN	4.5
1	E	4	MET	4.5
1	A	329	LEU	4.5
1	B	244	ASN	4.4
1	A	323	ASP	4.3
1	A	324	ASN	4.3
1	B	325	LYS	4.3
1	C	245	ASP	4.3
1	E	371	GLY	4.2
1	E	245	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	280	GLN	4.1
1	E	411	THR	4.1
1	A	421	VAL	4.0
1	F	244	ASN	4.0
1	B	432	LEU	4.0
1	C	277	ASP	3.9
1	A	120	TYR	3.9
1	D	363	VAL	3.8
1	C	121	MET	3.8
1	D	245	ASP	3.8
1	B	245	ASP	3.8
1	D	246	HIS	3.7
1	D	372	GLY	3.7
1	F	368	LEU	3.7
1	E	243	ASP	3.7
1	E	100	LEU	3.6
1	B	128	HIS	3.6
1	E	289	PRO	3.6
1	E	260	TYR	3.6
1	A	123	LEU	3.6
1	F	329	LEU	3.5
1	D	18	LEU	3.5
1	D	347	SER	3.5
1	A	288	LEU	3.4
1	B	333	TYR	3.4
1	D	208	TYR	3.4
1	B	4	MET	3.4
1	E	421	VAL	3.4
1	A	300	GLY	3.3
1	C	71	ASP	3.3
1	B	424	GLN	3.3
1	C	345	MET	3.3
1	D	136	ILE	3.3
1	D	124	HIS	3.2
1	A	82	THR	3.2
1	D	241	GLU	3.2
1	C	244	ASN	3.2
1	D	290	GLY	3.2
1	D	107	PHE	3.2
1	A	274	ALA	3.2
1	A	230	TYR	3.2
1	C	102	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	244	ASN	3.1
1	C	473	ILE	3.1
1	A	74	ALA	3.1
1	F	4	MET	3.1
1	A	302	GLY	3.0
1	F	26	GLU	3.0
1	A	226	ILE	3.0
1	D	413	GLU	3.0
1	F	292	ALA	3.0
1	C	323	ASP	3.0
1	E	24	LEU	3.0
1	F	417	PRO	3.0
1	A	446	HIS	3.0
1	D	106	GLN	3.0
1	F	118	MET	2.9
1	E	473	ILE	2.9
1	F	358	SER	2.9
1	A	136	ILE	2.9
1	E	280	GLN	2.9
1	D	259	GLU	2.9
1	B	247	GLU	2.9
1	C	123	LEU	2.9
1	F	379	LEU	2.9
1	D	122	ASN	2.8
1	F	148	TYR	2.8
1	B	246	HIS	2.8
1	F	324	ASN	2.8
1	C	304	GLY	2.8
1	F	473	ILE	2.8
1	C	124	HIS	2.8
1	F	363	VAL	2.8
1	C	390	ASP	2.8
1	F	277	ASP	2.8
1	B	423	LYS	2.8
1	C	412	PRO	2.8
1	D	100	LEU	2.8
1	D	118	MET	2.7
1	A	422	ALA	2.7
1	E	259	GLU	2.7
1	D	353	ASP	2.7
1	E	412	PRO	2.7
1	F	124	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	365	VAL	2.7
1	E	27	VAL	2.7
1	D	130	ASP	2.7
1	D	343	ALA	2.7
1	C	432	LEU	2.7
1	C	47	PRO	2.7
1	C	409	CYS	2.7
1	B	285	LEU	2.7
1	B	277	ASP	2.7
1	B	326	GLN	2.6
1	A	290	GLY	2.6
1	F	2	ARG	2.6
1	F	442	TYR	2.6
1	C	88	ASN	2.6
1	E	109	ASN	2.6
1	F	241	GLU	2.6
1	F	293	VAL	2.6
1	D	401	LYS	2.6
1	C	80	MET	2.5
1	D	148	TYR	2.5
1	D	170	TYR	2.5
1	D	301	TYR	2.5
1	F	454	LEU	2.5
1	D	364	GLU	2.5
1	B	121	MET	2.5
1	A	245	ASP	2.5
1	B	473	ILE	2.5
1	D	81	HIS	2.5
1	D	371	GLY	2.5
1	E	474	LYS	2.5
1	D	424	GLN	2.5
1	E	351	GLU	2.5
1	C	160	ILE	2.5
1	A	426	TRP	2.5
1	F	242	GLY	2.5
1	A	293	VAL	2.5
1	F	414	ALA	2.5
1	A	130	ASP	2.5
1	D	9	PHE	2.5
1	D	123	LEU	2.5
1	B	237	TYR	2.5
1	C	152	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	351	GLU	2.4
1	C	336	ASP	2.4
1	E	390	ASP	2.4
1	E	7	TYR	2.4
1	D	340	GLY	2.4
1	E	242	GLY	2.4
1	D	163	TRP	2.4
1	F	109	ASN	2.4
1	E	353	ASP	2.4
1	A	440	MET	2.4
1	C	416	MET	2.4
1	F	362	ARG	2.4
1	C	204	TRP	2.4
1	E	324	ASN	2.4
1	D	4	MET	2.4
1	C	411	THR	2.3
1	E	362	ARG	2.3
1	F	111	ILE	2.3
1	D	230	TYR	2.3
1	D	272	TYR	2.3
1	F	122	ASN	2.3
1	D	248	LYS	2.3
1	E	248	LYS	2.3
1	D	455	SER	2.3
1	D	120	TYR	2.3
1	E	256	GLN	2.3
1	C	415	GLU	2.3
1	F	48	VAL	2.3
1	F	151	TRP	2.3
1	C	120	TYR	2.3
1	E	255	TYR	2.3
1	E	225	GLU	2.2
1	F	18	LEU	2.2
1	B	82	THR	2.2
1	A	3	LYS	2.2
1	A	114	ASP	2.2
1	F	108	LEU	2.2
1	F	383	GLY	2.2
1	F	89	TRP	2.2
1	C	306	GLU	2.2
1	C	303	PHE	2.2
1	E	2	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	HIS	2.2
1	A	135	TYR	2.2
1	D	454	LEU	2.2
1	F	123	LEU	2.2
1	F	23	ALA	2.2
1	F	245	ASP	2.2
1	D	102	HIS	2.2
1	D	348	HIS	2.2
1	B	389	TYR	2.2
1	C	352	VAL	2.2
1	A	473	ILE	2.2
1	E	5	GLN	2.2
1	F	298	ILE	2.2
1	C	167	ALA	2.2
1	E	122	ASN	2.2
1	D	367	PRO	2.2
1	F	183	ASP	2.2
1	F	243	ASP	2.2
1	C	446	HIS	2.2
1	C	53	VAL	2.1
1	D	421	VAL	2.1
1	E	363	VAL	2.1
1	D	40	LYS	2.1
1	A	2	ARG	2.1
1	A	180	ARG	2.1
1	C	331	GLU	2.1
1	C	36	ASP	2.1
1	C	35	VAL	2.1
1	E	19	TYR	2.1
1	B	350	LEU	2.1
1	B	445	GLY	2.1
1	A	244	ASN	2.1
1	F	110	ASN	2.1
1	E	130	ASP	2.1
1	E	407	VAL	2.1
1	B	345	MET	2.1
1	F	104	ALA	2.1
1	C	183	ASP	2.1
1	D	323	ASP	2.1
1	F	45	ASP	2.1
1	A	67	ALA	2.1
1	C	354	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	275	PHE	2.1
1	E	34	LEU	2.1
1	B	124	HIS	2.1
1	A	243	ASP	2.1
1	C	4	MET	2.1
1	D	262	GLY	2.1
1	D	326	GLN	2.1
1	D	369	GLY	2.1
1	F	16	GLN	2.1
1	F	404	GLY	2.1
1	F	444	GLY	2.1
1	A	26	GLU	2.1
1	C	266	PHE	2.1
1	B	455	SER	2.0
1	D	295	LEU	2.0
1	E	252	ASN	2.0
1	C	280	GLN	2.0
1	F	367	PRO	2.0
1	D	206	VAL	2.0
1	A	109	ASN	2.0
1	C	341	HIS	2.0
1	C	447	HIS	2.0
1	F	220	GLY	2.0
1	E	288	LEU	2.0
1	E	450	LEU	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.