



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 1K9A / pdb_00001k9a
Title : Crystal structure analysis of full-length carboxyl-terminal Src kinase at 2.5 Å resolution
Authors : Ogawa, A.; Takayama, Y.; Nagata, A.; Chong, K.T.; Takeuchi, S.; Sakai, H.; Nakagawa, A.; Nada, S.; Okada, M.; Tsukihara, T.
Deposited on : 2001-10-28
Resolution : 2.50 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

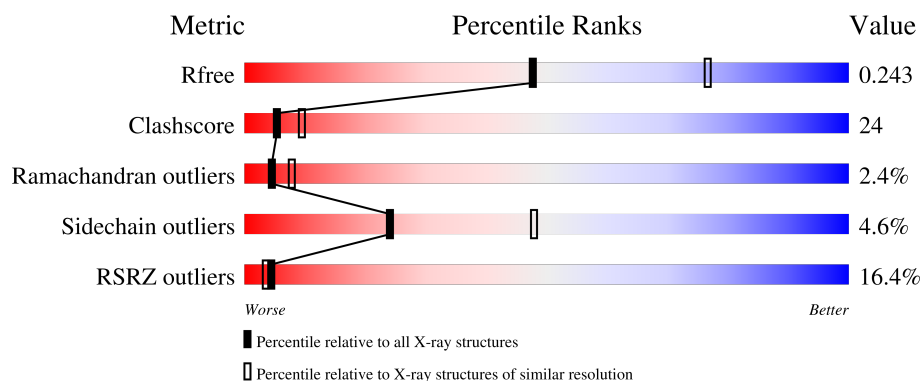
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	450	7% 63% 29% 5%
1	B	450	8% 63% 30% 5%
1	C	450	12% 60% 34%
1	D	450	13% 56% 35% 6%
1	E	450	15% 52% 39% 7%

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Mol	Chain	Length	Quality of chain
1	F	450	41% 45% 46% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21313 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 Carboxyl-terminal Src kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3491	2231	595	644	21			
1	B	441	Total	C	N	O	S	0	0	0
			3506	2241	598	646	21			
1	C	438	Total	C	N	O	S	0	0	0
			3482	2225	593	643	21			
1	D	433	Total	C	N	O	S	0	0	0
			3443	2201	587	634	21			
1	E	440	Total	C	N	O	S	0	0	0
			3495	2232	595	647	21			
1	F	436	Total	C	N	O	S	0	0	0
			3468	2216	591	640	21			

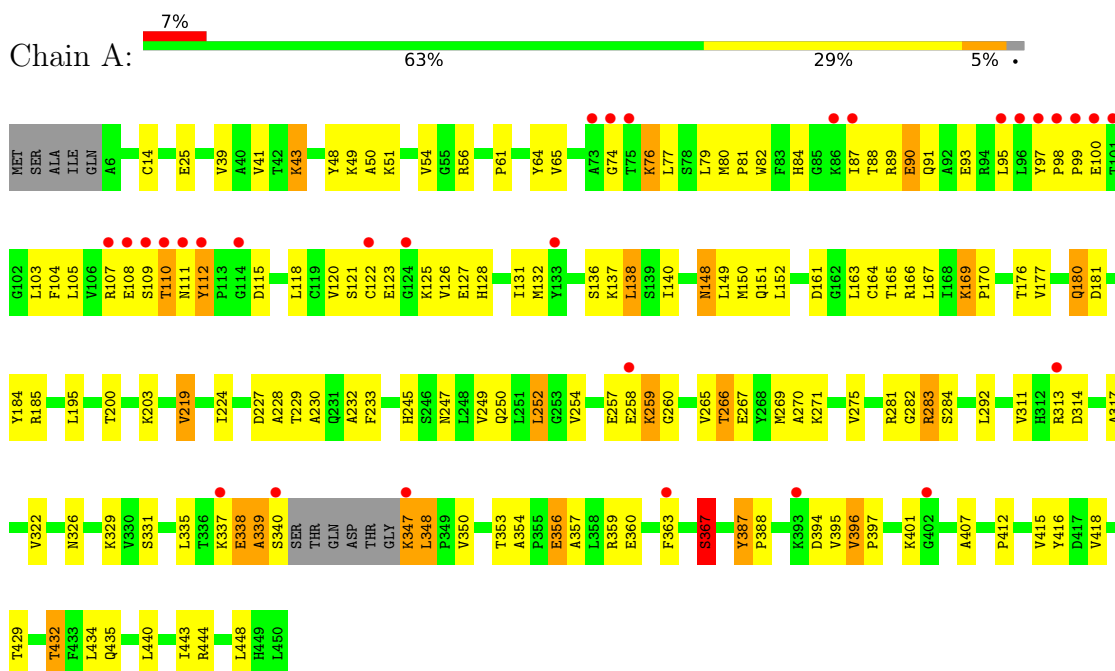
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	89	Total	O	0	0
			89	89		
2	C	79	Total	O	0	0
			79	79		
2	D	85	Total	O	0	0
			85	85		
2	E	40	Total	O	0	0
			40	40		
2	F	29	Total	O	0	0
			29	29		

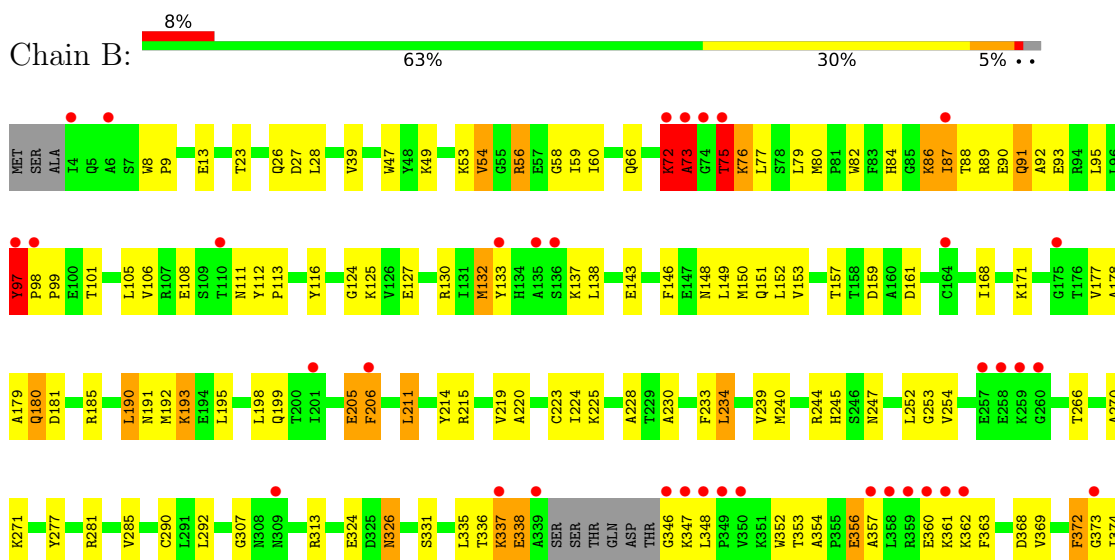
3 Residue-property plots

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: Carboxyl-terminal Src kinase

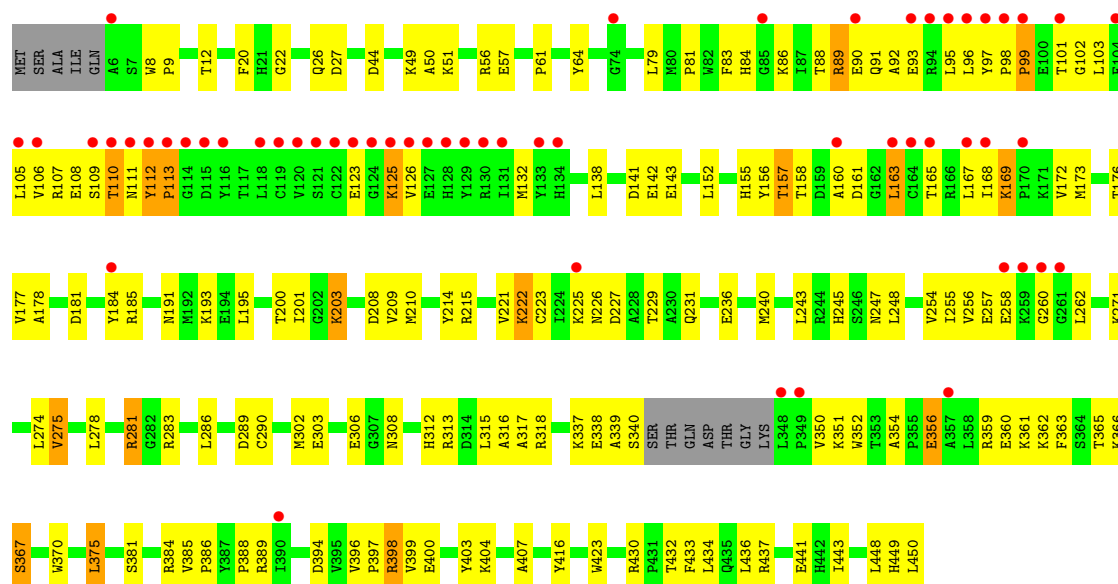


• Molecule 1: Carboxyl-terminal Src kinase

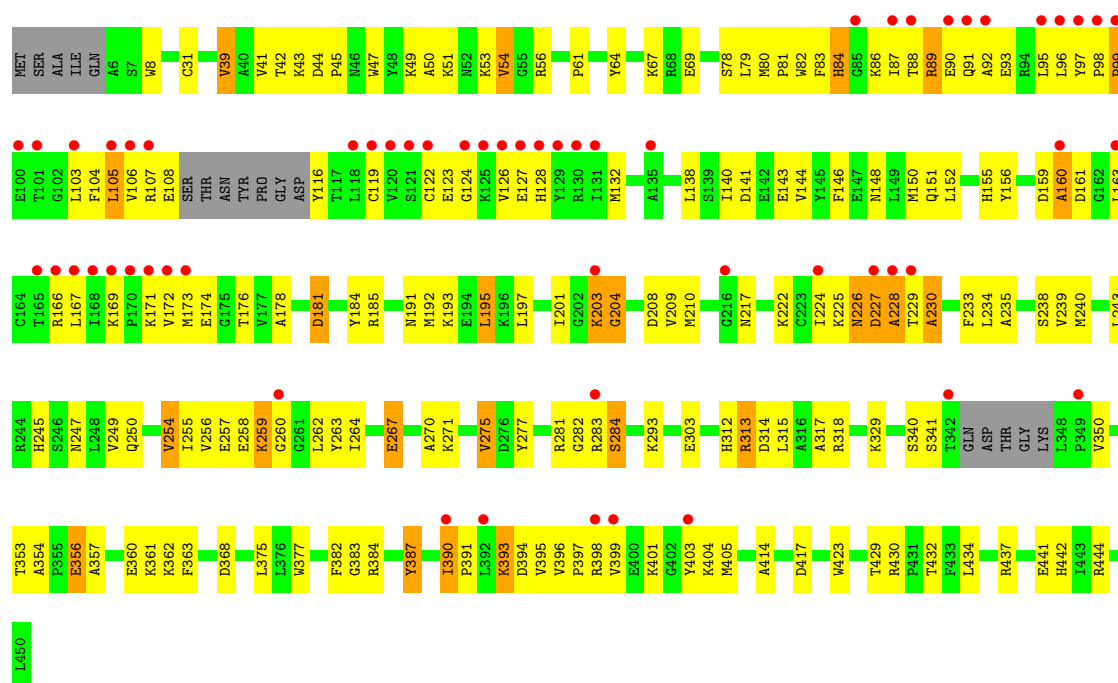




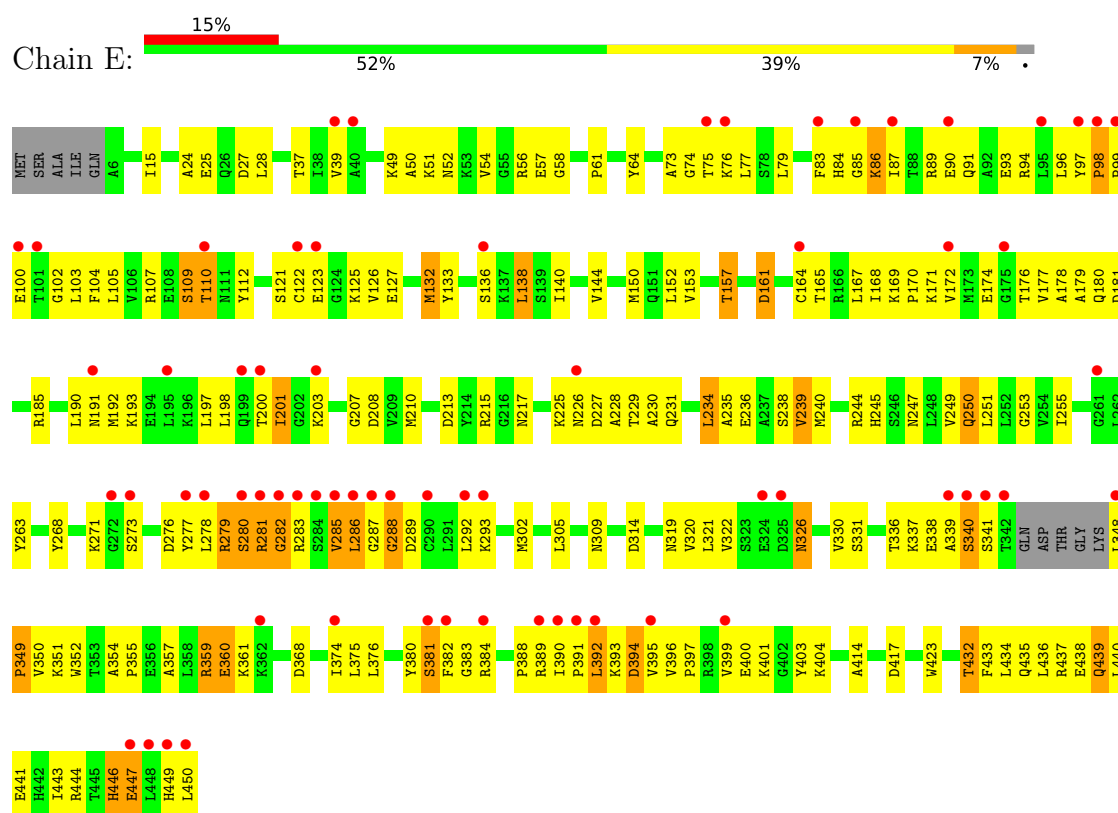
• Molecule 1: Carboxyl-terminal Src kinase



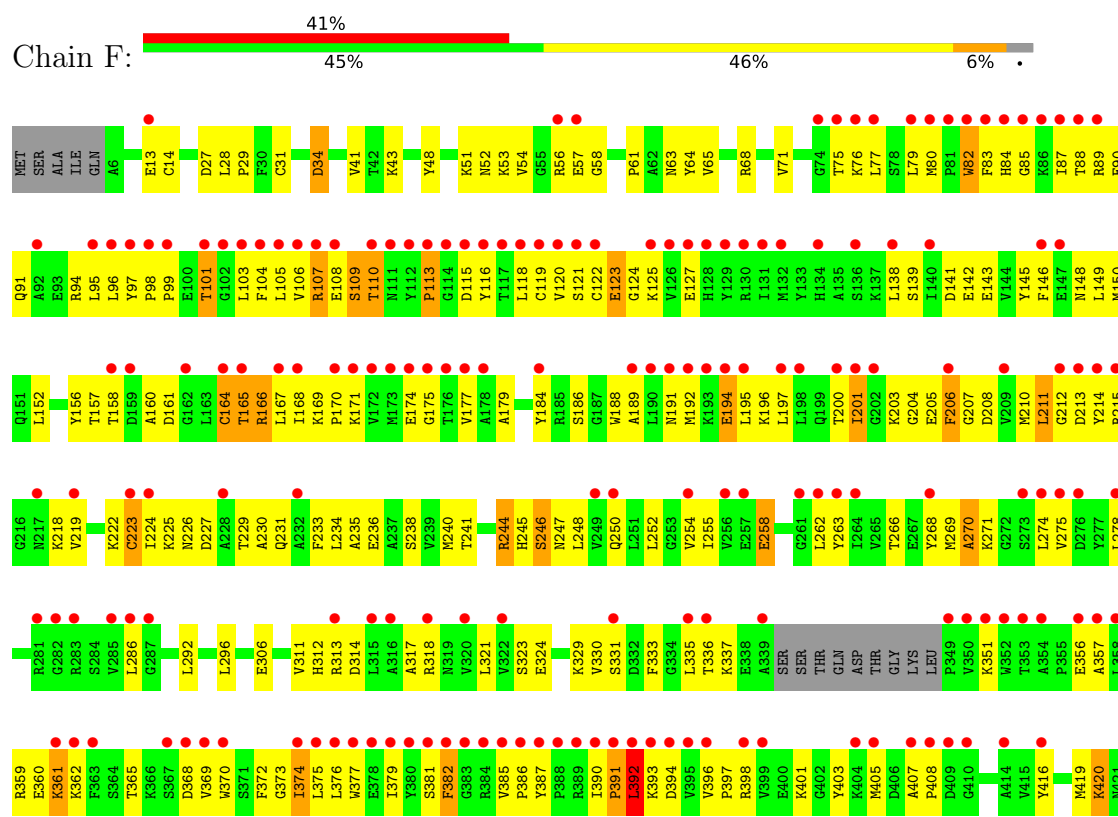
• Molecule 1: Carboxyl-terminal Src kinase



• Molecule 1: Carboxyl-terminal Src kinase



• Molecule 1: Carboxyl-terminal Src kinase



C422	W423	H424	L425	D426	A427	A428	T429	R430	F431	T432	F433	L436	R437	E438	Q439	L440	E441	H442	I443	R444	E447	L448	H449	L450
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.00Å 162.60Å 232.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.50 – 2.50 73.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (73.50-2.50) 98.2 (73.50-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.288 0.246 , 0.243	Depositor DCC
R_{free} test set	3007 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21313	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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	0.48	0/3570	0.97	21/4828 (0.4%)
1	B	0.47	0/3585	1.04	18/4848 (0.4%)
1	C	0.43	0/3561	0.92	12/4817 (0.2%)
1	D	0.45	0/3519	0.95	15/4757 (0.3%)
1	E	0.43	0/3574	0.95	15/4835 (0.3%)
1	F	0.39	0/3547	0.91	11/4797 (0.2%)
All	All	0.44	0/21356	0.96	92/28882 (0.3%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	LYS	N-CA-C	15.26	127.62	111.14
1	B	374	ILE	N-CA-C	-10.82	100.36	110.53
1	C	110	THR	N-CA-C	-10.25	102.11	112.97
1	A	326	ASN	N-CA-C	9.29	124.13	112.24
1	B	76	LYS	N-CA-C	-8.62	102.77	113.20
1	E	449	HIS	N-CA-C	-8.54	102.99	113.50
1	C	351	LYS	N-CA-C	8.22	122.27	111.75
1	D	270	ALA	N-CA-C	8.15	121.08	111.71
1	E	381	SER	N-CA-C	-8.06	93.63	110.80
1	B	372	PHE	N-CA-C	-7.82	98.71	110.28
1	F	157	THR	N-CA-C	-7.77	104.28	114.31
1	E	285	VAL	N-CA-C	-7.49	104.01	113.22
1	D	350	VAL	N-CA-C	7.46	118.39	112.12
1	B	331	SER	N-CA-C	7.41	126.59	110.80
1	E	109	SER	N-CA-C	7.36	120.65	110.35
1	C	271	LYS	N-CA-C	7.27	122.18	113.16
1	A	387	TYR	CA-C-N	7.20	126.73	119.24
1	A	387	TYR	C-N-CA	7.20	126.73	119.24
1	F	270	ALA	N-CA-C	7.20	121.69	112.34
1	E	157	THR	N-CA-C	-7.07	104.80	113.50
1	F	372	PHE	N-CA-C	-7.01	101.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	TYR	CA-C-N	-6.95	113.22	120.38
1	B	97	TYR	C-N-CA	-6.95	113.22	120.38
1	B	396	VAL	CB-CA-C	-6.95	107.10	113.70
1	D	387	TYR	CA-C-N	6.78	128.32	119.84
1	D	387	TYR	C-N-CA	6.78	128.32	119.84
1	B	91	GLN	N-CA-C	-6.69	104.06	111.82
1	F	201	ILE	N-CA-C	6.66	117.64	111.45
1	E	439	GLN	N-CA-C	-6.60	103.19	111.11
1	E	447	GLU	N-CA-C	-6.53	100.76	110.23
1	F	374	ILE	N-CA-C	-6.49	104.00	110.62
1	B	324	GLU	N-CA-C	-6.48	104.26	111.71
1	B	368	ASP	N-CA-C	-6.47	104.31	111.36
1	C	169	LYS	CA-C-N	6.38	126.35	120.03
1	C	169	LYS	C-N-CA	6.38	126.35	120.03
1	A	110	THR	N-CA-C	-6.37	103.63	111.40
1	A	270	ALA	N-CA-C	6.34	119.87	111.75
1	A	169	LYS	CA-C-N	6.20	125.96	119.76
1	A	169	LYS	C-N-CA	6.20	125.96	119.76
1	B	39	VAL	N-CA-C	-6.16	105.72	111.45
1	A	350	VAL	N-CA-C	6.15	116.82	110.36
1	B	157	THR	N-CA-C	-6.13	104.51	112.23
1	B	73	ALA	N-CA-C	6.10	123.78	110.80
1	E	446	HIS	N-CA-C	-6.09	99.48	109.40
1	A	232	ALA	N-CA-C	-6.06	104.75	111.36
1	C	157	THR	N-CA-C	-6.04	104.61	111.14
1	A	401	LYS	N-CA-C	-6.00	106.21	112.93
1	E	250	GLN	N-CA-C	5.96	119.24	109.76
1	A	112	TYR	CA-C-N	5.83	125.84	119.90
1	A	112	TYR	C-N-CA	5.83	125.84	119.90
1	B	211	LEU	N-CA-C	-5.83	101.66	110.28
1	F	110	THR	N-CA-C	-5.77	106.37	113.41
1	C	49	LYS	N-CA-C	-5.74	99.89	109.24
1	D	39	VAL	N-CA-C	-5.73	106.22	111.67
1	D	49	LYS	N-CA-C	-5.69	100.01	109.46
1	A	418	VAL	N-CA-C	-5.67	105.20	110.53
1	A	49	LYS	N-CA-C	-5.63	100.53	109.76
1	B	270	ALA	N-CA-C	5.60	118.91	111.75
1	E	201	ILE	N-CA-C	5.58	116.98	110.62
1	C	423	TRP	N-CA-C	5.53	119.12	112.93
1	A	250	GLN	N-CA-C	5.46	118.52	109.46
1	E	104	PHE	N-CA-C	5.42	115.69	108.38
1	D	8	TRP	CA-C-N	5.35	125.25	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	TRP	C-N-CA	5.35	125.25	119.85
1	D	250	GLN	N-CA-C	5.34	118.64	110.20
1	E	326	ASN	N-CA-C	5.33	118.60	111.24
1	C	432	THR	N-CA-C	-5.33	102.87	110.59
1	E	49	LYS	N-CA-C	-5.32	100.50	109.07
1	A	228	ALA	N-CA-C	5.31	117.75	111.33
1	D	284	SER	N-CA-C	-5.31	106.94	113.41
1	D	432	THR	N-CA-C	-5.30	103.69	110.53
1	D	423	TRP	N-CA-C	5.26	118.72	112.72
1	F	166	ARG	N-CA-C	-5.26	103.67	110.19
1	F	442	HIS	N-CA-C	-5.25	105.45	111.07
1	D	271	LYS	N-CA-C	5.24	118.98	112.59
1	A	348	LEU	N-CA-C	5.24	116.27	109.72
1	C	350	VAL	N-CA-C	5.24	120.23	109.34
1	D	234	LEU	N-CA-C	-5.20	105.69	111.36
1	B	143	GLU	N-CA-C	-5.18	107.62	114.04
1	F	211	LEU	N-CA-C	-5.13	103.27	110.35
1	A	252	LEU	N-CA-C	-5.11	107.60	113.88
1	C	275	VAL	CB-CA-C	-5.06	105.48	111.81
1	A	367	SER	N-CA-C	-5.04	105.88	112.23
1	A	108	GLU	N-CA-C	-5.04	103.94	110.19
1	B	49	LYS	N-CA-C	-5.04	101.03	109.24
1	C	27	ASP	N-CA-C	5.03	117.59	110.50
1	E	368	ASP	N-CA-C	-5.02	105.89	111.36
1	F	432	THR	N-CA-C	-5.02	102.64	110.42
1	A	440	LEU	N-CA-C	-5.01	106.01	111.82
1	E	423	TRP	N-CA-C	5.01	118.54	112.93
1	F	382	PHE	N-CA-C	5.00	118.30	111.39
1	D	442	HIS	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3491	0	3484	143	0
1	B	3506	0	3501	134	0
1	C	3482	0	3471	158	0
1	D	3443	0	3441	174	0
1	E	3495	0	3483	175	0
1	F	3468	0	3456	234	0
2	A	106	0	0	4	0
2	B	89	0	0	5	0
2	C	79	0	0	6	0
2	D	85	0	0	5	0
2	E	40	0	0	1	0
2	F	29	0	0	3	0
All	All	21313	0	20836	1005	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 (1005) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:H	1:A:259:LYS:HD2	1.02	1.13
1:B:193:LYS:H	1:B:193:LYS:HD2	1.11	1.12
1:B:73:ALA:HB3	1:B:77:LEU:HB2	1.32	1.09
1:E:432:THR:HG22	1:E:435:GLN:H	1.18	1.06
1:A:432:THR:HG22	1:A:435:GLN:H	1.12	1.05
1:F:191:ASN:HD21	1:F:194:GLU:HB2	1.20	1.04
1:D:203:LYS:H	1:D:203:LYS:HD2	1.19	1.04
1:D:105:LEU:HD23	1:D:171:LYS:HB3	1.41	1.01
1:C:125:LYS:HE2	1:C:126:VAL:HG22	1.45	0.99
1:E:277:TYR:HA	1:E:281:ARG:HG3	1.47	0.96
1:A:84:HIS:HB3	1:A:87:ILE:HD12	1.46	0.95
1:C:89:ARG:HB2	1:C:89:ARG:HH11	1.27	0.95
1:C:112:TYR:HB3	1:C:113:PRO:HD3	1.47	0.94
1:B:73:ALA:CB	1:B:77:LEU:HB2	1.97	0.94
1:D:84:HIS:NE2	1:D:105:LEU:HD21	1.85	0.92
1:C:102:GLY:HA3	1:C:168:ILE:HB	1.52	0.91
1:A:396:VAL:HG13	1:A:397:PRO:HD3	1.52	0.91
1:E:271:LYS:HB2	1:E:322:VAL:HB	1.52	0.91
1:D:313:ARG:HH11	1:D:363:PHE:HB2	1.32	0.90
1:B:437:ARG:HH11	1:B:437:ARG:HB3	1.35	0.89
1:A:347:LYS:HD3	1:A:348:LEU:H	1.35	0.89
1:F:148:ASN:HD22	1:F:150:MET:H	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:HD2	1:A:259:LYS:N	1.85	0.88
1:B:193:LYS:H	1:B:193:LYS:CD	1.82	0.88
1:A:43:LYS:H	1:A:43:LYS:HD2	1.36	0.88
1:E:97:TYR:HB3	1:E:98:PRO:HD3	1.56	0.87
1:C:281:ARG:HG2	1:C:281:ARG:HH11	1.39	0.87
1:E:447:GLU:HB2	1:E:450:LEU:HD12	1.57	0.86
1:A:89:ARG:HD3	1:A:89:ARG:H	1.38	0.86
1:D:103:LEU:HD11	1:D:171:LYS:HB2	1.55	0.86
1:D:313:ARG:NH1	1:D:363:PHE:HB2	1.90	0.85
1:E:190:LEU:HD13	1:E:253:GLY:HA3	1.58	0.85
1:A:88:THR:HG23	1:A:89:ARG:CZ	2.05	0.85
1:A:363:PHE:CE2	1:A:367:SER:HB2	2.11	0.85
1:E:289:ASP:O	1:E:293:LYS:HD3	1.76	0.85
1:C:125:LYS:HE2	1:C:126:VAL:H	1.40	0.84
1:E:391:PRO:HB2	1:E:394:ASP:HB2	1.60	0.84
1:F:196:LYS:HB2	1:F:213:ASP:OD2	1.77	0.83
1:A:347:LYS:HD3	1:A:348:LEU:N	1.93	0.83
1:C:163:LEU:H	1:C:163:LEU:HD23	1.42	0.82
1:A:97:TYR:HB3	1:A:98:PRO:HD3	1.62	0.82
1:B:84:HIS:HB3	1:B:87:ILE:HD12	1.62	0.81
1:E:79:LEU:HA	1:E:180:GLN:NE2	1.96	0.80
1:E:245:HIS:HE1	1:E:247:ASN:HD22	1.28	0.80
1:E:102:GLY:HA3	1:E:168:ILE:HB	1.64	0.80
1:D:140:ILE:HD12	1:D:156:TYR:HE1	1.47	0.79
1:F:138:LEU:HD13	1:F:149:LEU:HD23	1.64	0.79
1:F:391:PRO:HB2	1:F:394:ASP:CG	2.07	0.79
1:E:127:GLU:HG3	1:E:164:CYS:SG	2.22	0.79
1:B:220:ALA:HB3	1:B:266:THR:HG22	1.63	0.78
1:E:352:TRP:HA	1:E:374:ILE:HD13	1.64	0.78
1:A:127:GLU:HG3	1:A:164:CYS:SG	2.23	0.78
1:C:396:VAL:HB	1:C:397:PRO:HD3	1.64	0.78
1:D:97:TYR:HB3	1:D:98:PRO:HD3	1.64	0.78
1:F:51:LYS:HE2	1:F:57:GLU:HG2	1.67	0.77
1:F:200:THR:HG21	1:F:203:LYS:HE3	1.67	0.77
1:E:280:SER:O	1:E:281:ARG:HG2	1.84	0.77
1:F:258:GLU:H	1:F:258:GLU:CD	1.92	0.77
1:A:432:THR:HG22	1:A:435:GLN:N	1.96	0.76
1:E:157:THR:HG22	1:E:167:LEU:HB2	1.66	0.76
1:F:427:ALA:HA	1:F:430:ARG:NH1	1.99	0.76
1:B:72:LYS:CD	1:B:72:LYS:H	1.98	0.76
1:B:271:LYS:NZ	1:B:326:ASN:HD22	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LYS:HG2	1:C:338:GLU:N	1.99	0.76
1:B:220:ALA:HB3	1:B:266:THR:CG2	2.16	0.76
1:B:437:ARG:HB3	1:B:437:ARG:NH1	2.00	0.76
1:D:88:THR:HG22	1:D:91:GLN:HE21	1.51	0.76
1:B:348:LEU:HD22	1:B:363:PHE:CZ	2.20	0.76
1:D:150:MET:HE1	1:D:226:ASN:H	1.50	0.76
1:F:28:LEU:HB2	1:F:58:GLY:HA3	1.66	0.75
1:F:245:HIS:HE1	1:F:247:ASN:HD22	1.31	0.75
1:F:215:ARG:HD2	2:F:458:HOH:O	1.86	0.75
1:F:394:ASP:C	1:F:397:PRO:HD2	2.12	0.75
1:F:127:GLU:HG3	1:F:164:CYS:SG	2.26	0.75
1:B:271:LYS:HZ2	1:B:326:ASN:HD22	1.35	0.75
1:F:91:GLN:O	1:F:95:LEU:HG	1.85	0.75
1:A:80:MET:HE2	1:A:150:MET:HG3	1.69	0.75
1:D:88:THR:HG23	1:D:91:GLN:H	1.52	0.74
1:F:148:ASN:HD21	1:F:150:MET:HB2	1.52	0.74
1:F:275:VAL:HG23	1:F:317:ALA:C	2.12	0.74
1:F:89:ARG:H	1:F:89:ARG:HD2	1.53	0.74
1:F:118:LEU:HD23	1:F:119:CYS:N	2.03	0.73
1:B:193:LYS:HD2	1:B:193:LYS:N	1.97	0.73
1:B:245:HIS:HD2	1:B:247:ASN:H	1.35	0.73
1:E:90:GLU:HG3	1:E:91:GLN:H	1.53	0.73
1:F:97:TYR:HB3	1:F:98:PRO:HD3	1.71	0.73
1:A:84:HIS:CB	1:A:87:ILE:HD12	2.19	0.73
1:A:89:ARG:H	1:A:89:ARG:CD	2.01	0.73
1:A:43:LYS:H	1:A:43:LYS:CD	1.96	0.73
1:F:103:LEU:HD11	1:F:171:LYS:HD3	1.68	0.73
1:D:245:HIS:CD2	1:D:247:ASN:H	2.06	0.73
1:F:191:ASN:ND2	1:F:194:GLU:HB2	1.99	0.73
1:A:396:VAL:HG13	1:A:397:PRO:CD	2.18	0.73
1:F:392:LEU:HD23	1:F:392:LEU:H	1.52	0.72
1:E:357:ALA:O	1:E:361:LYS:HA	1.87	0.72
1:F:292:LEU:HD21	1:F:444:ARG:HB2	1.71	0.72
1:C:313:ARG:NH1	1:C:363:PHE:HB2	2.03	0.72
1:D:88:THR:HG22	1:D:91:GLN:NE2	2.04	0.72
1:E:302:MET:HE1	1:E:305:LEU:HD12	1.71	0.72
1:E:90:GLU:HG3	1:E:91:GLN:N	2.05	0.72
1:E:207:GLY:HA2	1:E:225:LYS:HG3	1.71	0.72
1:D:88:THR:H	1:D:91:GLN:HE21	1.34	0.71
1:B:245:HIS:CD2	1:B:247:ASN:H	2.07	0.71
1:D:437:ARG:O	1:D:441:GLU:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:C	1:B:105:LEU:HD12	2.15	0.71
1:E:122:CYS:SG	1:E:165:THR:HG22	2.31	0.70
1:B:396:VAL:HB	1:B:397:PRO:HD3	1.73	0.70
1:E:351:LYS:HE3	1:E:392:LEU:HD13	1.74	0.70
1:D:396:VAL:HB	1:D:397:PRO:HD3	1.71	0.70
1:C:157:THR:HA	1:C:167:LEU:HB2	1.73	0.70
1:D:312:HIS:HD2	1:D:314:ASP:H	1.38	0.70
1:F:324:GLU:CD	1:F:324:GLU:H	1.98	0.70
1:C:163:LEU:H	1:C:163:LEU:CD2	2.04	0.69
1:D:245:HIS:HD2	1:D:247:ASN:H	1.40	0.69
1:F:148:ASN:ND2	1:F:150:MET:HB2	2.07	0.69
1:F:53:LYS:NZ	1:F:215:ARG:HH22	1.89	0.69
1:C:223:CYS:SG	2:C:495:HOH:O	2.51	0.69
1:C:254:VAL:HG13	1:C:262:LEU:HD11	1.74	0.69
1:E:192:MET:HE3	1:E:192:MET:O	1.91	0.69
1:F:13:GLU:OE1	1:F:68:ARG:HD2	1.93	0.69
1:B:97:TYR:HB3	1:B:98:PRO:HD3	1.74	0.69
1:A:109:SER:HB3	1:A:112:TYR:O	1.93	0.68
1:C:125:LYS:CE	1:C:126:VAL:H	2.05	0.68
1:A:89:ARG:NH1	1:A:110:THR:HG21	2.07	0.68
1:E:79:LEU:HA	1:E:180:GLN:HE22	1.58	0.68
1:B:72:LYS:H	1:B:72:LYS:HD3	1.57	0.68
1:A:396:VAL:HG12	2:A:533:HOH:O	1.93	0.68
1:D:84:HIS:CD2	1:D:105:LEU:HD21	2.28	0.68
1:E:432:THR:HG22	1:E:435:GLN:N	2.03	0.68
1:D:96:LEU:HG	1:D:103:LEU:HD12	1.75	0.68
1:F:336:THR:O	1:F:337:LYS:HG3	1.94	0.68
1:A:181:ASP:HB2	1:A:185:ARG:NH1	2.09	0.68
1:C:275:VAL:HG23	1:C:317:ALA:C	2.19	0.68
1:E:61:PRO:HG2	1:E:64:TYR:HB2	1.76	0.67
1:C:84:HIS:HA	1:C:173:MET:HE2	1.75	0.67
1:C:163:LEU:HD23	1:C:163:LEU:N	2.09	0.67
1:B:437:ARG:HH11	1:B:437:ARG:CB	2.07	0.67
1:F:96:LEU:HD22	1:F:103:LEU:HD21	1.77	0.67
1:F:391:PRO:HB2	1:F:394:ASP:OD1	1.94	0.67
1:D:150:MET:HE1	1:D:226:ASN:N	2.09	0.67
1:E:302:MET:HA	1:E:302:MET:HE2	1.76	0.67
1:F:89:ARG:CZ	1:F:110:THR:HB	2.23	0.67
1:F:270:ALA:HB3	1:F:324:GLU:HG3	1.76	0.67
1:A:259:LYS:H	1:A:259:LYS:CD	1.89	0.66
1:C:97:TYR:O	1:C:99:PRO:HD3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:OG1	1:C:91:GLN:HG3	1.95	0.66
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.60	0.66
1:C:337:LYS:HG2	1:C:338:GLU:H	1.60	0.66
1:A:148:ASN:HD22	1:A:150:MET:H	1.42	0.66
1:E:93:GLU:HG2	1:E:126:VAL:HG11	1.77	0.66
1:D:293:LYS:HD3	1:D:444:ARG:HH12	1.60	0.66
1:A:283:ARG:HD3	1:A:284:SER:H	1.60	0.66
1:B:88:THR:OG1	1:B:91:GLN:HG3	1.95	0.65
1:D:394:ASP:O	1:D:397:PRO:HD2	1.96	0.65
1:E:320:VAL:O	1:E:321:LEU:HD23	1.95	0.65
1:A:89:ARG:HD3	1:A:89:ARG:N	2.11	0.65
1:E:381:SER:HB3	1:E:384:ARG:HG3	1.76	0.65
1:F:118:LEU:HD21	1:F:120:VAL:HG23	1.78	0.65
1:C:181:ASP:O	1:C:185:ARG:HB2	1.96	0.65
1:E:236:GLU:HG2	1:E:240:MET:CE	2.26	0.65
1:D:104:PHE:CE2	1:D:167:LEU:HB3	2.31	0.65
1:D:140:ILE:HD12	1:D:156:TYR:CE1	2.31	0.65
1:C:96:LEU:HG	1:C:103:LEU:HD12	1.77	0.65
1:B:290:CYS:SG	2:B:527:HOH:O	2.54	0.65
1:E:375:LEU:C	1:E:375:LEU:HD23	2.21	0.65
1:A:54:VAL:HG12	1:A:54:VAL:O	1.97	0.65
1:B:148:ASN:OD1	1:B:150:MET:HB2	1.97	0.65
1:D:393:LYS:H	1:D:393:LYS:HD2	1.62	0.65
1:D:105:LEU:HD13	1:D:106:VAL:N	2.11	0.64
1:F:152:LEU:C	1:F:152:LEU:HD23	2.21	0.64
1:F:351:LYS:HZ2	1:F:385:VAL:HG12	1.62	0.64
1:A:87:ILE:HD13	1:A:95:LEU:HD11	1.79	0.64
1:F:437:ARG:O	1:F:441:GLU:HG3	1.98	0.64
1:A:224:ILE:HD12	1:A:233:PHE:HA	1.80	0.64
1:B:97:TYR:O	1:B:98:PRO:C	2.37	0.64
1:F:396:VAL:HB	1:F:397:PRO:HD3	1.80	0.64
1:A:76:LYS:HG2	1:A:177:VAL:CG2	2.27	0.64
1:E:79:LEU:HD23	1:E:180:GLN:NE2	2.13	0.64
1:F:89:ARG:HG3	1:F:107:ARG:CZ	2.28	0.64
1:F:51:LYS:HE2	1:F:57:GLU:CG	2.28	0.64
1:F:387:TYR:HB3	1:F:390:ILE:HB	1.80	0.64
1:E:437:ARG:O	1:E:441:GLU:HG3	1.98	0.63
1:F:95:LEU:O	1:F:96:LEU:HD23	1.99	0.63
1:F:377:TRP:O	1:F:381:SER:HB2	1.98	0.63
1:C:193:LYS:HE2	2:C:515:HOH:O	1.97	0.63
1:A:356:GLU:HB3	1:A:360:GLU:OE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:HIS:HB3	1:A:87:ILE:CD1	2.25	0.63
1:C:254:VAL:CG1	1:C:262:LEU:HD11	2.28	0.63
1:D:257:GLU:HG2	1:D:258:GLU:H	1.64	0.63
1:D:356:GLU:O	1:D:360:GLU:HG2	1.98	0.63
1:F:274:LEU:HD12	1:F:317:ALA:HB1	1.81	0.63
1:F:422:CYS:O	1:F:430:ARG:HD3	1.99	0.63
1:E:302:MET:CE	1:E:305:LEU:HD12	2.27	0.63
1:C:84:HIS:HA	1:C:173:MET:CE	2.28	0.63
1:E:432:THR:HG23	1:E:434:LEU:H	1.62	0.63
1:C:101:THR:HG23	1:C:165:THR:HB	1.79	0.63
1:E:89:ARG:HG2	1:E:107:ARG:NH2	2.13	0.63
1:A:148:ASN:ND2	1:A:150:MET:HB2	2.13	0.63
1:C:394:ASP:O	1:C:398:ARG:HB2	1.99	0.63
1:D:81:PRO:HA	1:D:176:THR:HG21	1.81	0.63
1:E:153:VAL:O	1:E:157:THR:HG23	1.99	0.63
1:F:360:GLU:O	1:F:362:LYS:N	2.30	0.63
1:D:104:PHE:CD2	1:D:167:LEU:HB3	2.33	0.62
1:D:254:VAL:CG1	1:D:262:LEU:HD11	2.29	0.62
1:D:257:GLU:HG2	1:D:258:GLU:N	2.14	0.62
1:C:109:SER:OG	1:C:111:ASN:HB2	1.99	0.62
1:A:105:LEU:C	1:A:105:LEU:HD12	2.24	0.62
1:C:89:ARG:HH11	1:C:89:ARG:CB	2.06	0.62
1:C:107:ARG:NH2	1:C:111:ASN:HD22	1.97	0.62
1:F:141:ASP:OD2	1:F:143:GLU:HB2	1.99	0.62
1:F:191:ASN:ND2	1:F:194:GLU:H	1.96	0.62
1:A:151:GLN:HG2	1:A:260:GLY:HA3	1.81	0.62
1:C:398:ARG:HG3	1:C:398:ARG:HH11	1.64	0.62
1:A:148:ASN:HD22	1:A:150:MET:N	1.96	0.62
1:E:203:LYS:HG3	1:E:208:ASP:OD1	1.99	0.62
1:A:132:MET:HE1	2:A:541:HOH:O	2.00	0.62
1:D:151:GLN:HE21	1:D:259:LYS:HD3	1.65	0.62
1:C:315:LEU:HD23	1:C:316:ALA:N	2.14	0.62
1:E:105:LEU:HD12	1:E:105:LEU:C	2.25	0.61
1:F:118:LEU:CD2	1:F:120:VAL:HG23	2.29	0.61
1:A:314:ASP:HB2	1:A:335:LEU:HD12	1.82	0.61
1:A:115:ASP:HB3	1:A:131:ILE:O	2.01	0.61
1:A:245:HIS:CD2	1:A:247:ASN:H	2.18	0.61
1:C:79:LEU:HD12	1:C:225:LYS:O	2.00	0.61
1:F:76:LYS:HB3	1:F:175:GLY:O	2.00	0.61
1:A:76:LYS:H	1:A:76:LYS:HD3	1.65	0.61
1:A:257:GLU:HB3	1:A:259:LYS:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:HA	1:C:56:ARG:O	2.00	0.61
1:D:93:GLU:OE2	1:D:126:VAL:HG21	2.01	0.61
1:F:184:TYR:HA	1:F:189:ALA:HB2	1.83	0.61
1:E:109:SER:OG	1:E:112:TYR:HB2	2.01	0.61
1:E:359:ARG:C	1:E:361:LYS:H	2.09	0.61
1:F:88:THR:HB	1:F:91:GLN:HG3	1.82	0.61
1:C:281:ARG:HH11	1:C:281:ARG:CG	2.12	0.61
1:E:271:LYS:NZ	1:E:326:ASN:ND2	2.49	0.61
1:A:105:LEU:HD12	1:A:105:LEU:O	2.00	0.61
1:C:203:LYS:NZ	1:C:203:LYS:HB3	2.16	0.61
1:F:222:LYS:HE2	1:F:224:ILE:HG12	1.82	0.61
1:E:245:HIS:CE1	1:E:247:ASN:HD22	2.16	0.61
1:F:51:LYS:HA	1:F:56:ARG:O	2.00	0.60
1:C:209:VAL:HG12	1:C:222:LYS:HG2	1.83	0.60
1:C:245:HIS:CD2	1:C:247:ASN:H	2.20	0.60
1:D:254:VAL:HG22	1:D:264:ILE:HD13	1.83	0.60
1:F:245:HIS:CE1	1:F:247:ASN:HD22	2.17	0.60
1:C:105:LEU:HD22	1:C:106:VAL:H	1.67	0.60
1:D:103:LEU:HD13	1:D:104:PHE:N	2.17	0.60
1:D:105:LEU:HD13	1:D:106:VAL:H	1.67	0.60
1:B:435:GLN:HE21	1:C:308:ASN:ND2	1.99	0.60
1:C:95:LEU:C	1:C:96:LEU:HD12	2.26	0.60
1:C:107:ARG:HH21	1:C:109:SER:CB	2.13	0.60
1:B:193:LYS:HD3	2:B:502:HOH:O	2.01	0.60
1:C:84:HIS:CG	1:C:105:LEU:HD21	2.37	0.60
1:D:354:ALA:HB1	1:D:356:GLU:OE2	2.02	0.60
1:A:164:CYS:HB3	1:B:56:ARG:HE	1.67	0.60
1:D:184:TYR:CE1	1:D:256:VAL:HG23	2.37	0.60
1:E:271:LYS:HZ1	1:E:326:ASN:ND2	2.00	0.60
1:E:84:HIS:HB3	1:E:87:ILE:HD12	1.84	0.59
1:E:87:ILE:O	1:E:107:ARG:HD2	2.02	0.59
1:D:88:THR:HG22	1:D:91:GLN:HG2	1.85	0.59
1:D:387:TYR:HB3	1:D:390:ILE:HG23	1.85	0.59
1:E:89:ARG:HD2	1:E:110:THR:HG21	1.84	0.59
1:A:88:THR:HB	1:A:91:GLN:HG3	1.84	0.59
1:F:63:ASN:HB2	2:F:459:HOH:O	2.02	0.59
1:A:88:THR:HG22	1:A:90:GLU:HG3	1.83	0.59
1:E:190:LEU:CD1	1:E:253:GLY:HA3	2.32	0.59
1:F:105:LEU:C	1:F:105:LEU:HD12	2.28	0.59
1:A:148:ASN:ND2	1:A:151:GLN:H	1.99	0.59
1:B:76:LYS:O	1:B:177:VAL:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:GLU:HG2	1:E:240:MET:HE2	1.84	0.59
1:F:212:GLY:O	1:F:219:VAL:HG12	2.02	0.59
1:F:397:PRO:O	1:F:401:LYS:HG3	2.03	0.59
1:A:138:LEU:HD23	1:A:149:LEU:HD23	1.85	0.59
1:A:432:THR:HG23	1:A:434:LEU:H	1.68	0.59
1:D:203:LYS:HD2	1:D:203:LYS:N	2.03	0.59
1:E:28:LEU:HB2	1:E:58:GLY:HA3	1.83	0.59
1:A:258:GLU:HA	1:A:258:GLU:OE1	2.03	0.58
1:B:434:LEU:HG	1:B:437:ARG:HH12	1.68	0.58
1:C:275:VAL:HG23	1:C:318:ARG:N	2.18	0.58
1:E:359:ARG:O	1:E:361:LYS:N	2.37	0.58
1:F:53:LYS:HZ1	1:F:215:ARG:HH22	1.49	0.58
1:D:184:TYR:CZ	1:D:256:VAL:HG23	2.38	0.58
1:E:230:ALA:O	1:E:234:LEU:HD22	2.03	0.58
1:E:352:TRP:HA	1:E:374:ILE:CD1	2.34	0.58
1:F:271:LYS:HG3	1:F:323:SER:O	2.03	0.58
1:A:219:VAL:HG22	1:A:252:LEU:HD12	1.85	0.58
1:A:79:LEU:HA	1:A:180:GLN:HE22	1.69	0.58
1:D:191:ASN:HD21	1:D:193:LYS:HE3	1.68	0.58
1:B:87:ILE:HG23	1:B:91:GLN:HB2	1.85	0.58
1:B:108:GLU:HG2	1:B:116:TYR:CE2	2.39	0.58
1:A:122:CYS:SG	1:A:165:THR:HG22	2.44	0.58
1:B:75:THR:C	1:B:77:LEU:H	2.12	0.58
1:D:160:ALA:HB2	1:D:166:ARG:HB3	1.85	0.58
1:F:89:ARG:H	1:F:89:ARG:CD	2.15	0.58
1:E:54:VAL:HG12	1:E:54:VAL:O	2.03	0.58
1:F:109:SER:H	1:F:116:TYR:HA	1.69	0.58
1:F:311:VAL:HG22	1:F:337:LYS:O	2.04	0.58
1:C:102:GLY:HA3	1:C:168:ILE:CB	2.29	0.57
1:E:293:LYS:HZ1	1:E:444:ARG:HD2	1.68	0.57
1:B:148:ASN:CG	1:B:151:GLN:HG3	2.28	0.57
1:C:160:ALA:HA	1:C:163:LEU:HD21	1.86	0.57
1:B:97:TYR:O	1:B:99:PRO:N	2.38	0.57
1:B:99:PRO:HB3	1:B:124:GLY:HA2	1.86	0.57
1:C:275:VAL:HG22	1:C:317:ALA:HB3	1.86	0.57
1:A:249:VAL:HG21	1:A:331:SER:HB3	1.86	0.57
1:B:230:ALA:O	1:B:234:LEU:HD22	2.05	0.57
1:C:81:PRO:CG	1:C:178:ALA:HA	2.35	0.57
1:C:437:ARG:O	1:C:441:GLU:HG3	2.05	0.57
1:D:225:LYS:HB3	1:D:227:ASP:OD1	2.04	0.57
1:E:394:ASP:O	1:E:397:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:LYS:HG2	1:F:57:GLU:HG2	1.87	0.57
1:D:88:THR:N	1:D:91:GLN:HE21	2.00	0.57
1:F:188:TRP:O	1:F:254:VAL:HG12	2.04	0.57
1:C:61:PRO:HG2	1:C:64:TYR:HB2	1.87	0.57
1:E:109:SER:HB3	1:E:112:TYR:O	2.05	0.57
1:E:193:LYS:HD3	1:E:193:LYS:N	2.20	0.57
1:F:51:LYS:HE2	1:F:57:GLU:CD	2.30	0.57
1:C:243:LEU:HD13	1:C:248:LEU:HD13	1.87	0.56
1:D:108:GLU:HG2	1:D:116:TYR:HE2	1.70	0.56
1:D:225:LYS:HG2	1:D:226:ASN:H	1.69	0.56
1:D:258:GLU:H	1:D:258:GLU:CD	2.11	0.56
1:F:370:TRP:HE3	1:F:430:ARG:HE	1.53	0.56
1:D:160:ALA:CB	1:D:166:ARG:HB3	2.36	0.56
1:E:348:LEU:N	1:E:349:PRO:CD	2.69	0.56
1:C:184:TYR:CE1	1:C:256:VAL:HG23	2.39	0.56
1:F:196:LYS:N	1:F:196:LYS:HD2	2.21	0.56
1:A:76:LYS:HG2	1:A:177:VAL:HG21	1.86	0.56
1:C:173:MET:O	1:C:176:THR:HB	2.06	0.56
1:D:91:GLN:O	1:D:95:LEU:HG	2.04	0.56
1:D:108:GLU:HG2	1:D:116:TYR:CE2	2.40	0.56
1:E:86:LYS:HD3	1:E:86:LYS:H	1.71	0.56
1:E:432:THR:CG2	1:E:435:GLN:H	2.04	0.56
1:F:68:ARG:HA	1:F:186:SER:O	2.06	0.56
1:E:227:ASP:OD2	1:E:230:ALA:HA	2.06	0.56
1:D:89:ARG:O	1:D:93:GLU:HG3	2.06	0.56
1:A:164:CYS:HB3	1:B:56:ARG:NE	2.21	0.56
1:F:43:LYS:HG3	2:F:477:HOH:O	2.05	0.56
1:A:87:ILE:HG23	1:A:91:GLN:HB2	1.88	0.55
1:B:125:LYS:HE3	1:B:127:GLU:OE2	2.06	0.55
1:C:86:LYS:HG3	1:C:108:GLU:O	2.06	0.55
1:D:150:MET:CE	1:D:226:ASN:HB2	2.36	0.55
1:C:93:GLU:HG2	1:C:126:VAL:HG21	1.88	0.55
1:C:281:ARG:HG2	1:C:281:ARG:NH1	2.18	0.55
1:C:152:LEU:C	1:C:152:LEU:HD23	2.32	0.55
1:D:148:ASN:N	2:D:515:HOH:O	2.32	0.55
1:D:313:ARG:HB3	1:D:363:PHE:CD2	2.42	0.55
1:D:67:LYS:HE2	1:D:69:GLU:HB3	1.87	0.55
1:E:391:PRO:C	1:E:393:LYS:H	2.14	0.55
1:C:303:GLU:OE1	1:C:437:ARG:HD3	2.07	0.55
1:D:192:MET:HE1	1:D:263:TYR:CE1	2.41	0.55
1:C:354:ALA:HB1	1:C:356:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ALA:HA	1:D:95:LEU:HD12	1.88	0.55
1:D:160:ALA:HB2	1:D:166:ARG:CB	2.36	0.55
1:F:118:LEU:HD23	1:F:118:LEU:C	2.32	0.55
1:F:248:LEU:HD22	1:F:333:PHE:CE2	2.41	0.55
1:C:191:ASN:OD1	1:C:193:LYS:HE3	2.07	0.55
1:D:150:MET:HE2	1:D:226:ASN:HB2	1.88	0.55
1:F:306:GLU:CD	1:F:365:THR:HG21	2.31	0.55
1:C:356:GLU:O	1:C:360:GLU:HG2	2.06	0.55
1:D:90:GLU:C	1:D:92:ALA:H	2.14	0.55
1:E:191:ASN:ND2	1:E:215:ARG:HH12	2.04	0.55
1:E:271:LYS:NZ	1:E:326:ASN:HD21	2.03	0.55
1:A:271:LYS:HB2	1:A:322:VAL:HB	1.89	0.55
1:B:95:LEU:O	1:B:171:LYS:HE3	2.05	0.55
1:B:111:ASN:C	1:B:113:PRO:HD3	2.31	0.55
1:C:258:GLU:CD	1:C:258:GLU:H	2.15	0.55
1:D:54:VAL:HG22	1:E:140:ILE:CG2	2.37	0.55
1:D:107:ARG:HH12	1:D:128:HIS:CE1	2.24	0.55
1:F:94:ARG:C	1:F:96:LEU:H	2.14	0.55
1:C:125:LYS:HG3	1:C:126:VAL:N	2.20	0.54
1:D:201:ILE:HB	1:D:209:VAL:HG12	1.88	0.54
1:E:171:LYS:C	1:E:171:LYS:HD3	2.32	0.54
1:C:81:PRO:HG2	1:C:178:ALA:HA	1.88	0.54
1:F:89:ARG:HG3	1:F:107:ARG:NH2	2.21	0.54
1:F:375:LEU:HD23	1:F:375:LEU:O	2.07	0.54
1:A:88:THR:CG2	1:A:90:GLU:HG3	2.37	0.54
1:A:123:GLU:C	1:A:125:LYS:H	2.15	0.54
1:C:96:LEU:HG	1:C:103:LEU:CD1	2.37	0.54
1:E:74:GLY:C	1:E:76:LYS:H	2.14	0.54
1:E:235:ALA:O	1:E:239:VAL:HG23	2.07	0.54
1:A:148:ASN:ND2	1:A:151:GLN:HG3	2.21	0.54
1:F:109:SER:HB2	1:F:115:ASP:C	2.32	0.54
1:F:270:ALA:CB	1:F:324:GLU:HG3	2.38	0.54
1:D:203:LYS:H	1:D:203:LYS:CD	1.97	0.54
1:E:249:VAL:HG21	1:E:331:SER:HB3	1.90	0.54
1:E:348:LEU:O	1:E:350:VAL:N	2.41	0.54
1:F:398:ARG:O	1:F:401:LYS:HB2	2.08	0.54
1:D:54:VAL:HG22	1:E:140:ILE:HG22	1.90	0.54
1:E:39:VAL:HG23	1:E:50:ALA:HA	1.89	0.54
1:F:84:HIS:HB3	1:F:87:ILE:CG1	2.38	0.54
1:F:447:GLU:C	1:F:449:HIS:H	2.14	0.54
1:A:275:VAL:HG23	1:A:317:ALA:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:TYR:CD2	1:B:215:ARG:HG3	2.43	0.54
1:D:88:THR:H	1:D:91:GLN:NE2	2.04	0.54
1:F:236:GLU:HG2	1:F:240:MET:CE	2.38	0.54
1:F:258:GLU:CD	1:F:258:GLU:N	2.64	0.54
1:A:14:CYS:HB3	1:A:65:VAL:HB	1.90	0.54
1:B:354:ALA:HB1	1:B:356:GLU:OE1	2.08	0.54
1:C:83:PHE:O	1:C:173:MET:HE3	2.08	0.54
1:E:51:LYS:HG2	1:E:57:GLU:HB2	1.90	0.54
1:F:218:LYS:HD3	1:F:268:TYR:CD2	2.43	0.54
1:F:394:ASP:O	1:F:397:PRO:HD2	2.07	0.54
1:A:54:VAL:O	1:A:54:VAL:CG1	2.56	0.54
1:B:192:MET:HE3	1:B:192:MET:O	2.07	0.54
1:D:239:VAL:HG12	1:D:243:LEU:HD11	1.88	0.54
1:F:375:LEU:HD23	1:F:375:LEU:C	2.33	0.54
1:A:434:LEU:C	1:A:434:LEU:HD23	2.33	0.53
1:C:201:ILE:HB	1:C:209:VAL:HG23	1.91	0.53
1:E:97:TYR:HB3	1:E:98:PRO:CD	2.35	0.53
1:C:255:ILE:O	1:C:262:LEU:HD12	2.08	0.53
1:E:76:LYS:O	1:E:177:VAL:HG12	2.08	0.53
1:E:282:GLY:O	1:E:286:LEU:HG	2.09	0.53
1:B:388:PRO:O	1:B:389:ARG:HB2	2.08	0.53
1:C:105:LEU:HD22	1:C:106:VAL:N	2.23	0.53
1:C:236:GLU:O	1:C:240:MET:HG3	2.09	0.53
1:A:311:VAL:HG11	1:A:363:PHE:CD2	2.43	0.53
1:D:360:GLU:OE2	1:D:362:LYS:HB2	2.08	0.53
1:F:246:SER:O	1:F:329:LYS:HE2	2.09	0.53
1:D:82:TRP:CZ3	1:D:83:PHE:HB2	2.43	0.53
1:E:37:THR:O	1:E:50:ALA:HB1	2.09	0.53
1:E:73:ALA:HB2	1:E:238:SER:OG	2.09	0.53
1:E:84:HIS:CB	1:E:87:ILE:HD12	2.38	0.53
1:F:75:THR:HG23	1:F:76:LYS:HG3	1.90	0.53
1:D:393:LYS:H	1:D:393:LYS:CD	2.20	0.53
1:B:191:ASN:HB3	1:B:193:LYS:HD3	1.90	0.53
1:B:356:GLU:OE1	1:B:430:ARG:NH2	2.33	0.53
1:C:125:LYS:HE3	1:C:125:LYS:HA	1.91	0.53
1:E:293:LYS:NZ	1:E:444:ARG:HD2	2.24	0.53
1:A:88:THR:CG2	1:A:89:ARG:N	2.72	0.53
1:B:26:GLN:HG2	2:B:453:HOH:O	2.09	0.53
1:C:89:ARG:HG3	1:C:90:GLU:OE1	2.08	0.53
1:C:306:GLU:CD	1:C:365:THR:HG21	2.33	0.53
1:A:313:ARG:NH2	1:A:337:LYS:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLN:NE2	1:D:259:LYS:HD3	2.24	0.52
1:E:100:GLU:O	1:E:121:SER:HB3	2.08	0.52
1:F:200:THR:HG21	1:F:203:LYS:CE	2.36	0.52
1:A:61:PRO:HG2	1:A:64:TYR:HB2	1.91	0.52
1:B:198:LEU:HD12	1:B:211:LEU:HG	1.91	0.52
1:C:50:ALA:O	1:C:57:GLU:HA	2.08	0.52
1:D:156:TYR:CG	1:D:163:LEU:HD11	2.44	0.52
1:E:396:VAL:HB	1:E:397:PRO:HD3	1.90	0.52
1:B:190:LEU:HD22	1:B:253:GLY:C	2.34	0.52
1:F:370:TRP:HE3	1:F:430:ARG:NE	2.07	0.52
1:A:107:ARG:HH21	1:A:128:HIS:HD2	1.56	0.52
1:C:81:PRO:HA	1:C:176:THR:HG21	1.91	0.52
1:C:88:THR:HG23	1:C:91:GLN:HE21	1.73	0.52
1:F:79:LEU:HD23	1:F:179:ALA:HB3	1.90	0.52
1:C:97:TYR:N	1:C:98:PRO:CD	2.72	0.52
1:C:109:SER:C	1:C:111:ASN:H	2.17	0.52
1:E:283:ARG:HG2	1:E:283:ARG:HH11	1.75	0.52
1:A:90:GLU:O	1:A:93:GLU:HB2	2.09	0.52
1:D:51:LYS:HA	1:D:56:ARG:O	2.09	0.52
1:D:97:TYR:O	1:D:99:PRO:HD3	2.09	0.52
1:E:51:LYS:HA	1:E:56:ARG:O	2.10	0.52
1:A:354:ALA:HB1	1:A:356:GLU:OE2	2.08	0.52
1:C:399:VAL:HA	1:C:403:TYR:HB3	1.92	0.52
1:E:229:THR:O	1:E:230:ALA:HB3	2.09	0.52
1:B:191:ASN:HD22	1:B:215:ARG:HH12	1.58	0.52
1:F:82:TRP:CD1	1:F:82:TRP:H	2.25	0.52
1:A:43:LYS:HD2	1:A:43:LYS:N	2.15	0.52
1:A:219:VAL:HG11	1:A:265:VAL:HG13	1.92	0.52
1:A:283:ARG:HD3	1:A:283:ARG:N	2.25	0.52
1:F:398:ARG:HB3	1:F:403:TYR:HB2	1.90	0.52
1:B:337:LYS:HG3	1:B:338:GLU:H	1.74	0.52
1:A:161:ASP:OD1	1:B:53:LYS:NZ	2.34	0.51
1:A:257:GLU:HB3	1:A:259:LYS:CD	2.40	0.51
1:B:399:VAL:HA	1:B:403:TYR:HB3	1.91	0.51
1:D:81:PRO:HG3	1:D:178:ALA:HA	1.92	0.51
1:F:52:ASN:OD1	1:F:56:ARG:HB2	2.10	0.51
1:F:68:ARG:HD3	1:F:188:TRP:CZ2	2.45	0.51
1:F:275:VAL:CG2	1:F:317:ALA:HB3	2.40	0.51
1:C:366:LYS:NZ	1:C:430:ARG:O	2.41	0.51
1:F:106:VAL:HG11	1:F:149:LEU:HD13	1.91	0.51
1:F:351:LYS:NZ	1:F:385:VAL:HG12	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:MET:HE1	1:F:262:LEU:HD21	1.91	0.51
1:F:258:GLU:N	1:F:258:GLU:OE1	2.43	0.51
1:A:359:ARG:HD3	2:A:496:HOH:O	2.10	0.51
1:B:130:ARG:HD3	1:B:132:MET:HE2	1.92	0.51
1:B:223:CYS:O	1:B:223:CYS:SG	2.67	0.51
1:D:240:MET:HE2	1:D:249:VAL:O	2.10	0.51
1:A:151:GLN:HA	1:A:259:LYS:O	2.11	0.51
1:A:348:LEU:HD13	1:A:363:PHE:HE1	1.75	0.51
1:B:360:GLU:HG2	1:B:362:LYS:HB2	1.93	0.51
1:F:433:PHE:HA	1:F:436:LEU:HD12	1.92	0.51
1:C:141:ASP:OD2	1:C:143:GLU:HB2	2.11	0.51
1:E:447:GLU:CB	1:E:450:LEU:HD12	2.36	0.51
1:C:398:ARG:HG3	1:C:398:ARG:NH1	2.25	0.51
1:D:88:THR:HG22	1:D:91:GLN:CG	2.41	0.51
1:F:275:VAL:HG23	1:F:318:ARG:N	2.24	0.51
1:A:88:THR:HG22	1:A:89:ARG:N	2.25	0.51
1:B:214:TYR:CE2	1:B:215:ARG:HG3	2.46	0.51
1:C:92:ALA:O	1:C:96:LEU:HD13	2.11	0.51
1:E:152:LEU:C	1:E:152:LEU:HD23	2.36	0.51
1:E:302:MET:HE2	1:E:302:MET:CA	2.41	0.51
1:F:41:VAL:HB	1:F:48:TYR:CE2	2.46	0.51
1:F:224:ILE:HD12	1:F:233:PHE:HA	1.93	0.51
1:F:248:LEU:HD22	1:F:333:PHE:HE2	1.74	0.51
1:A:166:ARG:NH1	2:A:554:HOH:O	2.43	0.51
1:D:283:ARG:HA	1:D:382:PHE:CE2	2.46	0.51
1:F:398:ARG:HA	1:F:401:LYS:HD2	1.91	0.51
1:A:394:ASP:O	1:A:397:PRO:HG2	2.11	0.51
1:B:424:HIS:CD2	1:B:429:THR:HG22	2.46	0.51
1:E:359:ARG:C	1:E:361:LYS:N	2.69	0.51
1:F:195:LEU:CD2	1:F:214:TYR:HB2	2.41	0.51
1:A:219:VAL:CG1	1:A:265:VAL:HG13	2.41	0.50
1:F:84:HIS:HB3	1:F:87:ILE:HG12	1.92	0.50
1:F:255:ILE:HB	1:F:263:TYR:HB2	1.93	0.50
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.76	0.50
1:B:348:LEU:HD22	1:B:363:PHE:CE2	2.47	0.50
1:B:373:GLY:HA2	1:B:376:LEU:HB2	1.93	0.50
1:D:84:HIS:CE1	1:D:105:LEU:HD21	2.45	0.50
1:D:277:TYR:CZ	1:D:281:ARG:HD2	2.46	0.50
1:F:148:ASN:ND2	1:F:150:MET:H	1.97	0.50
1:B:338:GLU:HB3	2:B:522:HOH:O	2.12	0.50
1:D:225:LYS:C	1:D:227:ASP:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:HIS:CE1	1:F:450:LEU:HG	2.45	0.50
1:C:103:LEU:HA	1:C:169:LYS:O	2.11	0.50
1:D:208:ASP:OD1	1:D:209:VAL:HG23	2.12	0.50
1:A:313:ARG:NH2	1:A:340:SER:OG	2.44	0.50
1:D:160:ALA:HB2	1:D:166:ARG:HA	1.94	0.50
1:A:120:VAL:O	1:A:126:VAL:HA	2.11	0.50
1:A:140:ILE:HG22	1:B:54:VAL:HG22	1.93	0.50
1:B:75:THR:C	1:B:77:LEU:N	2.68	0.50
1:B:233:PHE:CZ	1:B:254:VAL:CG2	2.95	0.50
1:C:360:GLU:OE2	1:C:362:LYS:HB2	2.11	0.50
1:D:254:VAL:HG13	1:D:262:LEU:HD11	1.94	0.50
1:E:273:SER:HB3	1:E:276:ASP:OD2	2.12	0.50
1:F:275:VAL:HG23	1:F:317:ALA:HB3	1.92	0.50
1:C:443:ILE:HA	1:C:448:LEU:HD12	1.94	0.50
1:D:80:MET:HE2	1:D:226:ASN:CG	2.37	0.50
1:D:222:LYS:HE2	1:D:233:PHE:CZ	2.47	0.50
1:D:225:LYS:HG2	1:D:226:ASN:N	2.27	0.50
1:E:200:THR:HA	1:E:210:MET:HA	1.94	0.50
1:D:103:LEU:HA	1:D:169:LYS:O	2.11	0.50
1:F:141:ASP:O	1:F:143:GLU:HG3	2.12	0.50
1:F:191:ASN:HD22	1:F:194:GLU:H	1.59	0.50
1:F:375:LEU:O	1:F:379:ILE:HG13	2.12	0.50
1:B:82:TRP:CZ2	1:B:153:VAL:HG21	2.48	0.49
1:B:148:ASN:OD1	1:B:151:GLN:HG3	2.11	0.49
1:E:279:ARG:HG3	1:E:383:GLY:HA3	1.93	0.49
1:E:309:ASN:O	1:E:338:GLU:HG2	2.12	0.49
1:E:320:VAL:C	1:E:321:LEU:HD23	2.36	0.49
1:F:211:LEU:HG	1:F:212:GLY:H	1.77	0.49
1:B:180:GLN:CD	1:B:180:GLN:H	2.20	0.49
1:C:125:LYS:CE	1:C:126:VAL:HG22	2.28	0.49
1:E:193:LYS:HD3	1:E:193:LYS:H	1.77	0.49
1:F:101:THR:HA	1:F:121:SER:O	2.12	0.49
1:F:139:SER:HB2	1:F:145:TYR:CD2	2.47	0.49
1:C:101:THR:HG22	1:C:102:GLY:N	2.27	0.49
1:C:126:VAL:HG23	1:C:126:VAL:O	2.12	0.49
1:E:77:LEU:HA	1:E:177:VAL:HG13	1.93	0.49
1:F:286:LEU:HB2	1:F:382:PHE:HE2	1.76	0.49
1:C:315:LEU:HD23	1:C:315:LEU:C	2.37	0.49
1:C:433:PHE:HA	1:C:436:LEU:HD12	1.95	0.49
1:B:307:GLY:HA3	1:C:434:LEU:HD22	1.93	0.49
1:D:313:ARG:HH11	1:D:363:PHE:CB	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:GLU:CG	1:F:365:THR:HG21	2.43	0.49
1:F:386:PRO:C	1:F:387:TYR:HD1	2.21	0.49
1:C:281:ARG:CG	1:C:281:ARG:NH1	2.74	0.49
1:E:360:GLU:O	1:E:361:LYS:C	2.56	0.49
1:F:88:THR:HG22	1:F:89:ARG:N	2.28	0.49
1:F:425:LEU:H	1:F:425:LEU:HD22	1.78	0.49
1:D:43:LYS:HG2	2:D:527:HOH:O	2.12	0.49
1:D:197:LEU:HD13	1:D:210:MET:CE	2.43	0.49
1:D:357:ALA:O	1:D:361:LYS:HA	2.13	0.49
1:B:219:VAL:CG2	1:B:252:LEU:HD22	2.43	0.48
1:C:227:ASP:OD1	1:C:229:THR:HG22	2.13	0.48
1:D:88:THR:CG2	1:D:91:GLN:HG2	2.43	0.48
1:D:293:LYS:HD3	1:D:444:ARG:NH1	2.28	0.48
1:F:196:LYS:HD2	1:F:196:LYS:H	1.77	0.48
1:F:314:ASP:HB2	1:F:335:LEU:HD12	1.95	0.48
1:A:203:LYS:O	1:B:285:VAL:HG21	2.12	0.48
1:D:393:LYS:HD2	1:D:393:LYS:N	2.27	0.48
1:F:51:LYS:CE	1:F:57:GLU:HG2	2.41	0.48
1:A:76:LYS:H	1:A:76:LYS:CD	2.26	0.48
1:B:130:ARG:CD	1:B:132:MET:HE2	2.43	0.48
1:E:394:ASP:C	1:E:397:PRO:HD2	2.38	0.48
1:D:195:LEU:HD12	1:D:255:ILE:HD12	1.95	0.48
1:D:203:LYS:N	1:D:203:LYS:CD	2.71	0.48
1:D:258:GLU:C	1:D:260:GLY:H	2.22	0.48
1:E:292:LEU:HD21	1:E:444:ARG:HB2	1.96	0.48
1:F:219:VAL:HG23	1:F:266:THR:O	2.14	0.48
1:F:311:VAL:HG23	1:F:311:VAL:O	2.13	0.48
1:A:387:TYR:N	1:A:388:PRO:HD3	2.28	0.48
1:B:146:PHE:HB3	1:B:151:GLN:HB2	1.95	0.48
1:D:229:THR:HG23	1:D:230:ALA:N	2.28	0.48
1:F:76:LYS:O	1:F:177:VAL:HG12	2.14	0.48
1:C:339:ALA:O	1:C:340:SER:C	2.57	0.48
1:C:231:GLN:HB3	2:C:513:HOH:O	2.13	0.48
1:C:275:VAL:CG2	1:C:318:ARG:N	2.77	0.48
1:C:381:SER:HB3	1:C:384:ARG:HB3	1.96	0.48
1:D:375:LEU:O	1:D:375:LEU:HD12	2.14	0.48
1:F:141:ASP:O	1:F:142:GLU:C	2.57	0.48
1:F:387:TYR:HA	1:F:390:ILE:HD12	1.96	0.48
1:B:219:VAL:HG22	1:B:266:THR:O	2.14	0.48
1:C:245:HIS:HD2	1:C:247:ASN:H	1.59	0.48
1:E:91:GLN:HA	1:E:94:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ILE:HD11	1:E:268:TYR:HE1	1.79	0.48
1:E:395:VAL:O	1:E:399:VAL:HG23	2.13	0.48
1:F:77:LEU:CD1	1:F:177:VAL:HG13	2.43	0.48
1:F:184:TYR:HA	1:F:189:ALA:CB	2.44	0.48
1:B:360:GLU:CD	1:B:362:LYS:HD2	2.39	0.47
1:C:209:VAL:HG12	1:C:222:LYS:CG	2.43	0.47
1:E:52:ASN:OD1	1:E:52:ASN:C	2.56	0.47
1:F:416:TYR:CE2	1:F:420:LYS:HD3	2.50	0.47
1:A:281:ARG:HG3	1:A:281:ARG:NH1	2.28	0.47
1:D:391:PRO:HD2	1:D:394:ASP:OD2	2.14	0.47
1:E:24:ALA:O	1:E:27:ASP:HB2	2.14	0.47
1:E:197:LEU:O	1:E:198:LEU:HD23	2.14	0.47
1:E:213:ASP:HA	1:E:217:ASN:O	2.14	0.47
1:F:439:GLN:O	1:F:443:ILE:HG13	2.14	0.47
1:B:79:LEU:HD23	1:B:179:ALA:HB3	1.96	0.47
1:E:249:VAL:CG2	1:E:331:SER:HB3	2.44	0.47
1:A:100:GLU:O	1:A:121:SER:HB3	2.15	0.47
1:A:245:HIS:CD2	1:A:247:ASN:HB2	2.49	0.47
1:B:181:ASP:O	1:B:185:ARG:HG2	2.15	0.47
1:B:360:GLU:O	1:B:362:LYS:N	2.48	0.47
1:C:155:HIS:HE1	1:C:161:ASP:OD2	1.98	0.47
1:E:278:LEU:O	1:E:279:ARG:O	2.32	0.47
1:A:41:VAL:HB	1:A:48:TYR:CE2	2.49	0.47
1:B:108:GLU:HG2	1:B:116:TYR:HE2	1.78	0.47
1:D:303:GLU:OE1	1:D:437:ARG:HD3	2.15	0.47
1:F:96:LEU:HD22	1:F:103:LEU:CD2	2.41	0.47
1:A:51:LYS:HA	1:A:56:ARG:O	2.14	0.47
1:B:89:ARG:O	1:B:92:ALA:HB3	2.15	0.47
1:B:97:TYR:CD1	1:B:97:TYR:C	2.90	0.47
1:B:219:VAL:HG23	1:B:252:LEU:HD22	1.97	0.47
1:D:87:ILE:O	1:D:87:ILE:HG13	2.14	0.47
1:D:191:ASN:HD21	1:D:193:LYS:CE	2.27	0.47
1:E:302:MET:HE3	1:E:330:VAL:HG21	1.95	0.47
1:F:90:GLU:O	1:F:94:ARG:HG3	2.14	0.47
1:B:105:LEU:C	1:B:105:LEU:CD1	2.86	0.47
1:C:203:LYS:HB3	1:C:203:LYS:HZ3	1.80	0.47
1:C:303:GLU:OE2	1:C:437:ARG:NH1	2.48	0.47
1:E:74:GLY:C	1:E:76:LYS:N	2.73	0.47
1:F:278:LEU:HA	1:F:286:LEU:HD11	1.97	0.47
1:F:286:LEU:HB2	1:F:382:PHE:CE2	2.50	0.47
1:B:132:MET:HE1	2:B:470:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ILE:HG22	1:B:225:LYS:N	2.29	0.47
1:B:277:TYR:O	1:B:281:ARG:HG2	2.15	0.47
1:D:429:THR:HG22	1:D:429:THR:O	2.14	0.47
1:A:104:PHE:HB3	1:A:167:LEU:HD22	1.96	0.47
1:B:336:THR:O	1:B:337:LYS:HB2	2.15	0.47
1:D:181:ASP:O	1:D:185:ARG:HG3	2.15	0.47
1:F:373:GLY:HA2	1:F:376:LEU:HB2	1.96	0.47
1:C:20:PHE:CZ	1:C:22:GLY:HA2	2.50	0.46
1:C:352:TRP:CZ2	1:C:386:PRO:HG2	2.50	0.46
1:C:388:PRO:O	1:C:389:ARG:HG3	2.15	0.46
1:C:443:ILE:HG23	1:C:448:LEU:HB2	1.97	0.46
1:D:414:ALA:O	1:D:417:ASP:HB2	2.15	0.46
1:E:432:THR:HG23	1:E:434:LEU:N	2.30	0.46
1:F:275:VAL:HG23	1:F:317:ALA:CB	2.45	0.46
1:A:266:THR:HG22	1:A:267:GLU:O	2.15	0.46
1:B:133:TYR:CZ	1:B:228:ALA:HB2	2.50	0.46
1:F:160:ALA:HB2	1:F:166:ARG:N	2.30	0.46
1:B:159:ASP:OD1	1:B:161:ASP:N	2.48	0.46
1:C:396:VAL:HG12	1:C:400:GLU:OE1	2.15	0.46
1:D:283:ARG:HG2	2:D:522:HOH:O	2.14	0.46
1:E:79:LEU:CD2	1:E:180:GLN:HE21	2.27	0.46
1:E:302:MET:HB3	1:E:433:PHE:CE1	2.49	0.46
1:F:211:LEU:HG	1:F:212:GLY:N	2.31	0.46
1:A:123:GLU:C	1:A:125:LYS:N	2.72	0.46
1:B:205:GLU:HB2	1:B:206:PHE:CD1	2.51	0.46
1:F:447:GLU:C	1:F:449:HIS:N	2.73	0.46
1:A:76:LYS:HD3	1:A:76:LYS:N	2.29	0.46
1:C:81:PRO:HB3	1:C:172:VAL:HG13	1.97	0.46
1:C:112:TYR:HB3	1:C:113:PRO:CD	2.32	0.46
1:D:119:CYS:HA	1:D:127:GLU:O	2.15	0.46
1:A:76:LYS:HG2	1:A:177:VAL:HG23	1.96	0.46
1:B:152:LEU:HD23	1:B:152:LEU:C	2.41	0.46
1:B:435:GLN:HE21	1:C:308:ASN:HD22	1.61	0.46
1:C:367:SER:O	1:C:370:TRP:HB3	2.16	0.46
1:D:152:LEU:C	1:D:152:LEU:HD23	2.40	0.46
1:E:77:LEU:HD11	1:E:179:ALA:HA	1.97	0.46
1:E:388:PRO:O	1:E:389:ARG:HB2	2.14	0.46
1:F:244:ARG:HG3	1:F:250:GLN:OE1	2.16	0.46
1:A:148:ASN:HD22	1:A:148:ASN:C	2.24	0.46
1:A:292:LEU:HD21	1:A:444:ARG:HB2	1.97	0.46
1:C:200:THR:HA	1:C:210:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:GLY:O	1:E:288:GLY:C	2.58	0.46
1:E:432:THR:HB	1:E:435:GLN:OE1	2.15	0.46
1:D:47:TRP:CZ3	1:D:61:PRO:HB3	2.51	0.46
1:D:146:PHE:HA	1:D:151:GLN:OE1	2.15	0.46
1:D:155:HIS:HE1	1:D:161:ASP:OD2	1.96	0.46
1:D:387:TYR:HB3	1:D:390:ILE:CG2	2.45	0.46
1:F:219:VAL:CG2	1:F:266:THR:O	2.64	0.46
1:F:229:THR:OG1	1:F:231:GLN:HG3	2.16	0.46
1:D:191:ASN:OD1	1:D:193:LYS:HB2	2.16	0.46
1:F:109:SER:CB	1:F:115:ASP:C	2.88	0.46
1:C:110:THR:C	1:C:112:TYR:N	2.73	0.45
1:C:394:ASP:C	1:C:397:PRO:HD2	2.41	0.45
1:F:234:LEU:O	1:F:235:ALA:C	2.59	0.45
1:D:356:GLU:OE2	1:D:430:ARG:NH2	2.32	0.45
1:D:434:LEU:C	1:D:434:LEU:HD23	2.41	0.45
1:E:75:THR:HG22	1:E:75:THR:O	2.16	0.45
1:E:391:PRO:CB	1:E:394:ASP:HB2	2.38	0.45
1:F:127:GLU:CG	1:F:164:CYS:SG	3.02	0.45
1:F:369:VAL:HG13	1:F:436:LEU:HD11	1.98	0.45
1:B:132:MET:O	1:B:138:LEU:HA	2.16	0.45
1:D:78:SER:HB3	1:D:176:THR:HG23	1.99	0.45
1:E:94:ARG:C	1:E:96:LEU:N	2.74	0.45
1:B:233:PHE:HZ	1:B:254:VAL:CG2	2.29	0.45
1:B:239:VAL:HG13	1:B:240:MET:N	2.31	0.45
1:B:346:GLY:O	1:B:348:LEU:HD12	2.17	0.45
1:D:132:MET:O	1:D:138:LEU:HA	2.17	0.45
1:E:201:ILE:CD1	1:E:268:TYR:HE1	2.30	0.45
1:C:112:TYR:C	1:C:112:TYR:CD2	2.93	0.45
1:C:449:HIS:CE1	1:C:450:LEU:HG	2.51	0.45
1:D:86:LYS:HG3	1:D:108:GLU:OE1	2.16	0.45
1:E:132:MET:O	1:E:138:LEU:HA	2.17	0.45
1:F:443:ILE:HG23	1:F:448:LEU:HB2	1.98	0.45
1:A:122:CYS:SG	1:A:165:THR:CG2	3.04	0.45
1:A:269:MET:HE1	1:A:329:LYS:HG3	1.97	0.45
1:D:222:LYS:HE2	1:D:233:PHE:CE2	2.51	0.45
1:E:133:TYR:CZ	1:E:228:ALA:HB2	2.52	0.45
1:A:87:ILE:HD13	1:A:95:LEU:CD1	2.47	0.45
1:B:97:TYR:HB3	1:B:98:PRO:CD	2.45	0.45
1:F:85:GLY:O	1:F:108:GLU:HB2	2.16	0.45
1:A:39:VAL:HG23	1:A:50:ALA:HA	1.99	0.45
1:C:303:GLU:CD	1:C:437:ARG:HH11	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ASP:O	1:D:228:ALA:C	2.60	0.45
1:E:381:SER:O	1:E:382:PHE:CD1	2.70	0.45
1:A:412:PRO:HB2	1:A:415:VAL:HG23	1.99	0.45
1:E:229:THR:O	1:E:229:THR:HG22	2.15	0.45
1:E:436:LEU:O	1:E:440:LEU:HG	2.17	0.45
1:F:207:GLY:HA3	1:F:223:CYS:O	2.16	0.45
1:F:240:MET:HE3	1:F:240:MET:HB2	1.84	0.45
1:B:353:THR:HG22	1:B:357:ALA:HB3	1.99	0.45
1:C:226:ASN:O	1:C:227:ASP:C	2.60	0.45
1:D:79:LEU:HD11	1:D:224:ILE:HG22	1.99	0.45
1:D:90:GLU:C	1:D:92:ALA:N	2.74	0.45
1:D:156:TYR:CD1	1:D:163:LEU:HD11	2.52	0.45
1:D:197:LEU:HD13	1:D:210:MET:HE1	1.99	0.45
1:D:340:SER:OG	1:D:341:SER:N	2.51	0.45
1:E:87:ILE:HG23	1:E:91:GLN:HB2	1.98	0.45
1:F:425:LEU:H	1:F:425:LEU:CD2	2.29	0.45
1:A:103:LEU:HA	1:A:169:LYS:O	2.17	0.44
1:A:152:LEU:C	1:A:152:LEU:HD23	2.42	0.44
1:C:407:ALA:HB2	1:C:416:TYR:CD2	2.51	0.44
1:D:141:ASP:O	1:D:143:GLU:HG3	2.17	0.44
1:E:136:SER:HB2	1:E:226:ASN:OD1	2.16	0.44
1:F:68:ARG:HD3	1:F:188:TRP:CH2	2.51	0.44
1:F:84:HIS:HD2	1:F:105:LEU:HB2	1.81	0.44
1:F:312:HIS:O	1:F:313:ARG:HB2	2.17	0.44
1:C:89:ARG:HB3	1:C:107:ARG:HH12	1.82	0.44
1:C:172:VAL:HG11	1:C:176:THR:O	2.18	0.44
1:C:302:MET:SD	1:C:315:LEU:HD12	2.56	0.44
1:E:84:HIS:N	1:E:84:HIS:CD2	2.86	0.44
1:B:86:LYS:H	1:B:86:LYS:HD2	1.82	0.44
1:B:352:TRP:HE1	1:B:378:GLU:CD	2.23	0.44
1:E:414:ALA:O	1:E:417:ASP:HB2	2.17	0.44
1:F:105:LEU:HB3	1:F:171:LYS:HB3	1.99	0.44
1:F:227:ASP:OD2	1:F:230:ALA:HA	2.16	0.44
1:F:407:ALA:HB2	1:F:416:TYR:CG	2.52	0.44
1:E:351:LYS:O	1:E:374:ILE:HD13	2.18	0.44
1:E:390:ILE:HD11	1:E:403:TYR:OH	2.18	0.44
1:F:31:CYS:O	1:F:34:ASP:HB2	2.18	0.44
1:F:122:CYS:C	1:F:124:GLY:N	2.74	0.44
1:F:195:LEU:HD23	1:F:214:TYR:HB2	1.98	0.44
1:F:219:VAL:HG23	1:F:252:LEU:HD12	1.99	0.44
1:A:43:LYS:CD	1:A:43:LYS:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:CB	1:A:167:LEU:HD22	2.47	0.44
1:B:313:ARG:CZ	1:B:363:PHE:HB2	2.48	0.44
1:D:160:ALA:HB2	1:D:166:ARG:CA	2.46	0.44
1:E:83:PHE:CZ	1:E:85:GLY:HA2	2.52	0.44
1:E:180:GLN:CD	1:E:180:GLN:H	2.25	0.44
1:F:377:TRP:O	1:F:381:SER:CB	2.65	0.44
1:A:181:ASP:HA	1:A:184:TYR:HB3	2.00	0.44
1:F:236:GLU:O	1:F:240:MET:HE3	2.17	0.44
1:F:426:ASP:O	1:F:427:ALA:C	2.61	0.44
1:A:88:THR:HG23	1:A:89:ARG:NH1	2.32	0.44
1:B:73:ALA:HB1	1:B:77:LEU:HB2	1.94	0.44
1:C:132:MET:O	1:C:138:LEU:HA	2.18	0.44
1:C:132:MET:HE1	1:C:142:GLU:HG3	2.00	0.44
1:D:54:VAL:O	1:D:54:VAL:HG13	2.17	0.44
1:F:169:LYS:HA	1:F:170:PRO:HD3	1.83	0.44
1:F:245:HIS:O	1:F:247:ASN:N	2.51	0.44
1:F:391:PRO:O	1:F:394:ASP:OD1	2.36	0.44
1:A:76:LYS:HD3	1:A:77:LEU:N	2.32	0.44
1:B:133:TYR:HD1	1:B:137:LYS:O	2.00	0.44
1:D:53:LYS:HE3	1:E:161:ASP:O	2.18	0.44
1:D:122:CYS:O	1:D:124:GLY:N	2.51	0.44
1:D:403:TYR:O	1:D:404:LYS:HD3	2.17	0.44
1:F:360:GLU:O	1:F:362:LYS:HG2	2.16	0.44
1:C:44:ASP:C	1:C:44:ASP:OD1	2.61	0.44
1:C:81:PRO:HG3	1:C:178:ALA:HA	2.00	0.44
1:E:229:THR:HG21	1:E:231:GLN:HE21	1.82	0.44
1:F:71:VAL:O	1:F:238:SER:HB2	2.18	0.44
1:F:77:LEU:HD12	1:F:177:VAL:HG13	2.00	0.44
1:F:286:LEU:HD12	1:F:382:PHE:CE2	2.53	0.44
1:A:104:PHE:CD2	1:A:167:LEU:HB3	2.52	0.43
1:B:60:ILE:O	1:B:60:ILE:HG13	2.18	0.43
1:B:391:PRO:C	1:B:393:LYS:N	2.74	0.43
1:C:89:ARG:HB2	1:C:89:ARG:NH1	2.12	0.43
1:D:103:LEU:HD22	1:D:169:LYS:O	2.18	0.43
1:D:108:GLU:HA	1:D:116:TYR:HD2	1.82	0.43
1:E:250:GLN:HG3	1:E:251:LEU:O	2.17	0.43
1:A:180:GLN:H	1:A:180:GLN:NE2	2.15	0.43
1:B:190:LEU:HD22	1:B:254:VAL:N	2.33	0.43
1:C:274:LEU:O	1:C:278:LEU:HG	2.19	0.43
1:D:89:ARG:HB3	1:D:107:ARG:CZ	2.48	0.43
1:D:235:ALA:O	1:D:238:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:LEU:HD21	1:F:120:VAL:CG2	2.47	0.43
1:C:107:ARG:HH22	1:C:111:ASN:HD22	1.65	0.43
1:C:359:ARG:C	1:C:361:LYS:H	2.25	0.43
1:E:271:LYS:CB	1:E:322:VAL:HB	2.36	0.43
1:F:393:LYS:O	1:F:393:LYS:HG2	2.17	0.43
1:F:424:HIS:O	1:F:425:LEU:C	2.61	0.43
1:A:89:ARG:HH11	1:A:110:THR:HG21	1.82	0.43
1:D:312:HIS:O	1:D:368:ASP:OD1	2.36	0.43
1:F:192:MET:O	1:F:192:MET:HG3	2.17	0.43
1:F:197:LEU:HD13	1:F:210:MET:HE1	2.01	0.43
1:F:330:VAL:HG12	1:F:331:SER:N	2.33	0.43
1:A:229:THR:O	1:A:230:ALA:HB3	2.19	0.43
1:B:13:GLU:OE2	1:B:244:ARG:NH2	2.50	0.43
1:B:390:ILE:HA	1:B:391:PRO:HD3	1.88	0.43
1:E:97:TYR:O	1:E:99:PRO:HD3	2.18	0.43
1:E:438:GLU:O	1:E:439:GLN:C	2.60	0.43
1:F:229:THR:O	1:F:230:ALA:HB3	2.19	0.43
1:F:269:MET:CG	1:F:321:LEU:HD23	2.48	0.43
1:A:353:THR:HG22	1:A:357:ALA:HB3	2.01	0.43
1:C:257:GLU:HB3	1:C:260:GLY:O	2.19	0.43
1:C:315:LEU:CD2	1:C:375:LEU:HD23	2.48	0.43
1:D:41:VAL:HG22	1:D:42:THR:N	2.33	0.43
1:E:103:LEU:HA	1:E:169:LYS:O	2.17	0.43
1:E:255:ILE:HB	1:E:263:TYR:HB2	2.00	0.43
1:E:339:ALA:O	1:E:340:SER:C	2.62	0.43
1:F:274:LEU:HD12	1:F:317:ALA:CB	2.48	0.43
1:A:443:ILE:HG23	1:A:448:LEU:HB2	2.00	0.43
1:B:434:LEU:C	1:B:434:LEU:HD23	2.43	0.43
1:E:208:ASP:OD1	1:E:225:LYS:HE3	2.19	0.43
1:F:336:THR:C	1:F:337:LYS:HG3	2.44	0.43
1:C:338:GLU:O	1:C:339:ALA:C	2.62	0.43
1:E:283:ARG:O	1:E:285:VAL:HG23	2.19	0.43
1:F:150:MET:CE	1:F:262:LEU:HD21	2.49	0.43
1:F:386:PRO:C	1:F:387:TYR:CD1	2.97	0.43
1:A:163:LEU:HD23	1:B:54:VAL:HG21	2.01	0.43
1:A:200:THR:HG21	1:A:203:LYS:HG3	2.00	0.43
1:B:292:LEU:HD22	1:B:449:HIS:CG	2.54	0.43
1:D:39:VAL:HG23	1:D:50:ALA:HA	2.00	0.43
1:D:61:PRO:HG2	1:D:64:TYR:HB2	2.00	0.43
1:D:156:TYR:HB3	1:D:163:LEU:CD1	2.48	0.43
1:D:245:HIS:CD2	1:D:247:ASN:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:SER:HB2	1:F:116:TYR:N	2.34	0.43
1:F:206:PHE:CD1	1:F:206:PHE:N	2.87	0.43
1:F:387:TYR:CB	1:F:390:ILE:HD12	2.49	0.43
1:B:79:LEU:CD2	1:B:179:ALA:HB3	2.49	0.43
1:C:286:LEU:HD22	1:C:290:CYS:SG	2.59	0.43
1:E:286:LEU:HD11	1:E:382:PHE:HE2	1.84	0.43
1:E:375:LEU:HD23	1:E:375:LEU:O	2.19	0.43
1:F:104:PHE:CE2	1:F:167:LEU:HB3	2.54	0.43
1:F:201:ILE:HD11	1:F:211:LEU:HB2	2.00	0.43
1:A:97:TYR:O	1:A:99:PRO:HD3	2.20	0.42
1:B:23:THR:N	1:B:27:ASP:OD2	2.43	0.42
1:B:112:TYR:CE2	1:B:130:ARG:HD2	2.54	0.42
1:C:375:LEU:CD1	1:C:375:LEU:C	2.92	0.42
1:E:122:CYS:O	1:E:123:GLU:C	2.62	0.42
1:E:396:VAL:O	1:E:400:GLU:HG3	2.19	0.42
1:F:158:THR:HG22	1:F:158:THR:O	2.18	0.42
1:F:429:THR:O	1:F:429:THR:HG22	2.18	0.42
1:E:125:LYS:HG2	1:E:126:VAL:N	2.33	0.42
1:E:380:TYR:C	1:E:381:SER:O	2.61	0.42
1:F:152:LEU:C	1:F:152:LEU:CD2	2.91	0.42
1:F:269:MET:HB2	1:F:321:LEU:HD23	1.99	0.42
1:A:136:SER:O	1:A:137:LYS:HD3	2.19	0.42
1:B:387:TYR:N	1:B:388:PRO:HD3	2.35	0.42
1:C:125:LYS:HE2	1:C:126:VAL:CG2	2.32	0.42
1:C:375:LEU:C	1:C:375:LEU:HD13	2.44	0.42
1:D:227:ASP:O	1:D:229:THR:N	2.53	0.42
1:E:77:LEU:HD12	1:E:177:VAL:HG13	2.01	0.42
1:F:109:SER:O	1:F:113:PRO:HA	2.18	0.42
1:A:74:GLY:HA3	1:A:76:LYS:NZ	2.35	0.42
1:C:95:LEU:O	1:C:96:LEU:HD12	2.20	0.42
1:C:107:ARG:NH2	1:C:109:SER:OG	2.49	0.42
1:D:126:VAL:O	1:D:126:VAL:HG23	2.19	0.42
1:F:392:LEU:H	1:F:392:LEU:CD2	2.27	0.42
1:F:407:ALA:HB2	1:F:416:TYR:CD1	2.54	0.42
1:A:138:LEU:CD2	1:A:149:LEU:HD23	2.49	0.42
1:B:313:ARG:O	1:B:348:LEU:HD23	2.19	0.42
1:B:369:VAL:O	1:B:372:PHE:O	2.37	0.42
1:D:377:TRP:CE2	1:D:405:MET:SD	3.13	0.42
1:E:239:VAL:HG11	1:E:336:THR:HG22	2.02	0.42
1:F:188:TRP:NE1	1:F:241:THR:HB	2.34	0.42
1:A:407:ALA:HB2	1:A:416:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ARG:HG2	1:E:244:ARG:HH11	1.84	0.42
1:F:79:LEU:CD2	1:F:179:ALA:HB3	2.50	0.42
1:F:122:CYS:O	1:F:123:GLU:C	2.62	0.42
1:A:122:CYS:SG	1:A:164:CYS:C	3.02	0.42
1:B:80:MET:HB3	1:B:82:TRP:CZ3	2.55	0.42
1:C:26:GLN:HG2	2:C:467:HOH:O	2.19	0.42
1:C:97:TYR:O	1:C:99:PRO:CD	2.66	0.42
1:E:279:ARG:O	1:E:281:ARG:N	2.52	0.42
1:F:61:PRO:HG2	1:F:64:TYR:HB2	2.01	0.42
1:F:357:ALA:O	1:F:361:LYS:HA	2.19	0.42
1:A:82:TRP:HB3	1:A:170:PRO:HB3	2.02	0.42
1:A:227:ASP:OD2	1:A:230:ALA:HA	2.19	0.42
1:B:8:TRP:HA	1:B:9:PRO:HD3	1.85	0.42
1:B:447:GLU:HG2	1:B:450:LEU:HD12	2.01	0.42
1:C:9:PRO:O	1:C:12:THR:OG1	2.36	0.42
1:D:229:THR:O	1:D:230:ALA:C	2.62	0.42
1:F:80:MET:HE1	1:F:229:THR:HA	2.02	0.42
1:F:156:TYR:O	1:F:167:LEU:HG	2.20	0.42
1:F:419:MET:HB3	1:F:423:TRP:CH2	2.54	0.42
1:F:425:LEU:HD22	1:F:425:LEU:N	2.34	0.42
1:A:338:GLU:O	1:A:340:SER:N	2.52	0.42
1:B:245:HIS:CD2	1:B:247:ASN:HB2	2.54	0.42
1:C:89:ARG:HB3	1:C:107:ARG:NH1	2.35	0.42
1:D:31:CYS:SG	2:D:492:HOH:O	2.28	0.42
1:D:172:VAL:HG11	1:D:176:THR:O	2.20	0.42
1:D:208:ASP:O	1:D:222:LYS:HA	2.20	0.42
1:D:275:VAL:HG22	1:D:317:ALA:CB	2.50	0.42
1:D:383:GLY:O	1:D:384:ARG:C	2.62	0.42
1:F:387:TYR:CD1	1:F:387:TYR:N	2.88	0.42
1:B:101:THR:O	1:B:168:ILE:HD12	2.20	0.42
1:C:403:TYR:O	1:C:404:LYS:HD3	2.19	0.42
1:F:208:ASP:O	1:F:222:LYS:HA	2.19	0.42
1:D:173:MET:HG3	1:D:174:GLU:H	1.84	0.41
1:E:439:GLN:HA	2:E:471:HOH:O	2.20	0.41
1:F:27:ASP:O	1:F:29:PRO:HD3	2.20	0.41
1:F:274:LEU:CD1	1:F:278:LEU:HD11	2.50	0.41
1:C:97:TYR:CD1	1:C:98:PRO:HD3	2.55	0.41
1:D:96:LEU:HG	1:D:103:LEU:CD1	2.48	0.41
1:D:173:MET:CG	1:D:174:GLU:N	2.83	0.41
1:E:286:LEU:CD1	1:E:286:LEU:O	2.68	0.41
1:F:89:ARG:NH2	1:F:110:THR:HB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:GLU:HG2	1:F:240:MET:HE1	2.02	0.41
1:F:306:GLU:OE2	1:F:365:THR:HG21	2.20	0.41
1:B:429:THR:HG22	1:B:429:THR:O	2.21	0.41
1:D:44:ASP:HA	1:D:45:PRO:HD3	1.87	0.41
1:D:159:ASP:O	1:D:160:ALA:HB3	2.20	0.41
1:D:255:ILE:HB	1:D:263:TYR:HB2	2.02	0.41
1:F:77:LEU:HA	1:F:177:VAL:CG1	2.49	0.41
1:B:28:LEU:HB2	1:B:58:GLY:HA3	2.02	0.41
1:B:245:HIS:HD2	1:B:247:ASN:N	2.09	0.41
1:C:8:TRP:HA	1:C:9:PRO:HD3	1.95	0.41
1:F:28:LEU:HB2	1:F:58:GLY:CA	2.44	0.41
1:F:215:ARG:HG2	1:F:215:ARG:HH11	1.84	0.41
1:A:81:PRO:HA	1:A:176:THR:HG21	2.02	0.41
1:B:399:VAL:O	1:B:402:GLY:N	2.53	0.41
1:C:209:VAL:HA	1:C:221:VAL:O	2.20	0.41
1:E:348:LEU:N	1:E:349:PRO:HD3	2.35	0.41
1:F:374:ILE:HG13	1:F:423:TRP:HE1	1.86	0.41
1:A:140:ILE:CG2	1:B:54:VAL:HG22	2.50	0.41
1:B:111:ASN:O	1:B:113:PRO:HD3	2.20	0.41
1:D:353:THR:HG22	1:D:357:ALA:HB3	2.02	0.41
1:E:229:THR:CG2	1:E:231:GLN:HG3	2.50	0.41
1:F:201:ILE:HD11	1:F:211:LEU:CA	2.49	0.41
1:A:283:ARG:N	1:A:283:ARG:CD	2.83	0.41
1:A:338:GLU:O	1:A:339:ALA:C	2.63	0.41
1:D:104:PHE:CG	1:D:167:LEU:HD22	2.56	0.41
1:E:15:ILE:O	1:E:15:ILE:HG23	2.20	0.41
1:E:193:LYS:H	1:E:193:LYS:CD	2.33	0.41
1:E:390:ILE:HA	1:E:391:PRO:HD3	1.88	0.41
1:A:348:LEU:HD13	1:A:363:PHE:CE1	2.55	0.41
1:D:225:LYS:O	1:D:230:ALA:HB2	2.20	0.41
1:D:390:ILE:HA	1:D:391:PRO:HD3	1.90	0.41
1:B:47:TRP:HE3	1:B:59:ILE:HG22	1.85	0.41
1:C:184:TYR:CZ	1:C:256:VAL:HG23	2.56	0.41
1:C:275:VAL:HG22	1:C:317:ALA:CB	2.49	0.41
1:D:103:LEU:HD13	1:D:103:LEU:C	2.46	0.41
1:D:203:LYS:O	1:D:204:GLY:O	2.39	0.41
1:D:225:LYS:C	1:D:227:ASP:N	2.78	0.41
1:D:267:GLU:OE2	1:D:329:LYS:NZ	2.51	0.41
1:E:94:ARG:C	1:E:96:LEU:H	2.28	0.41
1:F:83:PHE:CE2	1:F:85:GLY:HA2	2.56	0.41
1:F:148:ASN:HD22	1:F:150:MET:N	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HD13	1:B:149:LEU:HD23	2.03	0.41
1:D:79:LEU:CD1	1:D:224:ILE:HG22	2.51	0.41
1:D:275:VAL:HG23	1:D:318:ARG:HA	2.03	0.41
1:F:14:CYS:HB3	1:F:65:VAL:HB	2.03	0.41
1:B:54:VAL:O	1:B:54:VAL:HG13	2.21	0.40
1:C:156:TYR:HB3	1:C:163:LEU:HD11	2.02	0.40
1:C:281:ARG:NH1	2:C:487:HOH:O	2.35	0.40
1:C:312:HIS:HD2	1:C:315:LEU:N	2.19	0.40
1:C:396:VAL:HG23	2:C:511:HOH:O	2.19	0.40
1:E:178:ALA:HB1	1:E:180:GLN:OE1	2.22	0.40
1:F:373:GLY:O	1:F:376:LEU:HB2	2.21	0.40
1:A:84:HIS:ND1	1:A:87:ILE:HD12	2.37	0.40
1:C:214:TYR:O	1:C:215:ARG:C	2.64	0.40
1:D:151:GLN:HB3	2:D:515:HOH:O	2.22	0.40
1:E:354:ALA:HA	1:E:355:PRO:HD3	1.98	0.40
1:E:443:ILE:O	1:E:446:HIS:O	2.39	0.40
1:F:391:PRO:C	1:F:393:LYS:H	2.29	0.40
1:A:245:HIS:HD2	1:A:247:ASN:HB2	1.85	0.40
1:A:429:THR:O	1:A:429:THR:HG22	2.20	0.40
1:B:356:GLU:H	1:B:356:GLU:HG3	1.55	0.40
1:E:169:LYS:HA	1:E:170:PRO:HD3	1.78	0.40
1:E:181:ASP:OD1	1:E:185:ARG:NH1	2.54	0.40
1:E:337:LYS:HG3	1:E:338:GLU:H	1.87	0.40
1:F:101:THR:HB	1:F:165:THR:HG21	2.02	0.40
1:F:225:LYS:O	1:F:226:ASN:C	2.64	0.40
1:F:262:LEU:C	1:F:263:TYR:CD2	2.99	0.40
1:A:148:ASN:ND2	1:A:148:ASN:C	2.79	0.40
1:B:90:GLU:O	1:B:93:GLU:HB2	2.22	0.40
1:B:106:VAL:HG11	1:B:149:LEU:HD13	2.02	0.40
1:E:79:LEU:HD23	1:E:180:GLN:HE21	1.81	0.40
1:E:168:ILE:HG22	1:E:169:LYS:N	2.36	0.40
1:E:314:ASP:OD1	1:E:319:ASN:ND2	2.54	0.40
1:E:397:PRO:O	1:E:401:LYS:HG3	2.20	0.40
1:C:176:THR:HG22	1:C:177:VAL:N	2.35	0.40
1:C:208:ASP:OD1	1:C:209:VAL:HG13	2.21	0.40
1:D:399:VAL:C	1:D:401:LYS:H	2.30	0.40
1:F:248:LEU:HD23	1:F:330:VAL:HB	2.03	0.40
1:F:292:LEU:HD21	1:F:444:ARG:CB	2.47	0.40
1:F:296:LEU:HD23	1:F:296:LEU:HA	1.92	0.40
1:F:387:TYR:HB3	1:F:390:ILE:HD12	2.03	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	435/450 (97%)	403 (93%)	29 (7%)	3 (1%)	18	34
1	B	437/450 (97%)	405 (93%)	23 (5%)	9 (2%)	5	9
1	C	434/450 (96%)	386 (89%)	43 (10%)	5 (1%)	10	20
1	D	427/450 (95%)	376 (88%)	39 (9%)	12 (3%)	4	6
1	E	436/450 (97%)	388 (89%)	33 (8%)	15 (3%)	3	4
1	F	432/450 (96%)	351 (81%)	63 (15%)	18 (4%)	2	2
All	All	2601/2700 (96%)	2309 (89%)	230 (9%)	62 (2%)	4	8

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	112	TYR
1	D	123	GLU
1	D	204	GLY
1	D	228	ALA
1	D	230	ALA
1	E	279	ARG
1	F	359	ARG
1	F	361	LYS
1	A	339	ALA
1	A	395	VAL
1	B	75	THR
1	B	347	LYS
1	B	361	LYS
1	C	123	GLU
1	D	282	GLY
1	D	395	VAL
1	E	110	THR
1	E	174	GLU
1	E	280	SER
1	E	288	GLY

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Mol	Chain	Res	Type
1	E	340	SER
1	E	341	SER
1	E	360	GLU
1	F	101	THR
1	F	109	SER
1	F	161	ASP
1	F	174	GLU
1	F	204	GLY
1	F	246	SER
1	F	392	LEU
1	B	97	TYR
1	B	338	GLU
1	C	113	PRO
1	C	158	THR
1	D	84	HIS
1	D	99	PRO
1	F	99	PRO
1	F	391	PRO
1	A	282	GLY
1	B	73	ALA
1	B	178	ALA
1	D	160	ALA
1	D	259	LYS
1	E	359	ARG
1	E	392	LEU
1	F	125	LYS
1	F	405	MET
1	B	395	VAL
1	C	99	PRO
1	D	226	ASN
1	D	313	ARG
1	E	161	ASP
1	E	281	ARG
1	E	282	GLY
1	E	349	PRO
1	B	199	GLN
1	F	54	VAL
1	F	107	ARG
1	F	168	ILE
1	F	113	PRO
1	E	98	PRO
1	F	408	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	376/385 (98%)	355 (94%)	21 (6%)	19	39
1	B	377/385 (98%)	357 (95%)	20 (5%)	20	42
1	C	375/385 (97%)	361 (96%)	14 (4%)	30	57
1	D	371/385 (96%)	353 (95%)	18 (5%)	22	45
1	E	377/385 (98%)	362 (96%)	15 (4%)	28	54
1	F	373/385 (97%)	357 (96%)	16 (4%)	26	51
All	All	2249/2310 (97%)	2145 (95%)	104 (5%)	24	48

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	43	LYS
1	A	76	LYS
1	A	90	GLU
1	A	111	ASN
1	A	118	LEU
1	A	138	LEU
1	A	148	ASN
1	A	180	GLN
1	A	195	LEU
1	A	219	VAL
1	A	254	VAL
1	A	259	LYS
1	A	266	THR
1	A	283	ARG
1	A	338	GLU
1	A	347	LYS
1	A	356	GLU
1	A	367	SER
1	A	396	VAL
1	A	432	THR
1	B	54	VAL

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Mol	Chain	Res	Type
1	B	56	ARG
1	B	66	GLN
1	B	72	LYS
1	B	75	THR
1	B	86	LYS
1	B	87	ILE
1	B	132	MET
1	B	180	GLN
1	B	190	LEU
1	B	193	LYS
1	B	195	LEU
1	B	205	GLU
1	B	206	PHE
1	B	234	LEU
1	B	326	ASN
1	B	335	LEU
1	B	337	LYS
1	B	356	GLU
1	B	437	ARG
1	C	89	ARG
1	C	125	LYS
1	C	163	LEU
1	C	195	LEU
1	C	203	LYS
1	C	222	LYS
1	C	281	ARG
1	C	283	ARG
1	C	289	ASP
1	C	356	GLU
1	C	367	SER
1	C	375	LEU
1	C	385	VAL
1	C	398	ARG
1	D	54	VAL
1	D	89	ARG
1	D	105	LEU
1	D	144	VAL
1	D	181	ASP
1	D	195	LEU
1	D	203	LYS
1	D	217	ASN
1	D	227	ASP

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Mol	Chain	Res	Type
1	D	254	VAL
1	D	267	GLU
1	D	275	VAL
1	D	284	SER
1	D	315	LEU
1	D	356	GLU
1	D	390	ILE
1	D	393	LYS
1	D	398	ARG
1	E	25	GLU
1	E	86	LYS
1	E	132	MET
1	E	138	LEU
1	E	144	VAL
1	E	150	MET
1	E	172	VAL
1	E	176	THR
1	E	234	LEU
1	E	239	VAL
1	E	286	LEU
1	E	376	LEU
1	E	394	ASP
1	E	404	LYS
1	E	432	THR
1	F	34	ASP
1	F	82	TRP
1	F	123	GLU
1	F	146	PHE
1	F	164	CYS
1	F	165	THR
1	F	194	GLU
1	F	205	GLU
1	F	206	PHE
1	F	223	CYS
1	F	244	ARG
1	F	258	GLU
1	F	356	GLU
1	F	368	ASP
1	F	392	LEU
1	F	420	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	148	ASN
1	A	180	GLN
1	A	199	GLN
1	A	226	ASN
1	A	245	HIS
1	A	247	ASN
1	A	326	ASN
1	B	63	ASN
1	B	191	ASN
1	B	231	GLN
1	B	245	HIS
1	B	247	ASN
1	B	326	ASN
1	B	424	HIS
1	C	91	GLN
1	C	111	ASN
1	C	155	HIS
1	C	191	ASN
1	C	245	HIS
1	C	308	ASN
1	C	312	HIS
1	C	446	HIS
1	D	91	GLN
1	D	245	HIS
1	D	247	ASN
1	D	308	ASN
1	D	312	HIS
1	D	326	ASN
1	D	442	HIS
1	D	446	HIS
1	E	63	ASN
1	E	134	HIS
1	E	180	GLN
1	E	191	ASN
1	E	231	GLN
1	E	247	ASN
1	E	250	GLN
1	E	326	ASN
1	F	84	HIS
1	F	148	ASN
1	F	191	ASN
1	F	226	ASN

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Mol	Chain	Res	Type
1	F	242	GLN
1	F	247	ASN
1	F	309	ASN
1	F	319	ASN
1	F	421	ASN
1	F	424	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	439/450 (97%)	0.36	30 (6%)	23 20	23, 45, 79, 100	0
1	B	441/450 (98%)	0.45	37 (8%)	17 15	29, 48, 78, 95	0
1	C	438/450 (97%)	0.71	56 (12%)	7 6	31, 52, 111, 124	0
1	D	433/450 (96%)	0.61	57 (13%)	7 6	24, 50, 101, 118	0
1	E	440/450 (97%)	0.93	66 (15%)	5 4	31, 58, 91, 107	0
1	F	436/450 (96%)	1.87	186 (42%)	0 0	40, 74, 118, 136	0
All	All	2627/2700 (97%)	0.82	432 (16%)	4 3	23, 54, 103, 136	0

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	352	TRP	6.9
1	F	350	VAL	6.7
1	F	390	ILE	6.4
1	A	122	CYS	6.2
1	E	348	LEU	5.8
1	F	121	SER	5.8
1	B	339	ALA	5.7
1	F	387	TYR	5.5
1	F	114	GLY	5.5
1	D	126	VAL	5.4
1	F	392	LEU	5.3
1	B	346	GLY	5.1
1	F	190	LEU	5.0
1	F	192	MET	4.9
1	E	342	THR	4.8
1	F	103	LEU	4.7
1	F	97	TYR	4.7
1	F	383	GLY	4.6
1	B	4	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	122	CYS	4.5
1	C	168	ILE	4.5
1	F	98	PRO	4.4
1	F	361	LYS	4.4
1	C	165	THR	4.4
1	F	88	THR	4.4
1	C	260	GLY	4.4
1	B	73	ALA	4.4
1	D	98	PRO	4.3
1	F	349	PRO	4.3
1	E	75	THR	4.3
1	F	193	LYS	4.3
1	E	98	PRO	4.3
1	B	74	GLY	4.3
1	B	110	THR	4.2
1	F	195	LEU	4.2
1	F	339	ALA	4.2
1	C	121	SER	4.2
1	F	125	LYS	4.2
1	F	136	SER	4.2
1	F	386	PRO	4.1
1	B	75	THR	4.1
1	F	184	TYR	4.0
1	C	112	TYR	4.0
1	C	111	ASN	4.0
1	C	99	PRO	4.0
1	E	285	VAL	4.0
1	F	191	ASN	3.9
1	E	110	THR	3.9
1	C	126	VAL	3.9
1	D	120	VAL	3.9
1	F	388	PRO	3.9
1	D	105	LEU	3.9
1	F	278	LEU	3.9
1	F	112	TYR	3.8
1	F	95	LEU	3.8
1	C	122	CYS	3.8
1	D	122	CYS	3.8
1	F	99	PRO	3.8
1	A	111	ASN	3.8
1	F	395	VAL	3.8
1	F	87	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	110	THR	3.7
1	F	382	PHE	3.7
1	F	126	VAL	3.7
1	C	115	ASP	3.7
1	E	282	GLY	3.6
1	D	99	PRO	3.6
1	F	75	THR	3.6
1	C	113	PRO	3.6
1	A	75	THR	3.6
1	F	351	LYS	3.5
1	F	404	LYS	3.5
1	C	120	VAL	3.5
1	C	96	LEU	3.5
1	C	105	LEU	3.5
1	F	358	LEU	3.5
1	A	87	ILE	3.5
1	F	170	PRO	3.5
1	B	360	GLU	3.5
1	C	106	VAL	3.5
1	F	101	THR	3.5
1	E	392	LEU	3.5
1	F	379	ILE	3.5
1	F	378	GLU	3.5
1	F	223	CYS	3.5
1	C	118	LEU	3.5
1	D	130	ARG	3.5
1	F	335	LEU	3.5
1	A	124	GLY	3.5
1	C	349	PRO	3.4
1	B	359	ARG	3.4
1	A	96	LEU	3.4
1	F	197	LEU	3.4
1	F	362	LYS	3.4
1	F	128	HIS	3.4
1	F	380	TYR	3.4
1	F	81	PRO	3.4
1	E	325	ASP	3.4
1	F	172	VAL	3.4
1	A	347	LYS	3.3
1	F	82	TRP	3.3
1	F	336	THR	3.3
1	E	288	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	95	LEU	3.3
1	D	97	TYR	3.3
1	D	96	LEU	3.3
1	F	376	LEU	3.3
1	F	111	ASN	3.3
1	C	170	PRO	3.3
1	A	340	SER	3.2
1	A	112	TYR	3.2
1	F	84	HIS	3.2
1	F	353	THR	3.2
1	E	95	LEU	3.2
1	E	97	TYR	3.2
1	F	396	VAL	3.2
1	C	85	GLY	3.2
1	D	342	THR	3.2
1	F	232	ALA	3.2
1	D	95	LEU	3.2
1	E	278	LEU	3.2
1	F	391	PRO	3.2
1	F	96	LEU	3.2
1	B	164	CYS	3.1
1	D	228	ALA	3.1
1	F	274	LEU	3.1
1	A	101	THR	3.1
1	E	384	ARG	3.1
1	F	407	ALA	3.1
1	E	281	ARG	3.1
1	F	130	ARG	3.1
1	F	212	GLY	3.1
1	C	160	ALA	3.1
1	B	348	LEU	3.1
1	D	167	LEU	3.1
1	E	286	LEU	3.1
1	F	118	LEU	3.1
1	B	257	GLU	3.0
1	E	83	PHE	3.0
1	F	74	GLY	3.0
1	D	127	GLU	3.0
1	A	86	LYS	3.0
1	F	104	PHE	3.0
1	F	140	ILE	2.9
1	F	168	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	370	TRP	2.9
1	F	198	LEU	2.9
1	F	83	PHE	2.9
1	A	109	SER	2.9
1	E	339	ALA	2.9
1	F	178	ALA	2.9
1	E	362	LYS	2.9
1	E	448	LEU	2.9
1	E	450	LEU	2.9
1	D	121	SER	2.9
1	E	280	SER	2.9
1	C	90	GLU	2.9
1	F	194	GLU	2.9
1	F	200	THR	2.9
1	E	122	CYS	2.9
1	F	375	LEU	2.9
1	D	173	MET	2.9
1	F	202	GLY	2.9
1	C	259	LYS	2.8
1	F	201	ILE	2.8
1	E	172	VAL	2.8
1	D	160	ALA	2.8
1	F	79	LEU	2.8
1	C	93	GLU	2.8
1	E	277	TYR	2.8
1	E	284	SER	2.8
1	F	132	MET	2.8
1	F	86	LYS	2.8
1	F	89	ARG	2.8
1	F	146	PHE	2.8
1	A	74	GLY	2.8
1	D	390	ILE	2.8
1	F	106	VAL	2.8
1	F	176	THR	2.8
1	D	128	HIS	2.8
1	B	349	PRO	2.8
1	D	106	VAL	2.8
1	C	125	LYS	2.8
1	F	76	LYS	2.8
1	F	215	ARG	2.8
1	D	260	GLY	2.7
1	D	168	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	377	TRP	2.7
1	F	331	SER	2.7
1	C	348	LEU	2.7
1	D	118	LEU	2.7
1	F	138	LEU	2.7
1	F	107	ARG	2.7
1	F	85	GLY	2.7
1	E	391	PRO	2.7
1	A	133	TYR	2.7
1	F	275	VAL	2.7
1	B	361	LYS	2.7
1	F	173	MET	2.7
1	F	316	ALA	2.7
1	D	119	CYS	2.7
1	E	87	ILE	2.7
1	B	98	PRO	2.7
1	F	105	LEU	2.7
1	F	414	ALA	2.7
1	D	227	ASP	2.7
1	E	382	PHE	2.7
1	C	167	LEU	2.7
1	F	283	ARG	2.7
1	F	389	ARG	2.7
1	D	88	THR	2.7
1	F	428	ALA	2.7
1	E	449	HIS	2.7
1	E	293	LYS	2.6
1	A	110	THR	2.6
1	F	393	LYS	2.6
1	A	95	LEU	2.6
1	D	392	LEU	2.6
1	F	209	VAL	2.6
1	E	340	SER	2.6
1	C	128	HIS	2.6
1	A	114	GLY	2.6
1	F	162	GLY	2.6
1	F	313	ARG	2.6
1	F	363	PHE	2.6
1	F	57	GLU	2.6
1	F	315	LEU	2.6
1	E	226	ASN	2.6
1	F	422	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	273	SER	2.6
1	C	101	THR	2.6
1	D	92	ALA	2.6
1	A	97	TYR	2.6
1	B	393	LYS	2.6
1	C	114	GLY	2.6
1	F	159	ASP	2.6
1	F	443	ILE	2.6
1	E	123	GLU	2.6
1	F	147	GLU	2.6
1	B	97	TYR	2.6
1	F	423	TRP	2.5
1	C	124	GLY	2.5
1	C	261	GLY	2.5
1	E	261	GLY	2.5
1	F	102	GLY	2.5
1	F	254	VAL	2.5
1	C	134	HIS	2.5
1	D	171	LYS	2.5
1	E	341	SER	2.5
1	F	354	ALA	2.5
1	D	124	GLY	2.5
1	F	175	GLY	2.5
1	F	410	GLY	2.5
1	F	224	ILE	2.5
1	B	258	GLU	2.5
1	C	163	LEU	2.5
1	F	249	VAL	2.5
1	F	92	ALA	2.5
1	C	109	SER	2.5
1	D	283	ARG	2.5
1	B	133	TYR	2.5
1	F	116	TYR	2.5
1	B	358	LEU	2.5
1	F	369	VAL	2.5
1	A	73	ALA	2.5
1	F	189	ALA	2.5
1	C	119	CYS	2.5
1	E	272	GLY	2.5
1	C	133	TYR	2.5
1	E	395	VAL	2.5
1	E	283	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	381	SER	2.5
1	C	98	PRO	2.4
1	F	134	HIS	2.4
1	A	107	ARG	2.4
1	F	119	CYS	2.4
1	F	287	GLY	2.4
1	D	163	LEU	2.4
1	F	77	LEU	2.4
1	F	268	TYR	2.4
1	B	350	VAL	2.4
1	F	120	VAL	2.4
1	D	229	THR	2.4
1	E	101	THR	2.4
1	E	200	THR	2.4
1	A	99	PRO	2.4
1	E	136	SER	2.4
1	F	286	LEU	2.4
1	D	403	TYR	2.4
1	C	104	PHE	2.4
1	F	219	VAL	2.4
1	F	217	ASN	2.4
1	F	427	ALA	2.4
1	D	349	PRO	2.4
1	E	90	GLU	2.4
1	F	158	THR	2.4
1	B	175	GLY	2.4
1	F	131	ILE	2.4
1	D	107	ARG	2.4
1	F	425	LEU	2.4
1	F	164	CYS	2.4
1	F	263	TYR	2.4
1	C	6	ALA	2.4
1	A	258	GLU	2.4
1	C	127	GLU	2.4
1	E	447	GLU	2.4
1	A	98	PRO	2.3
1	C	94	ARG	2.3
1	F	56	ARG	2.3
1	F	250	GLN	2.3
1	B	259	LYS	2.3
1	B	347	LYS	2.3
1	E	203	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	322	VAL	2.3
1	F	399	VAL	2.3
1	E	324	GLU	2.3
1	F	408	PRO	2.3
1	D	165	THR	2.3
1	F	117	THR	2.3
1	B	260	GLY	2.3
1	E	287	GLY	2.3
1	F	281	ARG	2.3
1	F	394	ASP	2.3
1	B	337	LYS	2.3
1	F	256	VAL	2.3
1	F	385	VAL	2.3
1	F	356	GLU	2.3
1	E	191	ASN	2.3
1	D	170	PRO	2.3
1	F	228	ALA	2.3
1	D	166	ARG	2.3
1	B	373	GLY	2.3
1	F	213	ASP	2.3
1	F	405	MET	2.3
1	A	100	GLU	2.3
1	D	90	GLU	2.3
1	D	100	GLU	2.3
1	E	399	VAL	2.3
1	B	136	SER	2.3
1	E	195	LEU	2.3
1	B	72	LYS	2.3
1	E	76	LYS	2.3
1	F	368	ASP	2.3
1	D	172	VAL	2.3
1	D	399	VAL	2.3
1	B	6	ALA	2.2
1	F	357	ALA	2.2
1	C	74	GLY	2.2
1	D	131	ILE	2.2
1	F	264	ILE	2.2
1	F	13	GLU	2.2
1	D	129	TYR	2.2
1	E	164	CYS	2.2
1	F	171	LYS	2.2
1	F	282	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	87	ILE	2.2
1	E	100	GLU	2.2
1	B	206	PHE	2.2
1	E	40	ALA	2.2
1	C	97	TYR	2.2
1	C	184	TYR	2.2
1	D	169	LYS	2.2
1	D	101	THR	2.2
1	F	80	MET	2.2
1	C	390	ILE	2.2
1	E	390	ILE	2.2
1	F	318	ARG	2.2
1	A	363	PHE	2.2
1	C	225	LYS	2.2
1	B	309	ASN	2.2
1	F	214	TYR	2.2
1	B	87	ILE	2.2
1	E	374	ILE	2.2
1	F	367	SER	2.2
1	F	127	GLU	2.2
1	A	393	LYS	2.2
1	B	362	LYS	2.2
1	D	203	LYS	2.2
1	F	206	PHE	2.2
1	F	262	LEU	2.1
1	C	130	ARG	2.1
1	C	258	GLU	2.1
1	F	409	ASP	2.1
1	A	337	LYS	2.1
1	D	125	LYS	2.1
1	E	99	PRO	2.1
1	D	91	GLN	2.1
1	D	135	ALA	2.1
1	D	85	GLY	2.1
1	D	216	GLY	2.1
1	E	292	LEU	2.1
1	F	165	THR	2.1
1	F	167	LEU	2.1
1	B	201	ILE	2.1
1	F	374	ILE	2.1
1	C	129	TYR	2.1
1	F	108	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	381	SER	2.1
1	F	115	ASP	2.1
1	F	276	ASP	2.1
1	F	113	PRO	2.1
1	E	39	VAL	2.1
1	E	199	GLN	2.1
1	E	175	GLY	2.1
1	F	110	THR	2.1
1	F	261	GLY	2.1
1	F	384	ARG	2.1
1	F	398	ARG	2.1
1	C	123	GLU	2.1
1	C	131	ILE	2.1
1	D	224	ILE	2.1
1	C	116	TYR	2.1
1	F	285	VAL	2.1
1	F	320	VAL	2.1
1	B	135	ALA	2.1
1	A	313	ARG	2.1
1	D	103	LEU	2.1
1	D	398	ARG	2.1
1	E	389	ARG	2.1
1	A	108	GLU	2.1
1	F	174	GLU	2.1
1	F	129	TYR	2.1
1	C	164	CYS	2.1
1	E	290	CYS	2.1
1	F	177	VAL	2.0
1	B	357	ALA	2.0
1	A	402	GLY	2.0
1	F	257	GLU	2.0
1	E	273	SER	2.0
1	C	357	ALA	2.0
1	E	85	GLY	2.0
1	F	416	TYR	2.0

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

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.