



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:51 PM UTC

PDB ID : 5I8I / pdb_00005i8i
Title : Crystal Structure of the K. lactis Urea Amidolyase
Authors : Zhao, J.; Xiang, S.
Deposited on : 2016-02-19
Resolution : 6.50 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:

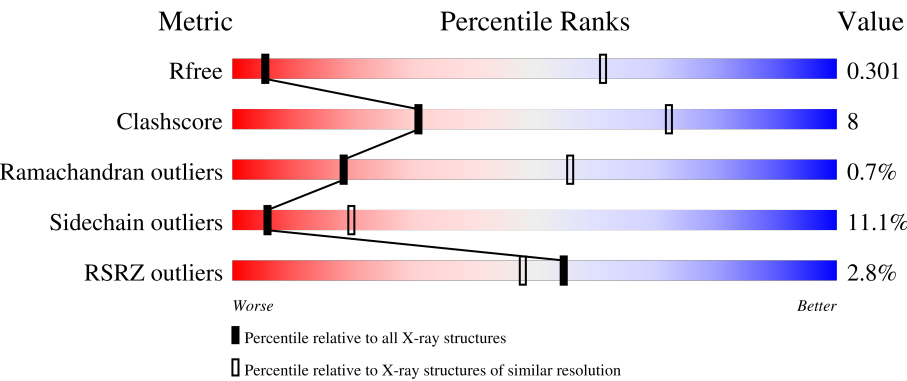
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	1829	4% 69%18%•9%
1	B	1829	2% 66%19%5%•9%
1	C	1829	2% 69%18%•9%
1	D	1829	2% 67%19%•9%

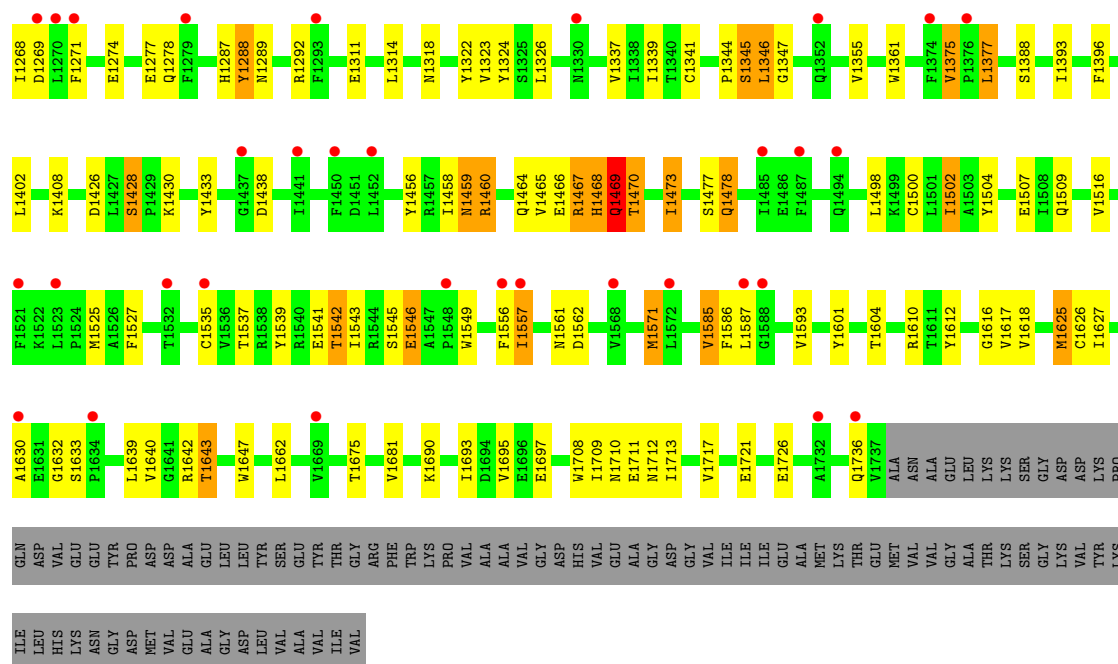
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 51722 atoms, of which 0 are hydrogens and 0 are deuteriums.

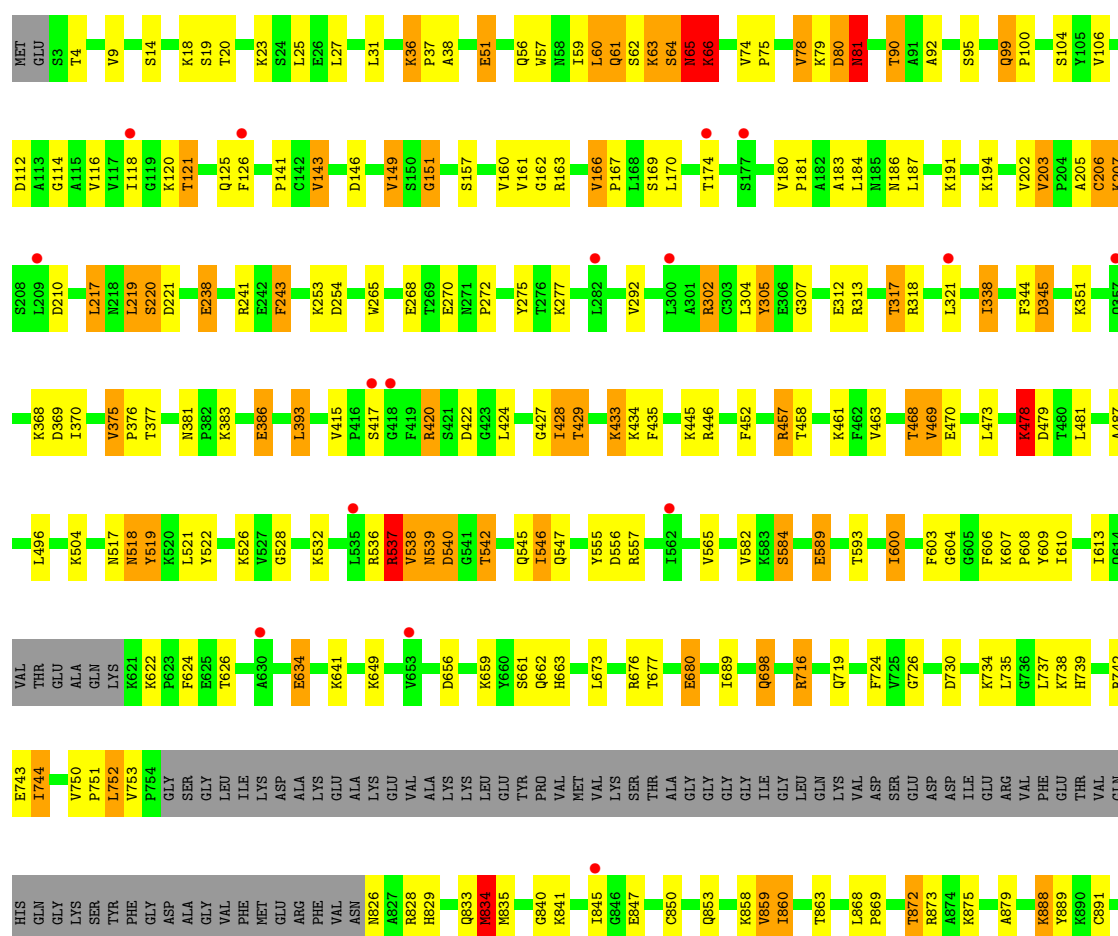
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Urea Amidolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0	0
			12939	8253	2183	2456	47			
1	B	1658	Total	C	N	O	S	0	0	0
			12922	8243	2181	2452	46			
1	C	1660	Total	C	N	O	S	0	0	0
			12939	8253	2183	2456	47			
1	D	1658	Total	C	N	O	S	0	0	0
			12922	8243	2181	2452	46			



• Molecule 1: Urea Amidolyase









4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.74Å 181.94Å 549.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 6.50 29.98 – 6.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.98-6.50) 94.7 (29.98-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 6.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.278 , 0.302 0.274 , 0.301	Depositor DCC
R_{free} test set	1017 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	216.1	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 331.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	51722	wwPDB-VP
Average B, all atoms (Å ²)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.53	8/13231 (0.1%)	1.02	44/17964 (0.2%)
1	B	0.66	10/13214 (0.1%)	1.19	100/17942 (0.6%)
1	C	0.51	0/13231	1.01	37/17964 (0.2%)
1	D	0.63	4/13214 (0.0%)	1.16	68/17942 (0.4%)
All	All	0.59	22/52890 (0.0%)	1.10	249/71812 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	6
All	All	0	13

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	LYS	CA-C	8.10	1.63	1.52
1	B	63	LYS	CA-C	7.89	1.63	1.52
1	B	61	GLN	CA-C	-7.22	1.42	1.52
1	A	64	SER	N-CA	7.16	1.54	1.46
1	B	64	SER	N-CA	7.12	1.54	1.46
1	B	1467	ARG	CA-C	-7.11	1.43	1.52
1	B	1542	THR	C-O	-7.01	1.15	1.23
1	A	1467	ARG	CA-C	-6.41	1.44	1.52
1	B	1468	HIS	N-CA	-5.79	1.38	1.46
1	B	1471	VAL	CA-CB	5.71	1.60	1.54
1	B	537	ARG	CA-C	5.67	1.60	1.52
1	D	393	LEU	CA-C	5.57	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	ARG	CA-C	5.50	1.59	1.52
1	A	1542	THR	C-O	-5.46	1.17	1.23
1	B	393	LEU	CA-C	5.43	1.60	1.52
1	D	180	VAL	CA-CB	5.35	1.57	1.54
1	A	61	GLN	CA-C	-5.34	1.45	1.52
1	A	1468	HIS	CA-C	-5.30	1.45	1.52
1	D	17	SER	CA-CB	5.17	1.61	1.53
1	A	1557	ILE	CA-CB	5.15	1.60	1.54
1	B	468	THR	CA-CB	5.12	1.62	1.53
1	A	1288	TYR	CA-C	5.08	1.59	1.52

All (249) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	TYR	N-CA-C	10.51	126.42	110.14
1	B	305	TYR	N-CA-C	10.26	122.22	111.14
1	D	305	TYR	N-CA-C	9.69	121.60	111.14
1	B	1303	LYS	N-CA-C	-9.66	93.52	109.07
1	D	556	ASP	N-CA-CB	-9.62	94.41	110.39
1	B	556	ASP	N-CA-CB	-9.46	94.69	110.39
1	C	38	ALA	CA-C-N	-9.26	110.56	120.47
1	C	38	ALA	C-N-CA	-9.26	110.56	120.47
1	B	542	THR	N-CA-C	9.17	123.20	112.93
1	B	496	LEU	CA-C-N	-9.12	108.44	119.84
1	B	496	LEU	C-N-CA	-9.12	108.44	119.84
1	C	898	ILE	N-CA-C	-9.00	97.13	109.55
1	A	38	ALA	CA-C-N	-8.97	110.87	120.47
1	A	38	ALA	C-N-CA	-8.97	110.87	120.47
1	D	422	ASP	N-CA-CB	-8.88	96.78	110.46
1	D	19	SER	N-CA-C	8.83	123.51	110.17
1	D	81	ASN	N-CA-C	-8.73	103.47	114.56
1	A	81	ASN	N-CA-C	-8.72	103.49	114.56
1	D	496	LEU	CA-C-N	-8.66	109.01	119.84
1	D	496	LEU	C-N-CA	-8.66	109.01	119.84
1	B	19	SER	N-CA-C	8.60	123.16	110.17
1	D	36	LYS	CA-C-N	-8.50	109.21	119.84
1	D	36	LYS	C-N-CA	-8.50	109.21	119.84
1	B	522	TYR	N-CA-C	8.32	122.46	109.07
1	B	1702	HIS	N-CA-C	-8.31	102.30	111.36
1	A	65	ASN	N-CA-C	-8.18	101.77	113.21
1	B	81	ASN	N-CA-C	-8.11	104.26	114.56
1	A	673	LEU	N-CA-C	-8.05	97.52	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	LYS	CA-C-N	-8.03	109.80	119.84
1	B	36	LYS	C-N-CA	-8.03	109.80	119.84
1	C	81	ASN	N-CA-C	-8.01	104.38	114.56
1	B	99	GLN	CA-C-N	7.93	127.86	119.85
1	B	99	GLN	C-N-CA	7.93	127.86	119.85
1	D	99	GLN	CA-C-N	7.86	127.79	119.85
1	D	99	GLN	C-N-CA	7.86	127.79	119.85
1	D	528	GLY	CA-C-N	-7.74	112.93	120.83
1	D	528	GLY	C-N-CA	-7.74	112.93	120.83
1	B	1570	ASN	N-CA-C	7.73	119.79	111.36
1	B	478	LYS	N-CA-C	7.72	119.69	111.28
1	A	1468	HIS	CA-C-N	-7.66	111.12	122.07
1	A	1468	HIS	C-N-CA	-7.66	111.12	122.07
1	D	673	LEU	N-CA-C	-7.65	98.15	110.32
1	D	565	VAL	CA-C-N	7.64	127.79	120.31
1	D	565	VAL	C-N-CA	7.64	127.79	120.31
1	D	478	LYS	N-CA-C	7.60	119.56	111.28
1	D	253	LYS	N-CA-C	-7.54	102.09	111.75
1	C	673	LEU	N-CA-C	-7.46	98.46	110.32
1	B	673	LEU	N-CA-C	-7.45	98.47	110.32
1	A	243	PHE	CA-C-N	-7.37	113.22	120.52
1	A	243	PHE	C-N-CA	-7.37	113.22	120.52
1	B	60	LEU	N-CA-C	7.36	119.30	111.28
1	D	941	ASP	N-CA-C	-7.34	101.63	110.44
1	D	542	THR	N-CA-C	7.21	121.67	113.02
1	B	528	GLY	CA-C-N	-7.18	113.50	120.83
1	B	528	GLY	C-N-CA	-7.18	113.50	120.83
1	D	254	ASP	CB-CA-C	-7.16	95.71	109.95
1	B	1469	GLN	CA-C-O	-7.12	113.28	121.54
1	A	941	ASP	N-CA-C	-7.11	101.90	110.44
1	D	304	LEU	N-CA-C	-7.08	103.50	111.07
1	B	254	ASP	CB-CA-C	-7.07	95.88	109.95
1	A	60	LEU	N-CA-C	7.07	118.98	111.28
1	B	833	GLN	N-CA-C	-7.01	97.82	109.46
1	B	203	VAL	CA-C-N	7.00	126.97	119.76
1	B	203	VAL	C-N-CA	7.00	126.97	119.76
1	B	64	SER	CB-CA-C	-6.99	99.89	111.13
1	C	243	PHE	CA-C-N	-6.98	113.61	120.52
1	C	243	PHE	C-N-CA	-6.98	113.61	120.52
1	B	253	LYS	N-CA-C	-6.95	102.85	111.75
1	B	1468	HIS	CA-C-N	-6.93	112.16	122.07
1	B	1468	HIS	C-N-CA	-6.93	112.16	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	PHE	CA-C-N	-6.86	113.73	120.52
1	B	243	PHE	C-N-CA	-6.86	113.73	120.52
1	B	304	LEU	N-CA-C	-6.85	103.74	111.07
1	D	20	THR	N-CA-C	-6.70	101.68	110.39
1	B	555	TYR	N-CA-C	-6.68	104.00	111.28
1	D	38	ALA	N-CA-C	6.67	118.20	109.93
1	D	446	ARG	CB-CA-C	-6.65	100.39	110.90
1	D	243	PHE	CA-C-N	-6.55	114.03	120.52
1	D	243	PHE	C-N-CA	-6.55	114.03	120.52
1	B	1470	THR	N-CA-C	6.55	119.86	110.24
1	A	1288	TYR	CA-CB-CG	-6.50	102.21	113.90
1	D	203	VAL	CA-C-N	6.48	126.44	119.76
1	D	203	VAL	C-N-CA	6.48	126.44	119.76
1	B	20	THR	N-CA-C	-6.47	101.98	110.39
1	B	446	ARG	CB-CA-C	-6.42	100.75	110.90
1	D	382	PRO	N-CA-C	6.39	120.45	110.80
1	D	207	LYS	N-CA-C	6.38	121.90	111.37
1	B	565	VAL	CA-C-N	6.34	127.57	120.66
1	B	565	VAL	C-N-CA	6.34	127.57	120.66
1	B	519	TYR	N-CA-CB	-6.33	101.10	110.85
1	B	532	LYS	CA-C-N	6.33	126.85	120.14
1	B	532	LYS	C-N-CA	6.33	126.85	120.14
1	D	945	PHE	N-CA-C	6.26	118.11	111.28
1	A	1467	ARG	N-CA-C	-6.26	104.54	111.36
1	A	1469	GLN	CA-C-O	-6.26	114.28	121.54
1	D	532	LYS	CA-C-N	6.24	126.76	120.14
1	D	532	LYS	C-N-CA	6.24	126.76	120.14
1	C	540	ASP	N-CA-C	-6.14	103.91	111.40
1	B	656	ASP	CA-C-N	-6.14	113.30	119.56
1	B	656	ASP	C-N-CA	-6.14	113.30	119.56
1	D	656	ASP	CA-C-N	-6.08	113.36	119.56
1	D	656	ASP	C-N-CA	-6.08	113.36	119.56
1	C	62	SER	CA-C-N	-6.07	112.74	121.42
1	C	62	SER	C-N-CA	-6.07	112.74	121.42
1	D	421	SER	N-CA-C	-6.07	103.98	111.75
1	C	656	ASP	CA-C-N	-6.07	113.37	119.56
1	C	656	ASP	C-N-CA	-6.07	113.37	119.56
1	B	834	MET	N-CA-C	6.01	119.20	109.40
1	B	542	THR	CA-C-N	-6.00	113.03	121.13
1	B	542	THR	C-N-CA	-6.00	113.03	121.13
1	D	1067	LYS	CA-C-N	5.99	126.30	119.83
1	D	1067	LYS	C-N-CA	5.99	126.30	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	ASP	N-CA-C	-5.99	104.10	111.40
1	A	66	LYS	N-CA-C	-5.98	101.81	110.24
1	A	656	ASP	CA-C-N	-5.98	113.46	119.56
1	A	656	ASP	C-N-CA	-5.98	113.46	119.56
1	C	895	VAL	N-CA-C	-5.96	99.77	108.11
1	B	207	LYS	N-CA-C	5.93	121.16	111.37
1	D	555	TYR	N-CA-C	-5.93	104.82	111.28
1	B	457	ARG	CG-CD-NE	5.90	124.99	112.00
1	D	151	GLY	N-CA-C	-5.86	105.39	112.48
1	A	945	PHE	N-CA-C	5.84	117.64	111.28
1	A	1067	LYS	CA-C-N	5.83	126.13	119.83
1	A	1067	LYS	C-N-CA	5.83	126.13	119.83
1	A	1593	VAL	CA-C-N	-5.82	113.94	119.76
1	A	1593	VAL	C-N-CA	-5.82	113.94	119.76
1	C	1067	LYS	CA-C-N	5.80	126.09	119.83
1	C	1067	LYS	C-N-CA	5.80	126.09	119.83
1	B	1575	ALA	N-CA-C	5.78	118.22	110.35
1	B	1067	LYS	CA-C-N	5.75	126.05	119.83
1	B	1067	LYS	C-N-CA	5.75	126.05	119.83
1	B	65	ASN	N-CA-C	-5.68	98.69	110.80
1	C	1060	VAL	N-CA-C	5.67	116.12	110.23
1	B	478	LYS	N-CA-CB	-5.66	101.80	110.12
1	A	1546	GLU	N-CA-C	5.66	118.68	109.06
1	B	469	VAL	N-CA-C	-5.66	107.99	113.53
1	B	1593	VAL	CA-C-N	-5.65	114.11	119.76
1	B	1593	VAL	C-N-CA	-5.65	114.11	119.76
1	B	556	ASP	N-CA-C	5.65	119.44	112.54
1	C	74	VAL	CA-C-N	-5.60	114.20	120.14
1	C	74	VAL	C-N-CA	-5.60	114.20	120.14
1	C	1228	SER	N-CA-C	5.60	118.58	109.06
1	D	546	ILE	N-CA-C	5.58	117.35	108.87
1	A	1643	THR	CB-CA-C	-5.57	104.40	113.37
1	A	74	VAL	CA-C-N	-5.57	114.23	120.14
1	A	74	VAL	C-N-CA	-5.57	114.23	120.14
1	D	1643	THR	CB-CA-C	-5.55	104.44	113.37
1	C	1049	LYS	N-CA-C	-5.53	105.34	111.36
1	C	1681	VAL	N-CA-C	-5.51	105.35	110.53
1	C	68	GLU	N-CA-C	-5.51	106.00	114.16
1	C	1593	VAL	CA-C-N	-5.50	114.27	119.76
1	C	1593	VAL	C-N-CA	-5.50	114.27	119.76
1	B	1049	LYS	N-CA-C	-5.49	105.37	111.36
1	B	828	ARG	CA-C-N	-5.49	115.36	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	ARG	C-N-CA	-5.49	115.36	123.05
1	D	478	LYS	N-CA-CB	-5.49	102.05	110.12
1	B	542	THR	CB-CA-C	-5.49	101.32	110.81
1	D	1228	SER	N-CA-C	5.46	118.35	109.06
1	D	1049	LYS	N-CA-C	-5.46	105.41	111.36
1	A	1228	SER	N-CA-C	5.45	118.33	109.06
1	B	344	PHE	N-CA-C	5.45	117.78	108.90
1	A	1469	GLN	N-CA-CB	-5.44	103.74	111.84
1	A	1060	VAL	N-CA-C	5.43	115.88	110.23
1	C	1643	THR	CB-CA-C	-5.43	104.62	113.37
1	B	151	GLY	N-CA-C	-5.41	105.94	112.48
1	B	1428	SER	CA-C-N	5.41	126.76	120.98
1	B	1428	SER	C-N-CA	5.41	126.76	120.98
1	B	66	LYS	CG-CD-CE	-5.40	98.87	111.30
1	D	1593	VAL	CA-C-N	-5.40	114.36	119.76
1	D	1593	VAL	C-N-CA	-5.40	114.36	119.76
1	B	945	PHE	N-CA-C	5.39	117.16	111.28
1	B	1706	LEU	CA-C-N	5.39	127.77	120.65
1	B	1706	LEU	C-N-CA	5.39	127.77	120.65
1	D	469	VAL	N-CA-C	-5.39	108.03	113.47
1	D	194	LYS	CD-CE-NZ	-5.38	94.70	111.90
1	D	345	ASP	CB-CA-C	-5.37	99.28	110.40
1	B	1467	ARG	O-C-N	5.37	127.81	122.12
1	C	1311	GLU	N-CA-C	5.37	118.62	111.75
1	A	68	GLU	N-CA-C	-5.37	106.22	114.16
1	B	1228	SER	N-CA-C	5.36	118.18	109.06
1	C	532	LYS	CA-C-N	5.36	125.82	120.14
1	C	532	LYS	C-N-CA	5.36	125.82	120.14
1	C	945	PHE	N-CA-C	5.35	117.11	111.28
1	D	556	ASP	N-CA-C	5.35	119.06	112.54
1	A	1535	CYS	N-CA-C	-5.34	105.54	111.36
1	D	344	PHE	N-CA-C	5.33	117.59	108.90
1	B	1467	ARG	N-CA-C	-5.31	105.50	111.28
1	D	318	ARG	N-CA-C	5.29	117.13	111.36
1	B	307	GLY	CA-C-N	-5.29	114.19	122.65
1	B	307	GLY	C-N-CA	-5.29	114.19	122.65
1	B	546	ILE	N-CA-C	5.28	116.90	108.87
1	A	1049	LYS	N-CA-C	-5.28	105.61	111.36
1	A	1470	THR	N-CA-C	5.27	117.98	110.24
1	C	893	GLY	CA-C-N	-5.26	113.65	122.92
1	C	893	GLY	C-N-CA	-5.26	113.65	122.92
1	D	1535	CYS	N-CA-C	-5.26	105.62	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	GLN	N-CA-C	5.26	116.83	108.67
1	B	1060	VAL	N-CA-C	5.26	115.70	110.23
1	B	217	LEU	N-CA-CB	5.24	118.62	110.44
1	D	1060	VAL	N-CA-C	5.24	115.68	110.23
1	A	622	LYS	CA-C-N	5.24	125.29	119.32
1	A	622	LYS	C-N-CA	5.24	125.29	119.32
1	B	1709	ILE	N-CA-C	-5.23	105.40	110.42
1	C	1502	ILE	CB-CA-C	-5.23	105.19	112.04
1	D	338	ILE	N-CA-C	5.22	117.58	111.05
1	B	318	ARG	N-CA-C	5.21	117.04	111.36
1	C	65	ASN	N-CA-C	-5.21	105.92	113.21
1	B	74	VAL	CA-C-N	-5.18	114.64	120.14
1	B	74	VAL	C-N-CA	-5.18	114.64	120.14
1	B	345	ASP	CB-CA-C	-5.18	99.68	110.40
1	A	64	SER	CB-CA-C	-5.18	102.79	111.13
1	A	1681	VAL	N-CA-C	-5.18	105.66	110.53
1	B	80	ASP	CA-C-N	5.17	129.98	122.08
1	B	80	ASP	C-N-CA	5.17	129.98	122.08
1	C	900	ASP	CA-C-N	5.16	127.20	120.28
1	C	900	ASP	C-N-CA	5.16	127.20	120.28
1	B	338	ILE	N-CA-C	5.16	117.50	111.05
1	A	919	HIS	CA-C-N	-5.15	114.30	119.56
1	A	919	HIS	C-N-CA	-5.15	114.30	119.56
1	A	324	ASN	CA-C-N	5.14	125.68	120.38
1	A	324	ASN	C-N-CA	5.14	125.68	120.38
1	B	1341	CYS	N-CA-C	5.12	118.63	112.38
1	A	1502	ILE	CB-CA-C	-5.12	105.33	112.04
1	B	537	ARG	CB-CG-CD	5.12	123.08	111.30
1	D	622	LYS	CA-C-N	5.12	125.16	119.32
1	D	622	LYS	C-N-CA	5.12	125.16	119.32
1	B	1535	CYS	N-CA-C	-5.12	105.78	111.36
1	B	381	ASN	CA-C-N	5.11	125.03	119.76
1	B	381	ASN	C-N-CA	5.11	125.03	119.76
1	D	553	VAL	N-CA-C	5.10	113.06	107.60
1	B	919	HIS	CA-C-N	-5.08	114.38	119.56
1	B	919	HIS	C-N-CA	-5.08	114.38	119.56
1	B	66	LYS	CD-CE-NZ	5.08	128.15	111.90
1	D	217	LEU	N-CA-CB	5.08	118.36	110.44
1	D	80	ASP	CA-C-N	5.07	129.84	122.08
1	D	80	ASP	C-N-CA	5.07	129.84	122.08
1	B	1643	THR	CB-CA-C	-5.07	105.21	113.37
1	D	434	LYS	CA-CB-CG	5.06	124.22	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ALA	N-CA-C	5.05	116.19	109.93
1	C	1238	GLU	N-CA-C	-5.05	102.87	110.24
1	C	1023	LEU	N-CA-C	-5.04	105.49	111.69
1	D	337	ILE	N-CA-C	-5.04	105.41	110.30
1	D	537	ARG	CB-CG-CD	5.04	122.89	111.30
1	A	1341	CYS	N-CA-C	5.03	118.52	112.38
1	B	254	ASP	N-CA-C	5.03	119.26	113.18
1	B	434	LYS	CA-CB-CG	5.03	124.16	114.10
1	D	556	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	1542	THR	O-C-N	-5.01	116.42	122.48
1	D	66	LYS	CG-CD-CE	-5.01	99.78	111.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1469	GLN	Mainchain
1	A	539	ASN	Peptide
1	B	1469	GLN	Mainchain
1	B	539	ASN	Peptide
1	C	1288	TYR	Mainchain
1	C	539	ASN	Peptide
1	C	896	GLU	Mainchain
1	D	101	THR	Mainchain
1	D	1288	TYR	Mainchain
1	D	382	PRO	Mainchain
1	D	422	ASP	Mainchain
1	D	517	ASN	Mainchain
1	D	539	ASN	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	12939	0	12896	234	0
1	B	12922	0	12878	228	1
1	C	12939	0	12896	214	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	12922	0	12878	226	0
All	All	51722	0	51548	853	1

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 8.

All (853) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:O	1:B:62:SER:OG	1.78	1.01
1:B:79:LYS:HA	1:B:121:THR:HG22	1.45	0.97
1:C:1509:GLN:NE2	1:D:101:THR:O	1.97	0.97
1:D:79:LYS:HA	1:D:121:THR:HG22	1.45	0.95
1:A:493:LEU:HB2	1:A:496:LEU:HD12	1.47	0.94
1:C:79:LYS:HA	1:C:121:THR:HG22	1.51	0.93
1:A:1546:GLU:HB2	1:D:1288:TYR:CD1	2.06	0.91
1:A:63:LYS:HA	1:B:1468:HIS:O	1.70	0.91
1:A:1288:TYR:OH	1:D:1541:GLU:HB3	1.72	0.89
1:A:1468:HIS:HE1	1:B:59:ILE:HG23	1.39	0.88
1:C:1459:ASN:HD21	1:C:1460:ARG:HH11	1.21	0.87
1:A:79:LYS:HA	1:A:121:THR:HG22	1.55	0.86
1:D:59:ILE:O	1:D:62:SER:OG	1.94	0.84
1:A:1459:ASN:HD21	1:A:1460:ARG:HH11	1.22	0.84
1:D:1459:ASN:HD21	1:D:1460:ARG:HH11	1.22	0.83
1:D:79:LYS:HG2	1:D:81:ASN:HB2	1.60	0.82
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.59	0.82
1:B:79:LYS:HG2	1:B:81:ASN:HB2	1.61	0.82
1:B:1459:ASN:HD21	1:B:1460:ARG:HH11	1.23	0.81
1:C:59:ILE:HG23	1:D:1468:HIS:HE1	1.43	0.80
1:C:79:LYS:HG2	1:C:81:ASN:HB2	1.64	0.80
1:A:1468:HIS:O	1:B:63:LYS:HA	1.82	0.80
1:A:58:ASN:O	1:A:62:SER:OG	2.01	0.79
1:D:859:VAL:HG23	1:D:860:ILE:HD12	1.63	0.79
1:D:186:ASN:HD21	1:D:458:THR:HG22	1.45	0.79
1:C:59:ILE:HG23	1:D:1468:HIS:CE1	2.17	0.78
1:A:859:VAL:HG23	1:A:860:ILE:HD12	1.65	0.77
1:B:1585:VAL:HG13	1:B:1586:PHE:CD1	2.21	0.76
1:D:1585:VAL:HG13	1:D:1586:PHE:CD1	2.21	0.76
1:A:64:SER:HA	1:B:1471:VAL:HG23	1.68	0.76
1:B:859:VAL:HG23	1:B:860:ILE:HD12	1.68	0.76
1:C:1585:VAL:HG13	1:C:1586:PHE:CD1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:859:VAL:HG23	1:C:860:ILE:HD12	1.65	0.76
1:A:1585:VAL:HG13	1:A:1586:PHE:CD1	2.21	0.75
1:A:1546:GLU:HB2	1:D:1288:TYR:HD1	1.49	0.75
1:B:1016:ARG:NH2	1:B:1051:PHE:O	2.19	0.75
1:B:1625:MET:HE1	1:B:1627:ILE:HG13	1.68	0.74
1:A:1625:MET:HE1	1:A:1627:ILE:HG13	1.69	0.74
1:A:1016:ARG:NH2	1:A:1051:PHE:O	2.21	0.73
1:C:62:SER:O	1:D:1470:THR:HA	1.89	0.73
1:C:1016:ARG:NH2	1:C:1051:PHE:O	2.22	0.73
1:B:186:ASN:HD21	1:B:458:THR:HG22	1.54	0.72
1:C:1625:MET:HE1	1:C:1627:ILE:HG13	1.71	0.72
1:C:1459:ASN:ND2	1:C:1460:ARG:HH11	1.87	0.72
1:D:1625:MET:HE1	1:D:1627:ILE:HG13	1.69	0.72
1:C:493:LEU:HB2	1:C:496:LEU:HD12	1.70	0.72
1:D:1016:ARG:NH2	1:D:1051:PHE:O	2.23	0.72
1:A:1459:ASN:ND2	1:A:1460:ARG:HH11	1.87	0.71
1:B:275:TYR:HD1	1:B:428:ILE:HD11	1.55	0.71
1:C:1464:GLN:O	1:C:1468:HIS:HD2	1.73	0.71
1:D:1459:ASN:ND2	1:D:1460:ARG:HH11	1.88	0.71
1:A:1470:THR:HA	1:B:62:SER:O	1.91	0.71
1:A:1542:THR:O	1:D:1541:GLU:HG3	1.90	0.71
1:A:59:ILE:HG23	1:B:1468:HIS:HE1	1.56	0.71
1:C:149:VAL:HG13	1:C:151:GLY:H	1.54	0.71
1:D:275:TYR:HD1	1:D:428:ILE:HD11	1.54	0.70
1:D:57:TRP:O	1:D:61:GLN:HG2	1.91	0.70
1:A:186:ASN:HD21	1:A:458:THR:HG22	1.57	0.70
1:A:1465:VAL:O	1:A:1469:GLN:N	2.25	0.69
1:B:1459:ASN:ND2	1:B:1460:ARG:HH11	1.90	0.69
1:C:186:ASN:HD21	1:C:458:THR:HG22	1.58	0.69
1:B:519:TYR:CE2	1:B:537:ARG:HB2	2.29	0.68
1:B:186:ASN:ND2	1:B:458:THR:HG22	2.08	0.67
1:B:1466:GLU:C	1:B:1469:GLN:H	2.03	0.67
1:D:1318:ASN:HD21	1:D:1605:LYS:H	1.43	0.67
1:C:1571:MET:HG2	1:C:1601:TYR:CE2	2.30	0.66
1:A:149:VAL:HG13	1:A:151:GLY:H	1.59	0.66
1:A:1287:HIS:CE1	1:A:1288:TYR:CE2	2.83	0.66
1:A:834:MET:HE1	1:A:889:TYR:CD2	2.31	0.66
1:D:275:TYR:CD1	1:D:428:ILE:HD11	2.31	0.66
1:B:1313:GLY:HA3	1:B:1318:ASN:HD22	1.61	0.66
1:A:62:SER:O	1:B:1470:THR:HA	1.96	0.66
1:A:504:LYS:O	1:A:557:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:HG22	1:B:92:ALA:H	1.62	0.65
1:C:464:ASP:HA	1:C:466:ARG:HH21	1.62	0.65
1:D:186:ASN:ND2	1:D:458:THR:HG22	2.11	0.65
1:A:377:THR:HA	1:A:429:THR:HG22	1.77	0.65
1:B:275:TYR:CD1	1:B:428:ILE:HD11	2.32	0.65
1:C:63:LYS:HA	1:D:1468:HIS:O	1.97	0.64
1:C:377:THR:HA	1:C:429:THR:HG22	1.78	0.64
1:B:1318:ASN:HD21	1:B:1605:LYS:H	1.46	0.64
1:D:1428:SER:O	1:D:1428:SER:OG	2.13	0.64
1:C:504:LYS:O	1:C:557:ARG:NH2	2.30	0.64
1:C:1075:ALA:HB3	1:C:1131:LYS:HG2	1.80	0.64
1:A:464:ASP:HA	1:A:466:ARG:HH21	1.62	0.64
1:C:62:SER:HB3	1:D:1504:TYR:OH	1.99	0.63
1:B:626:THR:HG22	1:B:649:LYS:HB2	1.79	0.63
1:B:834:MET:HE1	1:B:889:TYR:CD2	2.34	0.63
1:A:1468:HIS:ND1	1:B:62:SER:OG	2.31	0.63
1:D:1464:GLN:O	1:D:1468:HIS:HD2	1.81	0.63
1:D:121:THR:HG21	1:D:157:SER:OG	1.99	0.63
1:A:1288:TYR:OH	1:D:1541:GLU:OE2	2.10	0.63
1:B:205:ALA:O	1:B:206:CYS:HB2	1.99	0.63
1:B:1150:THR:HG23	1:B:1153:ASP:H	1.64	0.63
1:B:220:SER:HB2	1:B:470:GLU:O	1.99	0.63
1:A:1428:SER:O	1:A:1428:SER:OG	2.17	0.62
1:D:205:ALA:O	1:D:206:CYS:HB2	1.99	0.62
1:C:1470:THR:HA	1:D:62:SER:O	1.99	0.62
1:B:121:THR:HG21	1:B:157:SER:OG	1.99	0.62
1:C:1537:THR:O	1:C:1541:GLU:HG2	2.00	0.62
1:A:163:ARG:HG3	1:A:165:ILE:HD13	1.82	0.62
1:C:1150:THR:HG23	1:C:1153:ASP:H	1.64	0.62
1:D:834:MET:HE1	1:D:889:TYR:CD2	2.34	0.62
1:A:64:SER:N	1:B:1469:GLN:O	2.33	0.61
1:A:477:SER:OG	1:A:479:ASP:HB2	2.00	0.61
1:B:1075:ALA:HB3	1:B:1131:LYS:HG2	1.80	0.61
1:D:90:THR:HG22	1:D:92:ALA:H	1.64	0.61
1:A:1075:ALA:HB3	1:A:1131:LYS:HG2	1.82	0.61
1:C:162:GLY:HA2	1:C:187:LEU:HD21	1.83	0.61
1:D:220:SER:HB2	1:D:470:GLU:O	2.00	0.61
1:D:1150:THR:HG23	1:D:1153:ASP:H	1.65	0.61
1:B:1708:TRP:HE3	1:B:1709:ILE:HD12	1.63	0.61
1:C:101:THR:O	1:D:1509:GLN:NE2	2.33	0.61
1:C:205:ALA:O	1:C:206:CYS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1571:MET:HG2	1:D:1601:TYR:CE2	2.34	0.61
1:A:742:ARG:HH22	1:A:753:VAL:HB	1.66	0.61
1:A:1466:GLU:C	1:A:1469:GLN:H	2.07	0.61
1:B:1339:ILE:HG23	1:B:1344:PRO:HD2	1.82	0.61
1:B:1287:HIS:CE1	1:B:1288:TYR:CE2	2.89	0.61
1:A:90:THR:HG22	1:A:92:ALA:H	1.64	0.61
1:D:1075:ALA:HB3	1:D:1131:LYS:HG2	1.82	0.61
1:B:377:THR:HA	1:B:429:THR:HG22	1.83	0.61
1:B:57:TRP:O	1:B:61:GLN:HG2	2.01	0.60
1:A:59:ILE:HG23	1:B:1468:HIS:CE1	2.37	0.60
1:A:1150:THR:HG23	1:A:1153:ASP:H	1.66	0.60
1:C:834:MET:HE1	1:C:889:TYR:CD2	2.36	0.60
1:D:1260:VAL:HG12	1:D:1355:VAL:HA	1.84	0.60
1:A:205:ALA:O	1:A:206:CYS:HB2	2.00	0.60
1:D:149:VAL:HG13	1:D:151:GLY:H	1.67	0.60
1:B:149:VAL:HG13	1:B:151:GLY:H	1.66	0.60
1:D:600:ILE:HD11	1:D:609:TYR:CE1	2.36	0.60
1:C:90:THR:HG22	1:C:92:ALA:H	1.66	0.60
1:C:1339:ILE:HG23	1:C:1344:PRO:HD2	1.83	0.60
1:D:1313:GLY:HA3	1:D:1318:ASN:HD22	1.67	0.60
1:B:1465:VAL:O	1:B:1469:GLN:N	2.35	0.60
1:A:1259:GLY:HA2	1:A:1375:VAL:HG12	1.84	0.59
1:B:1500:CYS:HB3	1:B:1504:TYR:CZ	2.36	0.59
1:D:1339:ILE:HG23	1:D:1344:PRO:HD2	1.83	0.59
1:C:1468:HIS:HE1	1:D:59:ILE:HG12	1.66	0.59
1:D:60:LEU:HD11	1:D:114:GLY:HA2	1.83	0.59
1:A:162:GLY:HA2	1:A:187:LEU:HD21	1.85	0.59
1:B:375:VAL:HG12	1:B:429:THR:HG23	1.84	0.59
1:B:478:LYS:O	1:B:481:LEU:HG	2.02	0.59
1:C:1428:SER:O	1:C:1428:SER:OG	2.18	0.59
1:D:375:VAL:HG12	1:D:429:THR:HG23	1.85	0.59
1:A:61:GLN:O	1:A:66:LYS:NZ	2.29	0.59
1:B:143:VAL:HG13	1:B:461:LYS:HB3	1.84	0.59
1:D:1708:TRP:HE3	1:D:1709:ILE:HD12	1.67	0.59
1:C:163:ARG:HG3	1:C:165:ILE:HD13	1.84	0.59
1:D:626:THR:HG22	1:D:649:LYS:HB2	1.85	0.59
1:D:377:THR:HA	1:D:429:THR:HG22	1.84	0.59
1:A:1708:TRP:HE3	1:A:1709:ILE:HD12	1.68	0.59
1:B:1260:VAL:HG12	1:B:1355:VAL:HA	1.83	0.59
1:D:519:TYR:CE2	1:D:537:ARG:HB2	2.37	0.59
1:A:186:ASN:ND2	1:A:458:THR:HG22	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1428:SER:O	1:B:1428:SER:OG	2.18	0.59
1:C:1708:TRP:HE3	1:C:1709:ILE:HD12	1.66	0.59
1:C:626:THR:HG22	1:C:649:LYS:HB2	1.85	0.59
1:A:1469:GLN:HB3	1:B:64:SER:OG	2.02	0.58
1:B:1121:PRO:HG2	1:B:1189:ILE:H	1.68	0.58
1:C:186:ASN:ND2	1:C:458:THR:HG22	2.18	0.58
1:C:477:SER:OG	1:C:479:ASP:HB2	2.02	0.58
1:D:1121:PRO:HG2	1:D:1189:ILE:H	1.66	0.58
1:A:603:PHE:HB3	1:A:608:PRO:HB2	1.84	0.58
1:C:742:ARG:HH22	1:C:753:VAL:HB	1.69	0.58
1:D:1131:LYS:HB3	1:D:1171:SER:HB2	1.84	0.58
1:A:320:PHE:O	1:A:323:THR:HB	2.03	0.58
1:A:600:ILE:HD11	1:A:609:TYR:CZ	2.38	0.58
1:B:600:ILE:HD11	1:B:609:TYR:CE1	2.39	0.58
1:D:478:LYS:O	1:D:481:LEU:HG	2.03	0.58
1:A:1571:MET:HG2	1:A:1601:TYR:CE2	2.37	0.58
1:B:317:THR:HG21	1:B:338:ILE:HG21	1.84	0.58
1:A:1260:VAL:HG12	1:A:1355:VAL:HA	1.85	0.58
1:D:317:THR:HG21	1:D:338:ILE:HG21	1.85	0.58
1:B:1131:LYS:HB3	1:B:1171:SER:HB2	1.85	0.58
1:C:56:GLN:O	1:C:59:ILE:HB	2.03	0.58
1:B:742:ARG:HH22	1:B:753:VAL:HB	1.67	0.58
1:C:1131:LYS:HB3	1:C:1171:SER:HB2	1.86	0.58
1:C:1710:ASN:C	1:C:1712:ASN:H	2.12	0.58
1:A:1339:ILE:HG23	1:A:1344:PRO:HD2	1.84	0.58
1:B:1259:GLY:HA2	1:B:1375:VAL:HG12	1.86	0.58
1:A:1131:LYS:HB3	1:A:1171:SER:HB2	1.86	0.57
1:C:375:VAL:HG12	1:C:429:THR:HG23	1.85	0.57
1:C:1464:GLN:O	1:C:1468:HIS:CD2	2.55	0.57
1:D:853:GLN:HG2	1:D:858:LYS:HG2	1.86	0.57
1:C:600:ILE:HD11	1:C:609:TYR:CZ	2.39	0.57
1:D:1587:LEU:HB3	1:D:1647:TRP:CD2	2.39	0.57
1:A:1713:ILE:O	1:A:1717:VAL:HG23	2.05	0.57
1:C:603:PHE:HB3	1:C:608:PRO:HB2	1.86	0.57
1:D:1085:TYR:CD2	1:D:1108:ARG:HD3	2.39	0.57
1:A:1121:PRO:HG2	1:A:1189:ILE:H	1.70	0.57
1:B:603:PHE:HB3	1:B:608:PRO:HB2	1.86	0.57
1:C:1069:CYS:SG	1:C:1224:GLN:HB2	2.45	0.57
1:A:1710:ASN:C	1:A:1712:ASN:H	2.13	0.56
1:B:1587:LEU:HB3	1:B:1647:TRP:CD2	2.40	0.56
1:D:742:ARG:HH22	1:D:753:VAL:HB	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:TYR:CD2	1:C:1108:ARG:HD3	2.40	0.56
1:C:1121:PRO:HG2	1:C:1189:ILE:H	1.71	0.56
1:D:752:LEU:H	1:D:752:LEU:HD12	1.70	0.56
1:D:1315:HIS:HD2	1:D:1317:SER:H	1.52	0.56
1:A:752:LEU:HD12	1:A:752:LEU:H	1.71	0.56
1:B:417:SER:OG	1:B:427:GLY:HA2	2.04	0.56
1:B:1069:CYS:SG	1:B:1224:GLN:HB2	2.46	0.56
1:A:1085:TYR:CD2	1:A:1108:ARG:HD3	2.40	0.56
1:B:504:LYS:O	1:B:557:ARG:NH2	2.39	0.56
1:C:853:GLN:HG2	1:C:858:LYS:HG2	1.86	0.56
1:C:957:ILE:HG12	1:C:1023:LEU:HD22	1.86	0.56
1:A:1288:TYR:CD1	1:A:1288:TYR:C	2.83	0.56
1:A:1458:ILE:HG21	1:A:1478:GLN:HG2	1.88	0.56
1:D:265:TRP:CD2	1:D:272:PRO:HG3	2.41	0.56
1:C:320:PHE:O	1:C:323:THR:HB	2.06	0.56
1:B:853:GLN:HG2	1:B:858:LYS:HG2	1.88	0.56
1:C:1468:HIS:CE1	1:D:59:ILE:HG23	2.40	0.55
1:C:1587:LEU:HB3	1:C:1647:TRP:CD2	2.40	0.55
1:D:417:SER:OG	1:D:427:GLY:HA2	2.06	0.55
1:A:1587:LEU:HB3	1:A:1647:TRP:CD2	2.42	0.55
1:D:1710:ASN:C	1:D:1712:ASN:H	2.13	0.55
1:D:1713:ILE:O	1:D:1717:VAL:HG23	2.06	0.55
1:A:853:GLN:HG2	1:A:858:LYS:HG2	1.88	0.55
1:D:174:THR:OG1	1:D:210:ASP:OD1	2.24	0.55
1:C:57:TRP:O	1:C:61:GLN:HG2	2.06	0.55
1:D:1194:TYR:HE2	1:D:1206:MET:HE3	1.72	0.55
1:A:626:THR:HG22	1:A:649:LYS:HB2	1.88	0.55
1:B:1464:GLN:O	1:B:1468:HIS:HD2	1.88	0.55
1:B:1545:SER:C	1:B:1546:GLU:HG3	2.31	0.55
1:A:121:THR:HG21	1:A:157:SER:OG	2.06	0.55
1:A:375:VAL:HG12	1:A:429:THR:HG23	1.89	0.55
1:A:1500:CYS:HB3	1:A:1504:TYR:CZ	2.42	0.55
1:C:1571:MET:HG2	1:C:1601:TYR:HE2	1.70	0.55
1:B:80:ASP:OD1	1:B:90:THR:HB	2.07	0.55
1:C:1713:ILE:O	1:C:1717:VAL:HG23	2.06	0.55
1:B:1085:TYR:CD2	1:B:1108:ARG:HD3	2.42	0.54
1:B:1189:ILE:HG21	1:B:1220:LEU:HD23	1.89	0.54
1:A:57:TRP:O	1:A:61:GLN:HG2	2.07	0.54
1:B:1458:ILE:HG21	1:B:1478:GLN:HG2	1.89	0.54
1:C:1260:VAL:HG12	1:C:1355:VAL:HA	1.88	0.54
1:B:957:ILE:HG12	1:B:1023:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:LYS:O	1:D:557:ARG:NH2	2.39	0.54
1:A:1561:ASN:ND2	1:A:1601:TYR:HB3	2.21	0.54
1:D:80:ASP:OD1	1:D:90:THR:HB	2.07	0.54
1:A:65:ASN:O	1:A:68:GLU:HB2	2.07	0.54
1:A:611:GLU:C	1:A:613:ILE:H	2.15	0.54
1:B:847:GLU:OE2	1:B:873:ARG:NH1	2.41	0.54
1:C:1458:ILE:HG21	1:C:1478:GLN:HG2	1.90	0.54
1:A:295:GLU:HB3	1:A:296:PRO:HD3	1.90	0.54
1:A:607:LYS:HB2	1:A:608:PRO:CD	2.38	0.54
1:C:607:LYS:HB2	1:C:608:PRO:CD	2.38	0.54
1:A:1069:CYS:SG	1:A:1224:GLN:HB2	2.48	0.54
1:B:1194:TYR:HE2	1:B:1206:MET:HE3	1.73	0.54
1:D:9:VAL:HB	1:D:221:ASP:OD1	2.07	0.54
1:B:1561:ASN:ND2	1:B:1601:TYR:HB3	2.22	0.54
1:D:603:PHE:HB3	1:D:608:PRO:HB2	1.89	0.54
1:A:80:ASP:OD1	1:A:90:THR:HB	2.08	0.54
1:A:1184:SER:C	1:A:1185:ILE:HD13	2.33	0.54
1:A:1194:TYR:HE2	1:A:1206:MET:HE3	1.72	0.53
1:A:847:GLU:OE2	1:A:873:ARG:NH1	2.42	0.53
1:A:1200:THR:OG1	1:A:1208:GLY:HA3	2.09	0.53
1:A:1543:ILE:O	1:D:1542:THR:HA	2.08	0.53
1:B:487:ALA:HB3	1:B:584:SER:HB2	1.91	0.53
1:C:295:GLU:HB3	1:C:296:PRO:HD3	1.89	0.53
1:A:634:GLU:OE1	1:A:1008:LYS:HE2	2.09	0.53
1:D:1189:ILE:HG21	1:D:1220:LEU:HD23	1.90	0.53
1:A:62:SER:HB3	1:B:1504:TYR:CE2	2.44	0.53
1:A:624:PHE:HD1	1:A:698:GLN:HG3	1.74	0.53
1:C:592:TYR:OH	1:D:589:GLU:HG3	2.09	0.53
1:C:1194:TYR:HE2	1:C:1206:MET:HE3	1.72	0.53
1:B:265:TRP:CD2	1:B:272:PRO:HG3	2.44	0.53
1:C:634:GLU:OE1	1:C:1008:LYS:HE2	2.09	0.53
1:D:957:ILE:HG12	1:D:1023:LEU:HD22	1.90	0.53
1:A:957:ILE:HG12	1:A:1023:LEU:HD22	1.90	0.53
1:B:1459:ASN:ND2	1:B:1460:ARG:HD2	2.24	0.53
1:C:1503:ALA:HB1	1:D:55:HIS:CD2	2.44	0.53
1:D:1259:GLY:HA2	1:D:1375:VAL:HG12	1.91	0.53
1:A:1149:CYS:HB2	1:A:1156:ILE:HG22	1.91	0.52
1:B:1184:SER:C	1:B:1185:ILE:HD13	2.34	0.52
1:A:1459:ASN:ND2	1:A:1460:ARG:HD2	2.24	0.52
1:C:80:ASP:OD1	1:C:90:THR:HB	2.09	0.52
1:C:1184:SER:C	1:C:1185:ILE:HD13	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:VAL:HG13	1:D:376:PRO:O	2.09	0.52
1:A:92:ALA:HB3	1:A:125:GLN:HA	1.90	0.52
1:A:163:ARG:HG3	1:A:165:ILE:CD1	2.39	0.52
1:A:607:LYS:HB2	1:A:608:PRO:HD3	1.91	0.52
1:A:634:GLU:CD	1:A:1008:LYS:HE2	2.35	0.52
1:D:56:GLN:O	1:D:59:ILE:HB	2.10	0.52
1:A:125:GLN:HG2	1:A:126:PHE:CD1	2.45	0.52
1:B:174:THR:OG1	1:B:210:ASP:OD1	2.27	0.52
1:C:600:ILE:HD11	1:C:609:TYR:CE1	2.45	0.52
1:C:375:VAL:CG1	1:C:401:TRP:HB3	2.40	0.52
1:D:634:GLU:OE1	1:D:1008:LYS:HE2	2.09	0.52
1:D:1459:ASN:ND2	1:D:1460:ARG:HD2	2.24	0.52
1:A:1189:ILE:HG21	1:A:1220:LEU:HD23	1.91	0.52
1:A:1545:SER:C	1:A:1546:GLU:HG3	2.34	0.52
1:C:1459:ASN:ND2	1:C:1460:ARG:HD2	2.25	0.52
1:B:375:VAL:HG13	1:B:376:PRO:O	2.10	0.52
1:D:1571:MET:HG2	1:D:1601:TYR:HE2	1.75	0.52
1:A:592:TYR:OH	1:B:589:GLU:HG3	2.10	0.52
1:A:1203:MET:HE3	1:A:1633:SER:HB3	1.92	0.52
1:A:1265:HIS:HE1	1:A:1322:TYR:CZ	2.28	0.52
1:B:143:VAL:HG22	1:B:163:ARG:HG3	1.91	0.52
1:B:919:HIS:ND1	1:B:920:PRO:HD3	2.25	0.52
1:C:634:GLU:CD	1:C:1008:LYS:HE2	2.35	0.52
1:C:829:HIS:CD2	1:C:850:CYS:HB2	2.45	0.52
1:C:835:MET:HG2	1:C:933:TRP:HE3	1.75	0.52
1:D:1184:SER:C	1:D:1185:ILE:HD13	2.35	0.52
1:D:1200:THR:OG1	1:D:1208:GLY:HA3	2.09	0.52
1:D:1458:ILE:HG21	1:D:1478:GLN:HG2	1.91	0.52
1:A:835:MET:HG2	1:A:933:TRP:HE3	1.74	0.52
1:A:1288:TYR:CZ	1:D:1541:GLU:HB3	2.45	0.52
1:A:75:PRO:O	1:A:166:VAL:HG22	2.11	0.51
1:A:589:GLU:O	1:A:593:THR:HB	2.09	0.51
1:D:1618:VAL:HG13	1:D:1625:MET:HE3	1.92	0.51
1:B:9:VAL:HB	1:B:221:ASP:OD1	2.11	0.51
1:B:60:LEU:HD11	1:B:114:GLY:HA2	1.91	0.51
1:C:65:ASN:O	1:C:68:GLU:HB2	2.10	0.51
1:C:1189:ILE:HG21	1:C:1220:LEU:HD23	1.91	0.51
1:C:752:LEU:HD12	1:C:752:LEU:H	1.75	0.51
1:C:1259:GLY:HA2	1:C:1375:VAL:HG12	1.91	0.51
1:C:1469:GLN:HB2	1:D:63:LYS:HA	1.93	0.51
1:A:600:ILE:HD11	1:A:609:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:LYS:HB2	1:C:608:PRO:HD3	1.91	0.51
1:D:1498:LEU:O	1:D:1502:ILE:HG12	2.11	0.51
1:A:59:ILE:HD13	1:A:111:ARG:NH2	2.26	0.51
1:B:1315:HIS:HD2	1:B:1317:SER:H	1.58	0.51
1:B:1498:LEU:O	1:B:1502:ILE:HG12	2.11	0.51
1:C:92:ALA:HB3	1:C:125:GLN:HA	1.91	0.51
1:C:589:GLU:O	1:C:593:THR:HB	2.11	0.51
1:C:847:GLU:OE2	1:C:873:ARG:NH1	2.44	0.51
1:C:869:PRO:HD2	1:C:872:THR:CG2	2.41	0.51
1:D:487:ALA:HB3	1:D:584:SER:HB2	1.93	0.51
1:D:869:PRO:HD2	1:D:872:THR:CG2	2.41	0.51
1:B:351:LYS:HE3	1:B:351:LYS:O	2.11	0.51
1:A:63:LYS:O	1:A:66:LYS:NZ	2.34	0.51
1:B:1265:HIS:HE1	1:B:1322:TYR:CZ	2.28	0.51
1:D:829:HIS:CD2	1:D:850:CYS:HB2	2.47	0.50
1:C:125:GLN:HG2	1:C:126:PHE:CD1	2.47	0.50
1:C:62:SER:HB2	1:D:1468:HIS:HB3	1.93	0.50
1:A:1470:THR:HB	1:A:1473:ILE:HD12	1.93	0.50
1:B:1345:SER:OG	1:B:1346:LEU:N	2.44	0.50
1:C:290:VAL:HG12	1:C:292:VAL:HG23	1.92	0.50
1:C:1149:CYS:HB2	1:C:1156:ILE:HG22	1.93	0.50
1:D:677:THR:OG1	1:D:680:GLU:HB2	2.12	0.50
1:A:1466:GLU:O	1:A:1469:GLN:HG3	2.12	0.50
1:D:143:VAL:HG13	1:D:461:LYS:HB3	1.94	0.50
1:A:1288:TYR:OH	1:D:1541:GLU:CB	2.54	0.50
1:B:1149:CYS:HB2	1:B:1156:ILE:HG22	1.93	0.50
1:C:1200:THR:OG1	1:C:1208:GLY:HA3	2.11	0.50
1:D:1140:ILE:HD11	1:D:1185:ILE:HD12	1.94	0.50
1:C:1057:ALA:C	1:C:1059:LYS:H	2.20	0.50
1:A:62:SER:HB2	1:B:1468:HIS:ND1	2.27	0.50
1:A:750:VAL:HG22	1:A:879:ALA:HB1	1.94	0.50
1:A:1057:ALA:C	1:A:1059:LYS:H	2.20	0.50
1:D:219:LEU:HB3	1:D:473:LEU:HD21	1.94	0.50
1:D:1203:MET:HE3	1:D:1633:SER:HB3	1.93	0.50
1:B:317:THR:HG23	1:B:321:LEU:HD12	1.94	0.49
1:B:634:GLU:OE1	1:B:1008:LYS:HE2	2.13	0.49
1:A:194:LYS:HG2	1:A:211:CYS:SG	2.52	0.49
1:A:1287:HIS:CE1	1:A:1288:TYR:CZ	3.00	0.49
1:C:420:ARG:HG3	1:C:424:LEU:O	2.11	0.49
1:C:1618:VAL:HG13	1:C:1625:MET:HE3	1.94	0.49
1:D:677:THR:HG1	1:D:680:GLU:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1324:TYR:CZ	1:D:1347:GLY:HA3	2.47	0.49
1:A:417:SER:OG	1:A:427:GLY:HA2	2.12	0.49
1:A:487:ALA:HB3	1:A:584:SER:HB2	1.93	0.49
1:A:1498:LEU:O	1:A:1502:ILE:HG12	2.13	0.49
1:B:610:ILE:O	1:B:610:ILE:HG22	2.12	0.49
1:B:1464:GLN:O	1:B:1468:HIS:CD2	2.65	0.49
1:C:1345:SER:OG	1:C:1346:LEU:N	2.45	0.49
1:B:65:ASN:O	1:B:66:LYS:C	2.54	0.49
1:C:163:ARG:HG3	1:C:165:ILE:CD1	2.41	0.49
1:C:1115:GLY:HA2	1:C:1237:PHE:HB2	1.93	0.49
1:B:1057:ALA:C	1:B:1059:LYS:H	2.20	0.49
1:C:611:GLU:C	1:C:613:ILE:H	2.20	0.49
1:D:835:MET:HG2	1:D:933:TRP:HE3	1.77	0.49
1:A:1203:MET:CE	1:A:1633:SER:HB3	2.42	0.49
1:B:1618:VAL:HG13	1:B:1625:MET:HE3	1.93	0.49
1:C:1498:LEU:O	1:C:1502:ILE:HG12	2.13	0.49
1:D:847:GLU:OE2	1:D:873:ARG:NH1	2.46	0.49
1:D:1537:THR:O	1:D:1541:GLU:HG2	2.12	0.49
1:A:375:VAL:CG1	1:A:401:TRP:HB3	2.42	0.49
1:A:1464:GLN:O	1:A:1468:HIS:HD2	1.95	0.49
1:D:1269:ASP:OD2	1:D:1269:ASP:N	2.46	0.49
1:D:1500:CYS:HB3	1:D:1504:TYR:CZ	2.48	0.49
1:B:1200:THR:OG1	1:B:1208:GLY:HA3	2.13	0.49
1:D:634:GLU:CD	1:D:1008:LYS:HE2	2.37	0.49
1:A:1345:SER:OG	1:A:1346:LEU:N	2.46	0.49
1:A:1618:VAL:HG13	1:A:1625:MET:HE3	1.94	0.49
1:B:162:GLY:HA2	1:B:187:LEU:HD21	1.95	0.49
1:B:452:PHE:CD1	1:B:457:ARG:HG3	2.48	0.49
1:B:677:THR:OG1	1:B:680:GLU:HB2	2.13	0.49
1:B:869:PRO:HD2	1:B:872:THR:CG2	2.43	0.49
1:C:1468:HIS:CE1	1:D:59:ILE:HG12	2.48	0.49
1:D:1274:GLU:HA	1:D:1277:GLU:HG3	1.95	0.49
1:D:317:THR:HG23	1:D:321:LEU:HD12	1.95	0.49
1:D:1265:HIS:HE1	1:D:1322:TYR:CZ	2.31	0.49
1:A:66:LYS:O	1:A:67:GLU:HB2	2.13	0.48
1:A:1617:VAL:HG11	1:A:1639:LEU:HD22	1.95	0.48
1:B:180:VAL:HB	1:B:181:PRO:HD3	1.95	0.48
1:B:634:GLU:CD	1:B:1008:LYS:HE2	2.38	0.48
1:D:1057:ALA:C	1:D:1059:LYS:H	2.22	0.48
1:A:75:PRO:HB2	1:A:118:ILE:CD1	2.43	0.48
1:B:1470:THR:HB	1:B:1473:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1571:MET:HG2	1:B:1601:TYR:CE2	2.48	0.48
1:C:121:THR:HG21	1:C:157:SER:OG	2.12	0.48
1:C:1553:ASN:OD1	1:C:1606:TYR:OH	2.24	0.48
1:A:536:ARG:HD3	1:A:538:VAL:HG23	1.95	0.48
1:A:1537:THR:O	1:A:1541:GLU:HG2	2.14	0.48
1:B:420:ARG:HB2	1:B:422:ASP:HB2	1.95	0.48
1:B:1102:MET:HE1	1:B:1292:ARG:HA	1.95	0.48
1:C:1203:MET:HE3	1:C:1633:SER:HB3	1.95	0.48
1:D:539:ASN:O	1:D:540:ASP:O	2.31	0.48
1:A:290:VAL:HG12	1:A:292:VAL:HG23	1.95	0.48
1:B:1103:ASP:OD2	1:B:1361:TRP:HB2	2.14	0.48
1:B:1625:MET:CE	1:B:1627:ILE:HG13	2.41	0.48
1:C:536:ARG:HD3	1:C:538:VAL:HG23	1.94	0.48
1:C:1468:HIS:O	1:D:63:LYS:HA	2.13	0.48
1:D:92:ALA:HB3	1:D:125:GLN:HA	1.94	0.48
1:D:243:PHE:CZ	1:D:435:PHE:HA	2.49	0.48
1:A:1467:ARG:NH2	1:B:112:ASP:OD2	2.47	0.48
1:C:16:HIS:ND1	1:C:24:SER:HB2	2.28	0.48
1:C:1104:SER:O	1:C:1108:ARG:HG3	2.13	0.48
1:D:1069:CYS:SG	1:D:1224:GLN:HB2	2.53	0.48
1:B:99:GLN:NE2	1:B:100:PRO:HD2	2.28	0.48
1:C:1265:HIS:HE1	1:C:1322:TYR:CZ	2.31	0.48
1:D:7:TRP:O	1:D:167:PRO:HB3	2.14	0.48
1:D:1345:SER:OG	1:D:1346:LEU:N	2.47	0.48
1:A:919:HIS:ND1	1:A:920:PRO:HD3	2.28	0.48
1:A:1324:TYR:CZ	1:A:1347:GLY:HA3	2.49	0.48
1:C:624:PHE:HD1	1:C:698:GLN:HG3	1.79	0.48
1:D:610:ILE:O	1:D:610:ILE:HG22	2.14	0.48
1:A:1115:GLY:HA2	1:A:1237:PHE:HB2	1.94	0.48
1:D:162:GLY:HA2	1:D:187:LEU:HD21	1.96	0.48
1:A:1587:LEU:HD12	1:A:1630:ALA:HB2	1.96	0.48
1:B:219:LEU:HB3	1:B:473:LEU:HD21	1.95	0.48
1:B:539:ASN:O	1:B:540:ASP:O	2.32	0.48
1:D:1149:CYS:HB2	1:D:1156:ILE:HG22	1.96	0.48
1:D:1561:ASN:ND2	1:D:1601:TYR:HB3	2.28	0.48
1:A:1269:ASP:OD2	1:A:1269:ASP:N	2.46	0.47
1:C:377:THR:HA	1:C:429:THR:CG2	2.44	0.47
1:C:1324:TYR:CZ	1:C:1347:GLY:HA3	2.49	0.47
1:A:420:ARG:HG3	1:A:424:LEU:O	2.13	0.47
1:A:492:HIS:NE2	1:A:501:GLN:OE1	2.41	0.47
1:A:1542:THR:HB	1:D:1541:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1585:VAL:HG13	1:B:1586:PHE:HD1	1.75	0.47
1:D:919:HIS:ND1	1:D:920:PRO:HD3	2.29	0.47
1:D:1459:ASN:HD22	1:D:1460:ARG:HD2	1.80	0.47
1:C:85:LYS:HD3	1:D:1509:GLN:NE2	2.28	0.47
1:C:677:THR:OG1	1:C:680:GLU:HB2	2.14	0.47
1:D:351:LYS:O	1:D:351:LYS:HE3	2.14	0.47
1:A:1142:VAL:HA	1:A:1182:TYR:O	2.15	0.47
1:C:492:HIS:NE2	1:C:501:GLN:OE1	2.45	0.47
1:C:1587:LEU:HD12	1:C:1630:ALA:HB2	1.96	0.47
1:C:1708:TRP:CE3	1:C:1709:ILE:HD12	2.49	0.47
1:D:1103:ASP:OD2	1:D:1361:TRP:HB2	2.14	0.47
1:D:1464:GLN:O	1:D:1468:HIS:CD2	2.64	0.47
1:A:1059:LYS:HA	1:A:1059:LYS:HD2	1.75	0.47
1:B:546:ILE:N	1:B:546:ILE:HD12	2.30	0.47
1:B:1708:TRP:CE3	1:B:1709:ILE:HD12	2.48	0.47
1:C:919:HIS:ND1	1:C:920:PRO:HD3	2.29	0.47
1:D:78:VAL:HG22	1:D:120:LYS:HE3	1.96	0.47
1:D:1115:GLY:HA2	1:D:1237:PHE:HB2	1.96	0.47
1:A:862:GLU:OE1	1:A:1016:ARG:NH1	2.47	0.47
1:B:1587:LEU:HD12	1:B:1630:ALA:HB2	1.97	0.47
1:C:1585:VAL:HG13	1:C:1586:PHE:HD1	1.75	0.47
1:D:99:GLN:NE2	1:D:100:PRO:HD2	2.29	0.47
1:A:1468:HIS:O	1:A:1469:GLN:C	2.53	0.47
1:A:1616:GLY:C	1:A:1642:ARG:HG3	2.40	0.47
1:B:207:LYS:NZ	1:B:238:GLU:OE2	2.47	0.47
1:B:1259:GLY:HA3	1:B:1377:LEU:HD22	1.97	0.47
1:C:417:SER:OG	1:C:427:GLY:HA2	2.15	0.47
1:C:1561:ASN:ND2	1:C:1601:TYR:HB3	2.30	0.47
1:D:546:ILE:N	1:D:546:ILE:HD12	2.29	0.47
1:D:622:LYS:HB2	1:D:622:LYS:HE3	1.67	0.47
1:A:1459:ASN:HD22	1:A:1460:ARG:HD2	1.80	0.47
1:B:302:ARG:HE	1:B:302:ARG:HB3	1.47	0.47
1:B:1269:ASP:OD2	1:B:1269:ASP:N	2.47	0.47
1:A:78:VAL:HG22	1:A:120:LYS:HE3	1.96	0.46
1:A:521:LEU:HB2	1:A:546:ILE:HG12	1.97	0.46
1:A:1140:ILE:HD11	1:A:1185:ILE:HD12	1.96	0.46
1:A:1288:TYR:CD1	1:A:1289:ASN:N	2.84	0.46
1:B:14:SER:O	1:B:18:LYS:HG2	2.15	0.46
1:B:1275:TYR:HB2	1:B:1303:LYS:HG3	1.98	0.46
1:B:1713:ILE:O	1:B:1717:VAL:HG23	2.15	0.46
1:C:1:MET:HB2	1:C:2:GLU:H	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:GLN:O	1:C:66:LYS:NZ	2.40	0.46
1:A:38:ALA:HB1	1:A:39:PRO:HD3	1.97	0.46
1:A:377:THR:HA	1:A:429:THR:CG2	2.43	0.46
1:A:829:HIS:CD2	1:A:850:CYS:HB2	2.50	0.46
1:B:377:THR:HA	1:B:429:THR:CG2	2.45	0.46
1:B:518:ASN:O	1:B:538:VAL:HG23	2.15	0.46
1:B:1459:ASN:HD22	1:B:1460:ARG:HD2	1.80	0.46
1:C:38:ALA:HB1	1:C:39:PRO:HD3	1.97	0.46
1:C:750:VAL:HG22	1:C:879:ALA:HB1	1.97	0.46
1:D:1315:HIS:CD2	1:D:1317:SER:H	2.32	0.46
1:B:92:ALA:HB3	1:B:125:GLN:HA	1.96	0.46
1:C:1203:MET:HE1	1:C:1586:PHE:CG	2.51	0.46
1:D:207:LYS:NZ	1:D:238:GLU:OE2	2.46	0.46
1:A:1102:MET:HE1	1:A:1292:ARG:HA	1.96	0.46
1:B:206:CYS:HA	1:B:312:GLU:CB	2.46	0.46
1:C:1616:GLY:C	1:C:1642:ARG:HG3	2.40	0.46
1:C:1617:VAL:HG11	1:C:1639:LEU:HD22	1.96	0.46
1:D:716:ARG:HH11	1:D:716:ARG:HG3	1.81	0.46
1:B:56:GLN:O	1:B:59:ILE:HB	2.15	0.46
1:B:1537:THR:O	1:B:1541:GLU:HG2	2.16	0.46
1:D:377:THR:HA	1:D:429:THR:CG2	2.46	0.46
1:D:51:GLU:CD	1:D:51:GLU:H	2.24	0.46
1:A:79:LYS:C	1:A:81:ASN:H	2.24	0.46
1:A:1469:GLN:O	1:B:64:SER:HB3	2.16	0.46
1:B:742:ARG:HD3	1:B:752:LEU:HD23	1.97	0.46
1:B:1104:SER:O	1:B:1108:ARG:HG3	2.16	0.46
1:A:1585:VAL:HG13	1:A:1586:PHE:HD1	1.74	0.46
1:C:1123:LEU:HD12	1:C:1183:LEU:HD23	1.98	0.46
1:D:600:ILE:HD11	1:D:609:TYR:CZ	2.51	0.46
1:D:1085:TYR:CD1	1:D:1086:PRO:HA	2.51	0.46
1:A:677:THR:OG1	1:A:680:GLU:HB2	2.16	0.46
1:A:869:PRO:HD2	1:A:872:THR:CG2	2.45	0.46
1:A:1504:TYR:OH	1:B:62:SER:HB2	2.15	0.46
1:B:161:VAL:HG12	1:B:187:LEU:HD22	1.98	0.46
1:B:1274:GLU:HA	1:B:1277:GLU:HG3	1.98	0.46
1:D:75:PRO:O	1:D:167:PRO:HD2	2.15	0.46
1:D:1104:SER:O	1:D:1108:ARG:HG3	2.16	0.46
1:B:125:GLN:HG2	1:B:126:PHE:CD1	2.52	0.45
1:B:624:PHE:HD1	1:B:698:GLN:HG3	1.81	0.45
1:B:1085:TYR:CD1	1:B:1086:PRO:HA	2.52	0.45
1:B:1500:CYS:HB3	1:B:1504:TYR:OH	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:ARG:HE	1:D:302:ARG:HB3	1.48	0.45
1:D:624:PHE:HD1	1:D:698:GLN:HG3	1.81	0.45
1:B:51:GLU:CD	1:B:51:GLU:H	2.24	0.45
1:B:1268:ILE:HA	1:B:1271:PHE:O	2.16	0.45
1:D:1103:ASP:HA	1:D:1361:TRP:HA	1.98	0.45
1:A:1139:VAL:O	1:A:1140:ILE:HD12	2.17	0.45
1:A:1708:TRP:CE3	1:A:1709:ILE:HD12	2.50	0.45
1:B:1115:GLY:HA2	1:B:1237:PHE:HB2	1.99	0.45
1:B:1539:TYR:CD1	1:B:1610:ARG:HG2	2.52	0.45
1:D:180:VAL:HB	1:D:181:PRO:HD3	1.99	0.45
1:B:744:ILE:H	1:B:744:ILE:HG12	1.56	0.45
1:D:420:ARG:H	1:D:420:ARG:HG2	1.36	0.45
1:A:56:GLN:O	1:A:59:ILE:HB	2.16	0.45
1:A:1085:TYR:CD1	1:A:1086:PRO:HA	2.51	0.45
1:A:1203:MET:HE1	1:A:1586:PHE:CG	2.52	0.45
1:B:829:HIS:CD2	1:B:850:CYS:HB2	2.51	0.45
1:C:1085:TYR:CD1	1:C:1086:PRO:HA	2.52	0.45
1:C:1142:VAL:HA	1:C:1182:TYR:O	2.17	0.45
1:A:36:LYS:O	1:A:41:ASP:HB3	2.16	0.45
1:A:1542:THR:O	1:D:1541:GLU:CG	2.60	0.45
1:A:1571:MET:HG2	1:A:1601:TYR:HE2	1.79	0.45
1:A:1625:MET:CE	1:A:1627:ILE:HG13	2.42	0.45
1:B:1140:ILE:HD11	1:B:1185:ILE:HD12	1.98	0.45
1:B:1704:GLU:O	1:B:1707:ALA:HB3	2.17	0.45
1:A:1433:TYR:CE1	1:A:1502:ILE:HD13	2.52	0.45
1:D:522:TYR:O	1:D:533:PRO:HA	2.17	0.45
1:D:546:ILE:HA	1:D:604:GLY:O	2.16	0.45
1:D:1203:MET:CE	1:D:1633:SER:HB3	2.46	0.45
1:D:1625:MET:CE	1:D:1627:ILE:HG13	2.43	0.45
1:C:66:LYS:O	1:C:67:GLU:HB2	2.16	0.45
1:A:75:PRO:O	1:A:167:PRO:HD2	2.17	0.45
1:A:1274:GLU:HA	1:A:1277:GLU:HG3	1.99	0.45
1:B:521:LEU:HD23	1:B:600:ILE:CG2	2.47	0.45
1:C:194:LYS:HG2	1:C:211:CYS:SG	2.57	0.45
1:A:1259:GLY:HA3	1:A:1377:LEU:HD22	2.00	0.44
1:B:143:VAL:CG1	1:B:461:LYS:HB3	2.46	0.44
1:B:622:LYS:HB2	1:B:622:LYS:HE3	1.63	0.44
1:A:1103:ASP:OD2	1:A:1361:TRP:HB2	2.18	0.44
1:B:433:LYS:H	1:B:433:LYS:HG2	1.62	0.44
1:C:36:LYS:HD3	1:C:40:GLU:CD	2.42	0.44
1:C:271:ASN:OD1	1:C:420:ARG:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:LYS:HB3	1:C:641:LYS:HE3	1.58	0.44
1:A:75:PRO:HB2	1:A:118:ILE:HD11	1.99	0.44
1:A:828:ARG:NH2	1:A:866:PRO:O	2.43	0.44
1:A:1184:SER:O	1:A:1185:ILE:HD13	2.17	0.44
1:B:1203:MET:HE3	1:B:1633:SER:HB3	1.99	0.44
1:B:1612:TYR:CD1	1:B:1632:GLY:HA2	2.52	0.44
1:D:433:LYS:O	1:D:436:SER:OG	2.32	0.44
1:D:606:PHE:CZ	1:D:610:ILE:HD11	2.52	0.44
1:D:1539:TYR:CD1	1:D:1610:ARG:HG2	2.52	0.44
1:A:38:ALA:HB1	1:A:39:PRO:CD	2.48	0.44
1:C:66:LYS:H	1:C:66:LYS:HG3	1.55	0.44
1:C:75:PRO:O	1:C:166:VAL:HG22	2.18	0.44
1:A:36:LYS:HD3	1:A:40:GLU:CD	2.43	0.44
1:A:641:LYS:HE3	1:A:641:LYS:HB3	1.57	0.44
1:B:141:PRO:HB2	1:B:146:ASP:HA	1.99	0.44
1:B:1203:MET:HE1	1:B:1586:PHE:CG	2.52	0.44
1:C:1274:GLU:HA	1:C:1277:GLU:HG3	1.99	0.44
1:C:1612:TYR:CD1	1:C:1632:GLY:HA2	2.52	0.44
1:D:75:PRO:O	1:D:166:VAL:HG22	2.17	0.44
1:D:1203:MET:HE1	1:D:1586:PHE:CG	2.53	0.44
1:A:283:LYS:HB2	1:A:283:LYS:HE2	1.67	0.44
1:C:36:LYS:O	1:C:41:ASP:HB3	2.17	0.44
1:C:556:ASP:OD2	1:C:557:ARG:HG2	2.18	0.44
1:C:1103:ASP:OD2	1:C:1361:TRP:HB2	2.18	0.44
1:C:1433:TYR:CE1	1:C:1502:ILE:HD13	2.52	0.44
1:D:1710:ASN:O	1:D:1712:ASN:N	2.51	0.44
1:A:835:MET:HG2	1:A:933:TRP:CE3	2.53	0.44
1:A:1625:MET:HE2	1:A:1626:CYS:C	2.43	0.44
1:B:75:PRO:O	1:B:167:PRO:HD2	2.17	0.44
1:B:268:GLU:OE2	1:B:270:GLU:HB2	2.18	0.44
1:B:1549:TRP:HA	1:B:1556:PHE:HB2	2.00	0.44
1:C:894:THR:HG22	1:C:895:VAL:N	2.33	0.44
1:C:1459:ASN:HD22	1:C:1460:ARG:HD2	1.81	0.44
1:D:1468:HIS:O	1:D:1469:GLN:C	2.57	0.44
1:A:170:LEU:HD11	1:A:229:MET:HE1	1.99	0.44
1:A:375:VAL:HG13	1:A:401:TRP:HB3	1.99	0.44
1:A:556:ASP:OD2	1:A:557:ARG:HG2	2.18	0.44
1:A:1318:ASN:N	1:A:1318:ASN:HD22	2.16	0.44
1:C:38:ALA:HB1	1:C:39:PRO:CD	2.48	0.44
1:C:375:VAL:HG13	1:C:401:TRP:HB3	1.98	0.44
1:C:1215:LYS:N	1:C:1218:ASP:OD2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:SER:O	1:D:18:LYS:HG2	2.17	0.44
1:B:546:ILE:HA	1:B:604:GLY:O	2.18	0.43
1:B:716:ARG:HG3	1:B:716:ARG:HH11	1.83	0.43
1:D:1102:MET:HE1	1:D:1292:ARG:HA	1.99	0.43
1:A:849:ASP:OD1	1:A:851:SER:OG	2.29	0.43
1:A:1468:HIS:O	1:B:62:SER:O	2.35	0.43
1:B:78:VAL:O	1:B:120:LYS:HA	2.18	0.43
1:B:661:SER:OG	1:B:663:HIS:ND1	2.51	0.43
1:B:1323:VAL:HG21	1:B:1477:SER:HB3	2.00	0.43
1:B:1612:TYR:CD2	1:B:1612:TYR:C	2.97	0.43
1:C:78:VAL:HG22	1:C:120:LYS:HE3	2.00	0.43
1:C:567:GLU:HG2	1:C:568:PRO:HA	1.99	0.43
1:C:1318:ASN:N	1:C:1318:ASN:HD22	2.16	0.43
1:D:29:GLU:O	1:D:33:LYS:HG3	2.18	0.43
1:D:862:GLU:OE1	1:D:1016:ARG:NH1	2.51	0.43
1:A:452:PHE:CD1	1:A:457:ARG:HG3	2.53	0.43
1:B:1103:ASP:HA	1:B:1361:TRP:HA	2.00	0.43
1:C:283:LYS:HE2	1:C:283:LYS:HB2	1.68	0.43
1:C:1140:ILE:HD11	1:C:1185:ILE:HD12	1.99	0.43
1:D:1616:GLY:C	1:D:1642:ARG:HG3	2.43	0.43
1:D:1625:MET:HE2	1:D:1626:CYS:C	2.43	0.43
1:A:1104:SER:O	1:A:1108:ARG:HG3	2.18	0.43
1:B:78:VAL:HG22	1:B:120:LYS:HE3	2.00	0.43
1:B:1288:TYR:C	1:B:1288:TYR:CD1	2.96	0.43
1:B:1324:TYR:CZ	1:B:1347:GLY:HA3	2.53	0.43
1:B:1330:ASN:O	1:B:1336:PRO:HA	2.19	0.43
1:B:1571:MET:HG2	1:B:1601:TYR:HE2	1.83	0.43
1:C:521:LEU:HB2	1:C:546:ILE:HG12	2.00	0.43
1:C:1625:MET:CE	1:C:1627:ILE:HG13	2.44	0.43
1:D:420:ARG:C	1:D:422:ASP:N	2.73	0.43
1:D:834:MET:HG2	1:D:835:MET:N	2.33	0.43
1:A:1710:ASN:O	1:A:1712:ASN:N	2.51	0.43
1:B:1617:VAL:HG11	1:B:1639:LEU:HD22	2.01	0.43
1:D:988:VAL:HA	1:D:1008:LYS:O	2.18	0.43
1:D:1323:VAL:HG21	1:D:1477:SER:HB3	2.01	0.43
1:A:715:ASP:OD2	1:A:733:ARG:NH2	2.45	0.43
1:B:75:PRO:O	1:B:166:VAL:HG22	2.19	0.43
1:B:519:TYR:HB2	1:B:546:ILE:HD13	1.99	0.43
1:B:1139:VAL:O	1:B:1140:ILE:HD12	2.18	0.43
1:C:487:ALA:HB3	1:C:584:SER:HB2	1.99	0.43
1:C:1268:ILE:HA	1:C:1271:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:VAL:HG12	1:D:187:LEU:HD22	2.00	0.43
1:D:1059:LYS:HA	1:D:1059:LYS:HD2	1.77	0.43
1:A:1464:GLN:O	1:A:1468:HIS:CD2	2.71	0.43
1:A:1612:TYR:CD2	1:A:1612:TYR:C	2.96	0.43
1:C:1549:TRP:HA	1:C:1556:PHE:HB2	2.01	0.43
1:D:521:LEU:HD11	1:D:533:PRO:HB2	2.01	0.43
1:D:1549:TRP:HA	1:D:1556:PHE:HB2	2.01	0.43
1:A:716:ARG:HG3	1:A:716:ARG:HH11	1.84	0.43
1:C:1540:ARG:HH11	1:C:1540:ARG:HD2	1.66	0.43
1:D:1142:VAL:HA	1:D:1182:TYR:O	2.19	0.43
1:D:1617:VAL:HG11	1:D:1639:LEU:HD22	2.00	0.43
1:A:7:TRP:O	1:A:167:PRO:HB3	2.19	0.43
1:A:1690:LYS:HA	1:A:1690:LYS:HD3	1.82	0.43
1:B:36:LYS:HA	1:B:36:LYS:HD3	1.72	0.43
1:B:1123:LEU:HD12	1:B:1183:LEU:HD23	2.01	0.43
1:B:1523:LEU:HB3	1:B:1643:THR:HG21	2.01	0.43
1:C:840:GLY:N	1:C:888:LYS:HG3	2.33	0.43
1:C:1203:MET:CE	1:C:1633:SER:HB3	2.49	0.43
1:C:1243:PRO:HB2	1:C:1246:LEU:HG	2.01	0.43
1:D:268:GLU:OE2	1:D:270:GLU:HB2	2.18	0.43
1:D:437:ASP:OD1	1:D:437:ASP:N	2.52	0.43
1:D:1525:MET:HE3	1:D:1527:PHE:HA	2.01	0.43
1:D:1730:GLU:OE2	1:D:1730:GLU:HA	2.19	0.43
1:B:600:ILE:HD11	1:B:609:TYR:CZ	2.54	0.42
1:B:750:VAL:HG22	1:B:879:ALA:HB1	2.00	0.42
1:C:75:PRO:HB2	1:C:118:ILE:CD1	2.48	0.42
1:C:957:ILE:CG1	1:C:1023:LEU:HD22	2.49	0.42
1:C:1710:ASN:O	1:C:1712:ASN:N	2.52	0.42
1:A:567:GLU:HG2	1:A:568:PRO:HA	2.00	0.42
1:B:1625:MET:HE2	1:B:1626:CYS:C	2.44	0.42
1:C:1274:GLU:O	1:C:1278:GLN:HG3	2.19	0.42
1:D:143:VAL:CG2	1:D:163:ARG:HG3	2.49	0.42
1:D:556:ASP:HB3	1:D:557:ARG:HG2	2.01	0.42
1:D:716:ARG:HG3	1:D:716:ARG:NH1	2.34	0.42
1:D:1259:GLY:HA3	1:D:1377:LEU:HD22	2.01	0.42
1:A:66:LYS:O	1:A:67:GLU:CB	2.67	0.42
1:A:661:SER:OG	1:A:663:HIS:ND1	2.52	0.42
1:A:1323:VAL:HG21	1:A:1477:SER:HB3	2.00	0.42
1:C:661:SER:OG	1:C:663:HIS:ND1	2.51	0.42
1:C:835:MET:HG2	1:C:933:TRP:CE3	2.54	0.42
1:C:1585:VAL:HG13	1:C:1586:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:SER:HB3	1:D:169:SER:OG	2.18	0.42
1:A:1507:GLU:OE2	1:B:59:ILE:HG12	2.20	0.42
1:B:1102:MET:CE	1:B:1292:ARG:HA	2.50	0.42
1:C:15:PHE:HA	1:C:18:LYS:HE2	2.01	0.42
1:A:1103:ASP:HA	1:A:1361:TRP:HA	2.01	0.42
1:B:1304:TRP:CH2	1:B:1317:SER:HB3	2.54	0.42
1:C:716:ARG:HG3	1:C:716:ARG:HH11	1.85	0.42
1:D:66:LYS:H	1:D:66:LYS:HG3	1.59	0.42
1:D:1123:LEU:HD12	1:D:1183:LEU:HD23	2.00	0.42
1:D:1612:TYR:CD2	1:D:1612:TYR:C	2.97	0.42
1:A:81:ASN:HB3	1:A:82:ILE:HG13	2.01	0.42
1:A:744:ILE:H	1:A:744:ILE:HG12	1.55	0.42
1:B:1456:TYR:CZ	1:B:1460:ARG:HD3	2.54	0.42
1:C:180:VAL:HB	1:C:181:PRO:HD3	2.01	0.42
1:C:1346:LEU:HD13	1:C:1584:ASP:HB2	2.01	0.42
1:D:75:PRO:C	1:D:166:VAL:HG22	2.45	0.42
1:D:1243:PRO:HB2	1:D:1246:LEU:HG	2.02	0.42
1:D:1585:VAL:HG13	1:D:1586:PHE:HD1	1.77	0.42
1:D:1708:TRP:CE3	1:D:1709:ILE:HD12	2.50	0.42
1:A:1456:TYR:CZ	1:A:1460:ARG:HD3	2.55	0.42
1:A:1525:MET:HE3	1:A:1527:PHE:HA	2.02	0.42
1:B:420:ARG:H	1:B:420:ARG:HG2	1.31	0.42
1:B:609:TYR:CZ	1:B:613:ILE:HD11	2.55	0.42
1:B:1184:SER:O	1:B:1185:ILE:HD13	2.20	0.42
1:B:1585:VAL:HG13	1:B:1586:PHE:CE1	2.55	0.42
1:C:1625:MET:HE2	1:C:1626:CYS:C	2.44	0.42
1:D:1433:TYR:CE1	1:D:1502:ILE:HD13	2.55	0.42
1:B:936:ARG:HE	1:B:936:ARG:HB3	1.64	0.42
1:A:15:PHE:CZ	1:A:27:LEU:HD22	2.55	0.42
1:A:297:LEU:HD22	1:A:404:PHE:CD1	2.55	0.42
1:A:709:GLU:HG3	1:A:914:ARG:HD3	2.02	0.42
1:A:968:LYS:HA	1:A:968:LYS:HD2	1.87	0.42
1:B:1138:THR:OG1	1:B:1139:VAL:N	2.52	0.42
1:B:1142:VAL:HA	1:B:1182:TYR:O	2.20	0.42
1:C:79:LYS:C	1:C:81:ASN:H	2.28	0.42
1:C:1456:TYR:CZ	1:C:1460:ARG:HD3	2.55	0.42
1:D:622:LYS:HA	1:D:623:PRO:HD2	1.80	0.42
1:A:224:ILE:O	1:A:228:VAL:HG23	2.20	0.42
1:A:868:LEU:HA	1:A:869:PRO:HD3	1.89	0.42
1:B:860:ILE:HG23	1:B:957:ILE:CD1	2.50	0.42
1:C:724:PHE:CE2	1:C:726:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.86	0.42
1:D:1268:ILE:HA	1:D:1271:PHE:O	2.19	0.42
1:B:420:ARG:HG2	1:B:424:LEU:O	2.20	0.41
1:B:863:THR:HG23	1:B:925:VAL:HG11	2.01	0.41
1:C:1102:MET:HE1	1:C:1292:ARG:HA	2.02	0.41
1:C:1194:TYR:CE2	1:C:1206:MET:HE3	2.54	0.41
1:C:1730:GLU:HA	1:C:1730:GLU:OE2	2.20	0.41
1:D:265:TRP:CG	1:D:272:PRO:HG3	2.54	0.41
1:D:1184:SER:O	1:D:1185:ILE:HD13	2.19	0.41
1:D:1456:TYR:CZ	1:D:1460:ARG:HD3	2.55	0.41
1:A:1191:VAL:HG22	1:A:1192:PRO:HD2	2.01	0.41
1:B:1314:LEU:HD23	1:B:1314:LEU:HA	1.88	0.41
1:C:862:GLU:OE1	1:C:1016:ARG:NH1	2.53	0.41
1:C:1710:ASN:C	1:C:1712:ASN:N	2.78	0.41
1:D:1654:ASP:HB3	1:D:1691:PHE:O	2.20	0.41
1:A:622:LYS:HE3	1:A:622:LYS:HB2	1.67	0.41
1:D:194:LYS:HG2	1:D:211:CYS:SG	2.60	0.41
1:A:1539:TYR:CD1	1:A:1610:ARG:HG2	2.55	0.41
1:A:1549:TRP:HA	1:A:1556:PHE:HB2	2.02	0.41
1:A:1612:TYR:CD1	1:A:1632:GLY:HA2	2.55	0.41
1:B:243:PHE:CZ	1:B:435:PHE:HA	2.55	0.41
1:B:835:MET:HG2	1:B:933:TRP:HE3	1.85	0.41
1:C:533:PRO:HD3	1:C:606:PHE:CZ	2.55	0.41
1:C:1523:LEU:HB3	1:C:1643:THR:HG21	2.03	0.41
1:D:78:VAL:O	1:D:120:LYS:HA	2.21	0.41
1:A:180:VAL:HB	1:A:181:PRO:HD3	2.03	0.41
1:A:860:ILE:HG23	1:A:957:ILE:CD1	2.51	0.41
1:A:1268:ILE:HA	1:A:1271:PHE:O	2.19	0.41
1:B:183:ALA:HB2	1:B:377:THR:HG21	2.03	0.41
1:B:1433:TYR:CE1	1:B:1502:ILE:HD13	2.56	0.41
1:B:600:ILE:O	1:B:600:ILE:HG23	2.21	0.41
1:B:840:GLY:N	1:B:888:LYS:HG3	2.36	0.41
1:B:1356:ALA:O	1:B:1357:GLU:C	2.63	0.41
1:B:1523:LEU:HB3	1:B:1643:THR:CG2	2.50	0.41
1:C:15:PHE:HE2	1:C:24:SER:HA	1.85	0.41
1:C:270:GLU:HB3	1:C:420:ARG:HB3	2.03	0.41
1:C:677:THR:HG1	1:C:680:GLU:HB2	1.86	0.41
1:C:1057:ALA:C	1:C:1059:LYS:N	2.78	0.41
1:C:1500:CYS:HB3	1:C:1504:TYR:CZ	2.55	0.41
1:D:206:CYS:HA	1:D:312:GLU:CB	2.50	0.41
1:D:1525:MET:HE2	1:D:1573:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:O	1:A:18:LYS:HG3	2.21	0.41
1:A:1151:LEU:HB3	1:A:1156:ILE:HD13	2.02	0.41
1:A:1288:TYR:CD2	1:D:1540:ARG:NH1	2.88	0.41
1:A:1556:PHE:CZ	1:A:1604:THR:HG22	2.55	0.41
1:B:383:LYS:HB2	1:B:386:GLU:OE1	2.20	0.41
1:B:606:PHE:CZ	1:B:610:ILE:HD11	2.56	0.41
1:B:1556:PHE:CZ	1:B:1604:THR:HG22	2.56	0.41
1:B:1710:ASN:C	1:B:1712:ASN:H	2.28	0.41
1:C:1103:ASP:HA	1:C:1361:TRP:HA	2.02	0.41
1:C:1459:ASN:HD21	1:C:1460:ARG:NH1	2.03	0.41
1:C:1612:TYR:CD2	1:C:1612:TYR:C	2.98	0.41
1:D:840:GLY:N	1:D:888:LYS:HG3	2.36	0.41
1:D:1612:TYR:CD1	1:D:1632:GLY:HA2	2.56	0.41
1:A:16:HIS:ND1	1:A:24:SER:HB2	2.36	0.41
1:A:75:PRO:C	1:A:166:VAL:HG22	2.45	0.41
1:A:635:ILE:HD12	1:A:635:ILE:HA	1.88	0.41
1:B:1466:GLU:O	1:B:1469:GLN:N	2.52	0.41
1:D:1152:ASN:O	1:D:1153:ASP:HB2	2.20	0.41
1:D:1304:TRP:CG	1:D:1316:PRO:HB2	2.56	0.41
1:A:1274:GLU:O	1:A:1278:GLN:HG3	2.20	0.41
1:A:1314:LEU:HD23	1:A:1314:LEU:HA	1.88	0.41
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.89	0.41
1:B:868:LEU:HA	1:B:869:PRO:HD3	1.90	0.41
1:B:1468:HIS:O	1:B:1469:GLN:C	2.61	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.90	0.41
1:C:75:PRO:C	1:C:166:VAL:HG22	2.46	0.41
1:C:81:ASN:HB3	1:C:82:ILE:HG13	2.02	0.41
1:C:143:VAL:HG13	1:C:461:LYS:HB3	2.02	0.41
1:C:296:PRO:HG2	1:C:366:LEU:HD22	2.03	0.41
1:C:1184:SER:O	1:C:1185:ILE:HD13	2.20	0.41
1:C:1323:VAL:HG21	1:C:1477:SER:HB3	2.02	0.41
1:C:1539:TYR:CD1	1:C:1610:ARG:HG2	2.56	0.41
1:D:516:SER:O	1:D:518:ASN:N	2.52	0.41
1:D:701:ILE:HA	1:D:702:PRO:HD3	1.92	0.41
1:D:750:VAL:HG22	1:D:879:ALA:HB1	2.02	0.41
1:D:753:VAL:HA	1:D:754:PRO:HD3	1.95	0.41
1:D:968:LYS:HA	1:D:968:LYS:HD2	1.90	0.41
1:B:751:PRO:O	1:B:907:TYR:HA	2.21	0.41
1:B:1468:HIS:O	1:B:1469:GLN:HB2	2.20	0.41
1:B:1561:ASN:HD21	1:B:1601:TYR:HB3	1.86	0.41
1:C:81:ASN:O	1:C:203:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LYS:HD3	1:D:1509:GLN:HE22	1.85	0.41
1:C:860:ILE:HG23	1:C:957:ILE:CD1	2.50	0.41
1:C:1269:ASP:OD2	1:C:1269:ASP:N	2.47	0.41
1:D:851:SER:O	1:D:1058:THR:HA	2.21	0.41
1:D:1139:VAL:O	1:D:1140:ILE:HD12	2.20	0.41
1:A:1:MET:HB2	1:A:2:GLU:H	1.59	0.40
1:A:1469:GLN:CB	1:B:64:SER:H	2.34	0.40
1:C:90:THR:HG22	1:C:92:ALA:N	2.32	0.40
1:C:524:LEU:HB2	1:C:532:LYS:O	2.20	0.40
1:C:737:LEU:HB2	1:C:740:SER:OG	2.21	0.40
1:C:1468:HIS:O	1:C:1469:GLN:C	2.63	0.40
1:C:1524:PRO:O	1:C:1643:THR:HG23	2.22	0.40
1:D:1138:THR:OG1	1:D:1139:VAL:N	2.54	0.40
1:A:78:VAL:HG23	1:A:82:ILE:HB	2.02	0.40
1:A:1102:MET:CE	1:A:1292:ARG:HA	2.50	0.40
1:A:1194:TYR:CE2	1:A:1206:MET:HG2	2.56	0.40
1:B:724:PHE:CE2	1:B:726:GLY:HA3	2.56	0.40
1:B:1151:LEU:HB3	1:B:1156:ILE:HD13	2.04	0.40
1:B:1616:GLY:C	1:B:1642:ARG:HG3	2.46	0.40
1:C:894:THR:O	1:C:911:VAL:HG13	2.21	0.40
1:C:1151:LEU:HB3	1:C:1156:ILE:HD13	2.02	0.40
1:D:1523:LEU:HB3	1:D:1643:THR:HG21	2.03	0.40
1:A:1006:LEU:HD23	1:A:1006:LEU:HA	1.96	0.40
1:A:1085:TYR:CE2	1:A:1108:ARG:HD3	2.56	0.40
1:B:1191:VAL:HG22	1:B:1192:PRO:HD2	2.04	0.40
1:C:75:PRO:O	1:C:167:PRO:HD2	2.21	0.40
1:C:375:VAL:HG13	1:C:376:PRO:O	2.21	0.40
1:D:1085:TYR:CE2	1:D:1108:ARG:HD3	2.56	0.40
1:D:1302:PRO:HG3	1:D:1331:PHE:CE2	2.56	0.40
1:D:1391:LYS:HA	1:D:1391:LYS:HD2	1.93	0.40
1:D:1459:ASN:HD21	1:D:1460:ARG:NH1	2.04	0.40
1:A:925:VAL:HG23	1:A:926:THR:HG23	2.04	0.40
1:B:1730:GLU:OE2	1:B:1730:GLU:HA	2.20	0.40
1:C:170:LEU:HD11	1:C:229:MET:HE1	2.03	0.40
1:C:622:LYS:HB2	1:C:622:LYS:HE3	1.71	0.40
1:D:1057:ALA:C	1:D:1059:LYS:N	2.79	0.40
1:B:157:SER:HB3	1:B:169:SER:OG	2.21	0.40
1:B:519:TYR:CB	1:B:546:ILE:HD13	2.52	0.40
1:B:1057:ALA:C	1:B:1059:LYS:N	2.79	0.40
1:B:1151:LEU:HD11	1:B:1168:ASP:HB3	2.04	0.40
1:C:1059:LYS:HA	1:C:1059:LYS:HD2	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:ILE:HG23	1:D:957:ILE:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:TYR:OH	1:C:1541:GLU:OE2[2_455]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1654/1829 (90%)	1540 (93%)	101 (6%)	13 (1%)	16	54
1	B	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	18	56
1	C	1654/1829 (90%)	1539 (93%)	102 (6%)	13 (1%)	16	54
1	D	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	18	56
All	All	6612/7316 (90%)	6167 (93%)	397 (6%)	48 (1%)	18	56

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	1166	ARG
1	A	1711	GLU
1	B	1166	ARG
1	C	38	ALA
1	C	1166	ARG
1	C	1711	GLU
1	D	1166	ARG
1	D	1711	GLU

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Mol	Chain	Res	Type
1	A	206	CYS
1	A	479	ASP
1	A	1438	ASP
1	B	206	CYS
1	B	479	ASP
1	B	540	ASP
1	B	1438	ASP
1	C	206	CYS
1	C	479	ASP
1	C	1438	ASP
1	D	206	CYS
1	D	479	ASP
1	D	540	ASP
1	D	1438	ASP
1	A	891	CYS
1	B	104	SER
1	B	891	CYS
1	C	891	CYS
1	D	104	SER
1	D	891	CYS
1	A	104	SER
1	A	517	ASN
1	A	612	HIS
1	C	104	SER
1	C	517	ASN
1	C	612	HIS
1	A	1003	ASP
1	A	1058	THR
1	B	65	ASN
1	B	1003	ASP
1	C	1003	ASP
1	C	1058	THR
1	D	1003	ASP
1	D	1058	THR
1	B	1058	THR
1	A	37	PRO
1	C	37	PRO
1	B	37	PRO
1	D	37	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	1413/1547 (91%)	1263 (89%)	150 (11%)	6	21
1	B	1411/1547 (91%)	1248 (88%)	163 (12%)	5	18
1	C	1413/1547 (91%)	1262 (89%)	151 (11%)	6	21
1	D	1411/1547 (91%)	1250 (89%)	161 (11%)	5	18
All	All	5648/6188 (91%)	5023 (89%)	625 (11%)	6	20

All (625) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	4	THR
1	A	18	LYS
1	A	60	LEU
1	A	62	SER
1	A	66	LYS
1	A	67	GLU
1	A	78	VAL
1	A	90	THR
1	A	95	SER
1	A	106	VAL
1	A	116	VAL
1	A	121	THR
1	A	143	VAL
1	A	149	VAL
1	A	160	VAL
1	A	165	ILE
1	A	166	VAL
1	A	170	LEU
1	A	188	ILE
1	A	191	LYS
1	A	194	LYS
1	A	202	VAL

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Mol	Chain	Res	Type
1	A	203	VAL
1	A	219	LEU
1	A	231	LYS
1	A	238	GLU
1	A	241	ARG
1	A	262	GLU
1	A	269	THR
1	A	283	LYS
1	A	292	VAL
1	A	305	TYR
1	A	310	VAL
1	A	323	THR
1	A	356	ARG
1	A	368	LYS
1	A	375	VAL
1	A	385	GLU
1	A	387	VAL
1	A	393	LEU
1	A	415	VAL
1	A	420	ARG
1	A	429	THR
1	A	434	LYS
1	A	445	LYS
1	A	463	VAL
1	A	469	VAL
1	A	494	LYS
1	A	538	VAL
1	A	540	ASP
1	A	547	GLN
1	A	582	VAL
1	A	593	THR
1	A	600	ILE
1	A	634	GLU
1	A	641	LYS
1	A	659	LYS
1	A	662	GLN
1	A	676	ARG
1	A	680	GLU
1	A	689	ILE
1	A	698	GLN
1	A	716	ARG
1	A	719	GLN

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Mol	Chain	Res	Type
1	A	730	ASP
1	A	734	LYS
1	A	735	LEU
1	A	737	LEU
1	A	738	LYS
1	A	739	HIS
1	A	743	GLU
1	A	744	ILE
1	A	752	LEU
1	A	826	ASN
1	A	834	MET
1	A	841	LYS
1	A	845	ILE
1	A	859	VAL
1	A	860	ILE
1	A	872	THR
1	A	875	LYS
1	A	888	LYS
1	A	944	ASP
1	A	951	GLU
1	A	952	VAL
1	A	957	ILE
1	A	978	THR
1	A	979	SER
1	A	988	VAL
1	A	993	LYS
1	A	999	SER
1	A	1011	VAL
1	A	1016	ARG
1	A	1042	LEU
1	A	1044	SER
1	A	1055	LYS
1	A	1074	LEU
1	A	1079	ASN
1	A	1103	ASP
1	A	1125	ILE
1	A	1131	LYS
1	A	1140	ILE
1	A	1147	VAL
1	A	1150	THR
1	A	1156	ILE
1	A	1165	LYS

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Mol	Chain	Res	Type
1	A	1172	VAL
1	A	1191	VAL
1	A	1216	LEU
1	A	1224	GLN
1	A	1227	LEU
1	A	1252	THR
1	A	1311	GLU
1	A	1326	LEU
1	A	1337	VAL
1	A	1345	SER
1	A	1346	LEU
1	A	1375	VAL
1	A	1377	LEU
1	A	1388	SER
1	A	1393	ILE
1	A	1396	PHE
1	A	1402	LEU
1	A	1408	LYS
1	A	1426	ASP
1	A	1428	SER
1	A	1430	LYS
1	A	1459	ASN
1	A	1460	ARG
1	A	1473	ILE
1	A	1478	GLN
1	A	1509	GLN
1	A	1516	VAL
1	A	1557	ILE
1	A	1562	ASP
1	A	1571	MET
1	A	1585	VAL
1	A	1625	MET
1	A	1640	VAL
1	A	1643	THR
1	A	1662	LEU
1	A	1675	THR
1	A	1693	ILE
1	A	1695	VAL
1	A	1697	GLU
1	A	1721	GLU
1	A	1726	GLU
1	A	1736	GLN

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Mol	Chain	Res	Type
1	B	4	THR
1	B	23	LYS
1	B	25	LEU
1	B	27	LEU
1	B	31	LEU
1	B	51	GLU
1	B	66	LYS
1	B	78	VAL
1	B	81	ASN
1	B	90	THR
1	B	95	SER
1	B	106	VAL
1	B	116	VAL
1	B	118	ILE
1	B	121	THR
1	B	143	VAL
1	B	149	VAL
1	B	160	VAL
1	B	166	VAL
1	B	170	LEU
1	B	184	LEU
1	B	191	LYS
1	B	194	LYS
1	B	202	VAL
1	B	203	VAL
1	B	217	LEU
1	B	219	LEU
1	B	220	SER
1	B	238	GLU
1	B	241	ARG
1	B	277	LYS
1	B	292	VAL
1	B	302	ARG
1	B	305	TYR
1	B	313	ARG
1	B	317	THR
1	B	345	ASP
1	B	368	LYS
1	B	369	ASP
1	B	370	ILE
1	B	375	VAL
1	B	386	GLU

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Mol	Chain	Res	Type
1	B	393	LEU
1	B	415	VAL
1	B	420	ARG
1	B	428	ILE
1	B	429	THR
1	B	433	LYS
1	B	445	LYS
1	B	463	VAL
1	B	468	THR
1	B	469	VAL
1	B	478	LYS
1	B	517	ASN
1	B	518	ASN
1	B	526	LYS
1	B	536	ARG
1	B	537	ARG
1	B	538	VAL
1	B	542	THR
1	B	547	GLN
1	B	582	VAL
1	B	584	SER
1	B	589	GLU
1	B	593	THR
1	B	600	ILE
1	B	607	LYS
1	B	634	GLU
1	B	641	LYS
1	B	659	LYS
1	B	662	GLN
1	B	676	ARG
1	B	680	GLU
1	B	689	ILE
1	B	698	GLN
1	B	716	ARG
1	B	719	GLN
1	B	730	ASP
1	B	734	LYS
1	B	735	LEU
1	B	737	LEU
1	B	738	LYS
1	B	739	HIS
1	B	743	GLU

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Mol	Chain	Res	Type
1	B	744	ILE
1	B	752	LEU
1	B	826	ASN
1	B	834	MET
1	B	841	LYS
1	B	845	ILE
1	B	859	VAL
1	B	860	ILE
1	B	872	THR
1	B	875	LYS
1	B	888	LYS
1	B	944	ASP
1	B	951	GLU
1	B	952	VAL
1	B	957	ILE
1	B	978	THR
1	B	979	SER
1	B	988	VAL
1	B	993	LYS
1	B	999	SER
1	B	1011	VAL
1	B	1016	ARG
1	B	1042	LEU
1	B	1044	SER
1	B	1055	LYS
1	B	1074	LEU
1	B	1079	ASN
1	B	1103	ASP
1	B	1125	ILE
1	B	1131	LYS
1	B	1140	ILE
1	B	1147	VAL
1	B	1150	THR
1	B	1156	ILE
1	B	1165	LYS
1	B	1172	VAL
1	B	1191	VAL
1	B	1216	LEU
1	B	1224	GLN
1	B	1227	LEU
1	B	1252	THR
1	B	1301	LYS

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Mol	Chain	Res	Type
1	B	1303	LYS
1	B	1311	GLU
1	B	1326	LEU
1	B	1337	VAL
1	B	1345	SER
1	B	1346	LEU
1	B	1375	VAL
1	B	1377	LEU
1	B	1388	SER
1	B	1393	ILE
1	B	1396	PHE
1	B	1402	LEU
1	B	1408	LYS
1	B	1426	ASP
1	B	1428	SER
1	B	1430	LYS
1	B	1459	ASN
1	B	1460	ARG
1	B	1473	ILE
1	B	1478	GLN
1	B	1509	GLN
1	B	1516	VAL
1	B	1557	ILE
1	B	1562	ASP
1	B	1571	MET
1	B	1585	VAL
1	B	1625	MET
1	B	1640	VAL
1	B	1643	THR
1	B	1662	LEU
1	B	1675	THR
1	B	1693	ILE
1	B	1695	VAL
1	B	1697	GLU
1	B	1721	GLU
1	B	1726	GLU
1	B	1736	GLN
1	C	1	MET
1	C	2	GLU
1	C	4	THR
1	C	18	LYS
1	C	60	LEU

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Mol	Chain	Res	Type
1	C	62	SER
1	C	66	LYS
1	C	67	GLU
1	C	78	VAL
1	C	90	THR
1	C	95	SER
1	C	106	VAL
1	C	116	VAL
1	C	121	THR
1	C	143	VAL
1	C	149	VAL
1	C	160	VAL
1	C	165	ILE
1	C	166	VAL
1	C	170	LEU
1	C	188	ILE
1	C	191	LYS
1	C	194	LYS
1	C	202	VAL
1	C	203	VAL
1	C	219	LEU
1	C	231	LYS
1	C	238	GLU
1	C	241	ARG
1	C	262	GLU
1	C	269	THR
1	C	283	LYS
1	C	292	VAL
1	C	305	TYR
1	C	310	VAL
1	C	323	THR
1	C	356	ARG
1	C	368	LYS
1	C	370	ILE
1	C	375	VAL
1	C	385	GLU
1	C	387	VAL
1	C	393	LEU
1	C	415	VAL
1	C	420	ARG
1	C	429	THR
1	C	434	LYS

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Mol	Chain	Res	Type
1	C	445	LYS
1	C	463	VAL
1	C	469	VAL
1	C	494	LYS
1	C	538	VAL
1	C	540	ASP
1	C	546	ILE
1	C	547	GLN
1	C	582	VAL
1	C	593	THR
1	C	600	ILE
1	C	634	GLU
1	C	641	LYS
1	C	659	LYS
1	C	662	GLN
1	C	676	ARG
1	C	680	GLU
1	C	689	ILE
1	C	698	GLN
1	C	716	ARG
1	C	719	GLN
1	C	730	ASP
1	C	734	LYS
1	C	735	LEU
1	C	737	LEU
1	C	738	LYS
1	C	739	HIS
1	C	743	GLU
1	C	744	ILE
1	C	752	LEU
1	C	826	ASN
1	C	834	MET
1	C	841	LYS
1	C	845	ILE
1	C	859	VAL
1	C	860	ILE
1	C	872	THR
1	C	875	LYS
1	C	888	LYS
1	C	944	ASP
1	C	951	GLU
1	C	952	VAL

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Mol	Chain	Res	Type
1	C	957	ILE
1	C	978	THR
1	C	979	SER
1	C	988	VAL
1	C	993	LYS
1	C	999	SER
1	C	1011	VAL
1	C	1016	ARG
1	C	1042	LEU
1	C	1044	SER
1	C	1055	LYS
1	C	1074	LEU
1	C	1079	ASN
1	C	1103	ASP
1	C	1125	ILE
1	C	1131	LYS
1	C	1140	ILE
1	C	1147	VAL
1	C	1150	THR
1	C	1156	ILE
1	C	1165	LYS
1	C	1172	VAL
1	C	1191	VAL
1	C	1216	LEU
1	C	1224	GLN
1	C	1227	LEU
1	C	1252	THR
1	C	1311	GLU
1	C	1326	LEU
1	C	1345	SER
1	C	1346	LEU
1	C	1375	VAL
1	C	1377	LEU
1	C	1388	SER
1	C	1393	ILE
1	C	1396	PHE
1	C	1402	LEU
1	C	1408	LYS
1	C	1426	ASP
1	C	1428	SER
1	C	1430	LYS
1	C	1459	ASN

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Mol	Chain	Res	Type
1	C	1460	ARG
1	C	1473	ILE
1	C	1478	GLN
1	C	1509	GLN
1	C	1516	VAL
1	C	1557	ILE
1	C	1562	ASP
1	C	1571	MET
1	C	1585	VAL
1	C	1625	MET
1	C	1640	VAL
1	C	1643	THR
1	C	1662	LEU
1	C	1675	THR
1	C	1693	ILE
1	C	1695	VAL
1	C	1697	GLU
1	C	1721	GLU
1	C	1726	GLU
1	C	1736	GLN
1	D	4	THR
1	D	23	LYS
1	D	25	LEU
1	D	27	LEU
1	D	31	LEU
1	D	51	GLU
1	D	66	LYS
1	D	78	VAL
1	D	81	ASN
1	D	90	THR
1	D	95	SER
1	D	106	VAL
1	D	116	VAL
1	D	118	ILE
1	D	121	THR
1	D	143	VAL
1	D	149	VAL
1	D	160	VAL
1	D	166	VAL
1	D	170	LEU
1	D	184	LEU
1	D	191	LYS

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Mol	Chain	Res	Type
1	D	194	LYS
1	D	202	VAL
1	D	203	VAL
1	D	217	LEU
1	D	219	LEU
1	D	220	SER
1	D	238	GLU
1	D	241	ARG
1	D	277	LYS
1	D	292	VAL
1	D	302	ARG
1	D	305	TYR
1	D	313	ARG
1	D	317	THR
1	D	345	ASP
1	D	368	LYS
1	D	369	ASP
1	D	370	ILE
1	D	375	VAL
1	D	386	GLU
1	D	393	LEU
1	D	415	VAL
1	D	420	ARG
1	D	428	ILE
1	D	429	THR
1	D	433	LYS
1	D	445	LYS
1	D	458	THR
1	D	463	VAL
1	D	468	THR
1	D	469	VAL
1	D	478	LYS
1	D	517	ASN
1	D	518	ASN
1	D	526	LYS
1	D	536	ARG
1	D	537	ARG
1	D	538	VAL
1	D	542	THR
1	D	547	GLN
1	D	582	VAL
1	D	584	SER

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Mol	Chain	Res	Type
1	D	589	GLU
1	D	593	THR
1	D	600	ILE
1	D	607	LYS
1	D	634	GLU
1	D	641	LYS
1	D	659	LYS
1	D	662	GLN
1	D	676	ARG
1	D	680	GLU
1	D	689	ILE
1	D	698	GLN
1	D	716	ARG
1	D	719	GLN
1	D	730	ASP
1	D	734	LYS
1	D	735	LEU
1	D	737	LEU
1	D	738	LYS
1	D	739	HIS
1	D	743	GLU
1	D	744	ILE
1	D	752	LEU
1	D	826	ASN
1	D	834	MET
1	D	841	LYS
1	D	845	ILE
1	D	859	VAL
1	D	860	ILE
1	D	872	THR
1	D	875	LYS
1	D	888	LYS
1	D	944	ASP
1	D	951	GLU
1	D	952	VAL
1	D	957	ILE
1	D	978	THR
1	D	979	SER
1	D	988	VAL
1	D	993	LYS
1	D	999	SER
1	D	1011	VAL

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Mol	Chain	Res	Type
1	D	1016	ARG
1	D	1042	LEU
1	D	1044	SER
1	D	1055	LYS
1	D	1074	LEU
1	D	1079	ASN
1	D	1103	ASP
1	D	1125	ILE
1	D	1131	LYS
1	D	1140	ILE
1	D	1147	VAL
1	D	1150	THR
1	D	1156	ILE
1	D	1165	LYS
1	D	1172	VAL
1	D	1191	VAL
1	D	1216	LEU
1	D	1224	GLN
1	D	1227	LEU
1	D	1252	THR
1	D	1311	GLU
1	D	1326	LEU
1	D	1345	SER
1	D	1346	LEU
1	D	1375	VAL
1	D	1377	LEU
1	D	1388	SER
1	D	1393	ILE
1	D	1396	PHE
1	D	1402	LEU
1	D	1408	LYS
1	D	1426	ASP
1	D	1428	SER
1	D	1430	LYS
1	D	1459	ASN
1	D	1460	ARG
1	D	1473	ILE
1	D	1478	GLN
1	D	1509	GLN
1	D	1516	VAL
1	D	1557	ILE
1	D	1562	ASP

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Mol	Chain	Res	Type
1	D	1571	MET
1	D	1585	VAL
1	D	1625	MET
1	D	1640	VAL
1	D	1643	THR
1	D	1662	LEU
1	D	1675	THR
1	D	1693	ILE
1	D	1695	VAL
1	D	1697	GLU
1	D	1721	GLU
1	D	1726	GLU
1	D	1736	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	58	ASN
1	A	99	GLN
1	A	186	ASN
1	A	230	ASN
1	A	284	ASN
1	A	829	HIS
1	A	1459	ASN
1	A	1688	ASN
1	B	10	GLN
1	B	55	HIS
1	B	230	ASN
1	B	517	ASN
1	B	594	GLN
1	B	829	HIS
1	B	1315	HIS
1	B	1318	ASN
1	B	1459	ASN
1	B	1509	GLN
1	B	1688	ASN
1	C	10	GLN
1	C	55	HIS
1	C	58	ASN
1	C	99	GLN
1	C	284	ASN

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Mol	Chain	Res	Type
1	C	829	HIS
1	C	1459	ASN
1	C	1468	HIS
1	C	1509	GLN
1	C	1659	HIS
1	C	1688	ASN
1	D	10	GLN
1	D	230	ASN
1	D	517	ASN
1	D	539	ASN
1	D	594	GLN
1	D	829	HIS
1	D	1315	HIS
1	D	1318	ASN
1	D	1459	ASN
1	D	1468	HIS
1	D	1509	GLN
1	D	1688	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1660/1829 (90%)	0.14	68 (4%) 41 41	236, 291, 352, 387	0
1	B	1658/1829 (90%)	-0.00	44 (2%) 56 48	245, 295, 361, 403	0
1	C	1660/1829 (90%)	-0.02	34 (2%) 65 56	269, 323, 368, 413	0
1	D	1658/1829 (90%)	0.08	43 (2%) 57 49	254, 306, 345, 377	0
All	All	6636/7316 (90%)	0.05	189 (2%) 55 48	236, 307, 356, 413	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1568	VAL	10.5
1	D	1568	VAL	7.6
1	A	1557	ILE	6.9
1	B	1548	PRO	6.8
1	A	1587	LEU	5.8
1	D	1735	ILE	5.5
1	A	303	CYS	5.5
1	C	1568	VAL	5.5
1	A	1279	PHE	5.2
1	A	1669	VAL	5.1
1	A	1572	LEU	5.0
1	C	126	PHE	4.9
1	D	1127	LEU	4.9
1	C	934	MET	4.9
1	A	1270	LEU	4.8
1	B	118	ILE	4.7
1	D	931	VAL	4.7
1	B	535	LEU	4.7
1	C	1735	ILE	4.6
1	D	1258	ILE	4.5
1	D	1556	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	1557	ILE	4.4
1	D	126	PHE	4.4
1	B	1735	ILE	4.4
1	D	374	CYS	4.3
1	C	535	LEU	4.3
1	B	357	GLN	4.3
1	D	1452	LEU	4.2
1	B	1279	PHE	4.2
1	C	125	GLN	4.2
1	B	1634	PRO	4.2
1	A	1634	PRO	4.2
1	B	1339	ILE	4.1
1	C	1634	PRO	4.1
1	D	28	LEU	4.1
1	B	1374	PHE	4.1
1	B	1620	ILE	4.0
1	A	1556	PHE	4.0
1	D	1557	ILE	4.0
1	D	1560	VAL	4.0
1	A	845	ILE	3.9
1	B	1270	LEU	3.9
1	B	1143	SER	3.8
1	D	1572	LEU	3.7
1	A	571	ILE	3.6
1	D	1270	LEU	3.5
1	B	321	LEU	3.4
1	D	1326	LEU	3.4
1	A	1271	PHE	3.4
1	D	1607	ASN	3.4
1	D	1279	PHE	3.3
1	C	175	ALA	3.3
1	A	1548	PRO	3.3
1	B	1009	ILE	3.3
1	D	1455	CYS	3.2
1	A	1630	ALA	3.2
1	C	387	VAL	3.2
1	D	1620	ILE	3.2
1	C	1557	ILE	3.2
1	A	1532	THR	3.1
1	C	127	ALA	3.1
1	C	725	VAL	3.1
1	B	1568	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	282	LEU	3.1
1	A	430	LEU	3.0
1	B	1258	ILE	3.0
1	A	297	LEU	3.0
1	A	386	GLU	3.0
1	A	1521	PHE	2.9
1	B	1547	ALA	2.9
1	A	1142	VAL	2.9
1	B	418	GLY	2.9
1	A	1269	ASP	2.9
1	B	1326	LEU	2.9
1	A	860	ILE	2.8
1	D	321	LEU	2.8
1	A	1588	GLY	2.8
1	A	1181	ALA	2.8
1	D	495	GLY	2.8
1	B	1413	TYR	2.8
1	C	403	ASN	2.8
1	D	170	LEU	2.8
1	B	417	SER	2.8
1	D	935	LEU	2.8
1	C	1045	ILE	2.6
1	A	1265	HIS	2.6
1	B	1452	LEU	2.6
1	B	562	ILE	2.6
1	B	1382	ALA	2.6
1	A	1096	VAL	2.6
1	C	1560	VAL	2.6
1	C	304	LEU	2.6
1	A	1487	PHE	2.6
1	C	846	GLY	2.6
1	D	125	GLN	2.6
1	A	296	PRO	2.6
1	A	133	THR	2.5
1	A	1494	GLN	2.5
1	A	1452	LEU	2.5
1	C	170	LEU	2.5
1	A	427	GLY	2.5
1	C	174	THR	2.5
1	A	1736	GLN	2.5
1	A	639	ILE	2.5
1	B	174	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1332	THR	2.4
1	C	1070	ALA	2.4
1	A	300	LEU	2.4
1	D	915	LEU	2.4
1	B	1549	TRP	2.4
1	D	574	VAL	2.4
1	A	1376	PRO	2.4
1	C	614	GLN	2.4
1	D	1146	THR	2.4
1	A	1071	PHE	2.4
1	C	1071	PHE	2.4
1	A	415	VAL	2.4
1	C	1736	GLN	2.4
1	D	93	CYS	2.4
1	B	1142	VAL	2.4
1	D	1096	VAL	2.4
1	C	297	LEU	2.4
1	C	1265	HIS	2.4
1	D	1346	LEU	2.4
1	D	1634	PRO	2.3
1	B	630	ALA	2.3
1	A	992	VAL	2.3
1	B	967	VAL	2.3
1	B	653	VAL	2.3
1	C	558	PHE	2.3
1	C	1551	PRO	2.3
1	D	1732	ALA	2.3
1	D	375	VAL	2.3
1	A	1523	LEU	2.3
1	B	1344	PRO	2.3
1	A	118	ILE	2.3
1	B	1276	ILE	2.3
1	A	1450	PHE	2.3
1	D	1548	PRO	2.3
1	B	209	LEU	2.3
1	B	845	ILE	2.3
1	B	1144	GLY	2.3
1	D	1078	ALA	2.3
1	A	126	PHE	2.3
1	A	1051	PHE	2.3
1	D	1271	PHE	2.3
1	D	1551	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	300	LEU	2.3
1	A	1330	ASN	2.2
1	A	1535	CYS	2.2
1	A	377	THR	2.2
1	A	938	ALA	2.2
1	A	1133	LEU	2.2
1	A	1437	GLY	2.2
1	A	1352	GLN	2.2
1	A	1441	ILE	2.2
1	D	639	ILE	2.2
1	A	212	VAL	2.2
1	A	1732	ALA	2.2
1	B	1372	ILE	2.2
1	A	735	LEU	2.2
1	B	1523	LEU	2.2
1	B	1280	PHE	2.2
1	A	374	CYS	2.2
1	A	852	LEU	2.1
1	C	1620	ILE	2.1
1	C	1332	THR	2.1
1	A	183	ALA	2.1
1	C	374	CYS	2.1
1	A	1293	PHE	2.1
1	C	1483	VAL	2.1
1	A	1485	ILE	2.1
1	D	1437	GLY	2.1
1	A	401	TRP	2.1
1	B	1622	GLY	2.1
1	D	1559	ASP	2.1
1	C	1545	SER	2.1
1	A	189	GLY	2.1
1	A	1266	GLY	2.1
1	A	1374	PHE	2.1
1	A	610	ILE	2.0
1	C	713	PHE	2.0
1	C	1258	ILE	2.0
1	B	177	SER	2.0
1	D	53	LEU	2.0
1	B	126	PHE	2.0
1	D	379	PRO	2.0
1	A	174	THR	2.0
1	A	931	VAL	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.