



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:34 PM UTC

PDB ID : 8J9B / pdb_00008j9b
Title : LnaB-actin binary complex
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2023-05-03
Resolution : 3.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

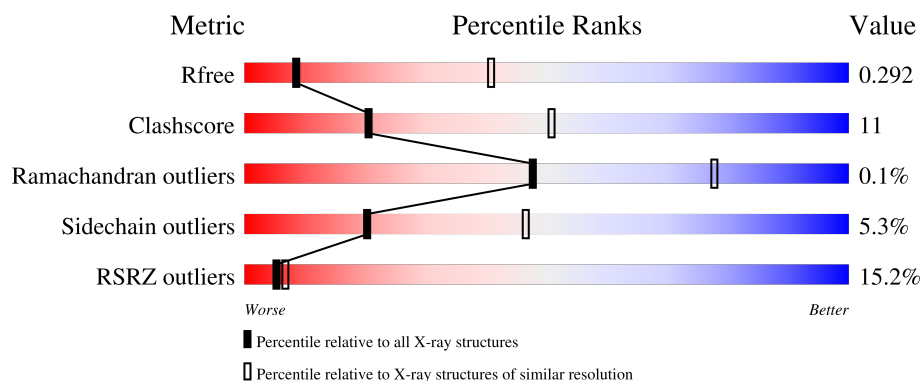
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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.



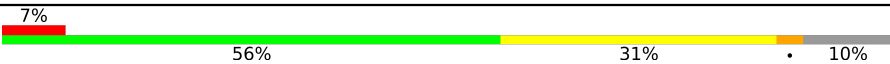
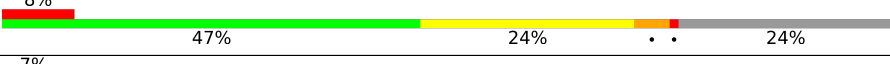
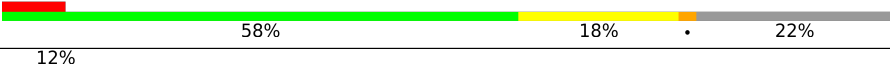
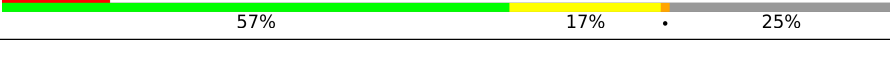
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	375	36% 49% 31% 6% 14%
1	B	375	30% 52% 31% 8% 9%
1	C	375	7% 57% 28% 6% 9%
1	D	375	8% 54% 35% 6% 6%
1	E	375	9% 54% 27% 15%

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Mol	Chain	Length	Quality of chain
1	F	375	
2	H	441	
2	I	441	
2	J	441	
2	K	441	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26804 atoms, of which 0 are hydrogens and 0 are deuteriums.

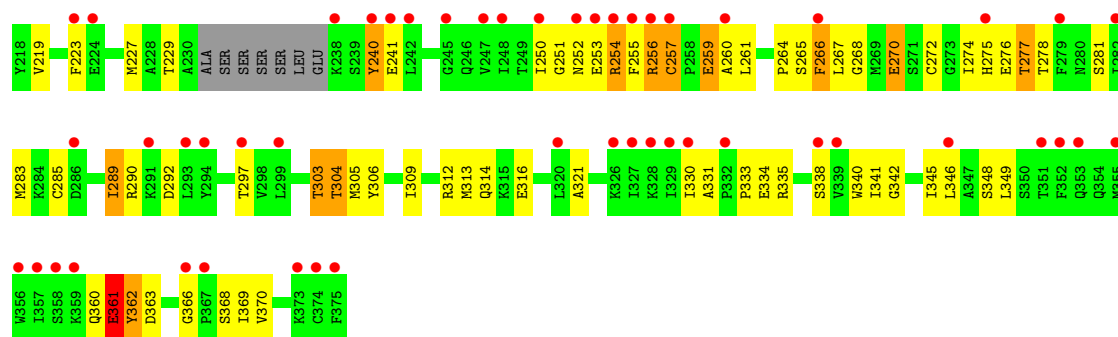
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin gamma 1.

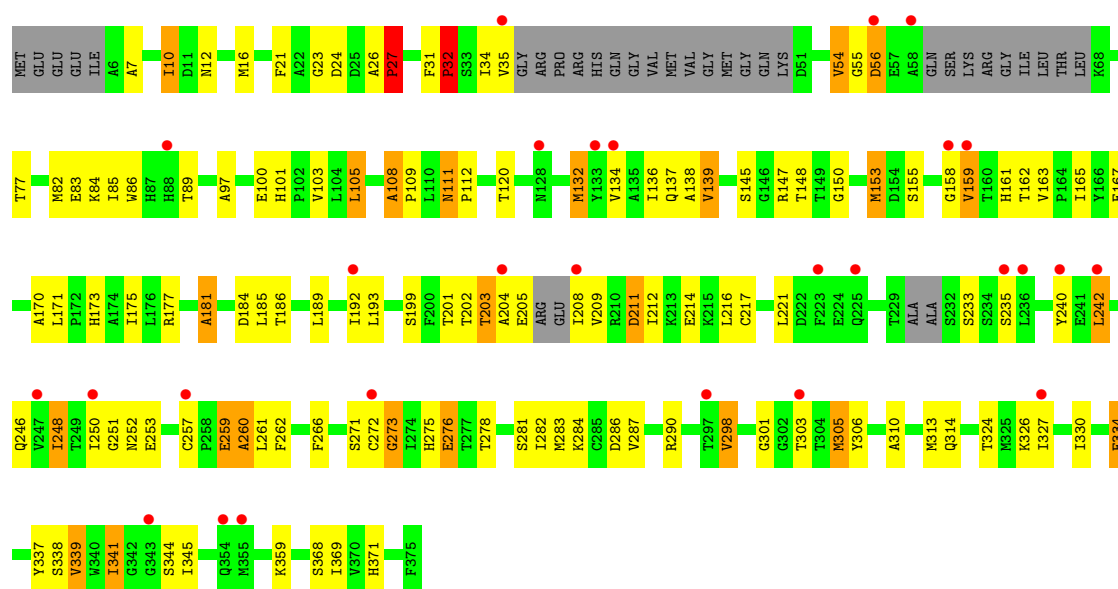
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2538	1619	420	479	20			
1	B	343	Total	C	N	O	S	0	0	0
			2683	1706	446	511	20			
1	C	342	Total	C	N	O	S	0	0	0
			2673	1700	439	514	20			
1	D	354	Total	C	N	O	S	0	0	0
			2774	1763	462	529	20			
1	E	318	Total	C	N	O	S	0	0	0
			2488	1585	410	474	19			
1	F	338	Total	C	N	O	S	0	0	0
			2641	1676	443	502	20			

- Molecule 2 is a protein called Type IV secretion protein Dot.

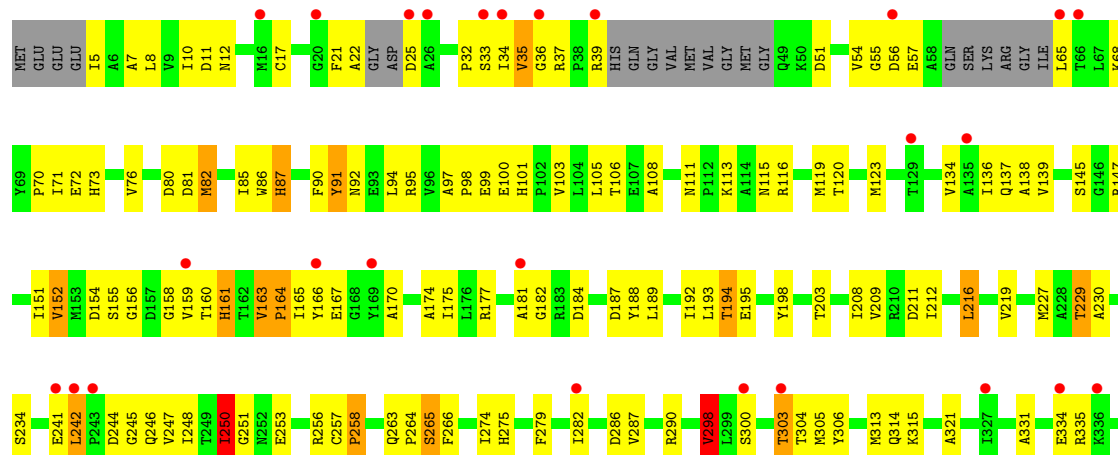
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	348	Total	C	N	O	S	0	0	0
			2826	1803	462	556	5			
2	I	335	Total	C	N	O	S	0	0	0
			2707	1723	444	535	5			
2	J	343	Total	C	N	O	S	0	0	0
			2780	1772	457	546	5			
2	K	331	Total	C	N	O	S	0	0	0
			2694	1726	442	521	5			



• Molecule 1: Actin gamma 1

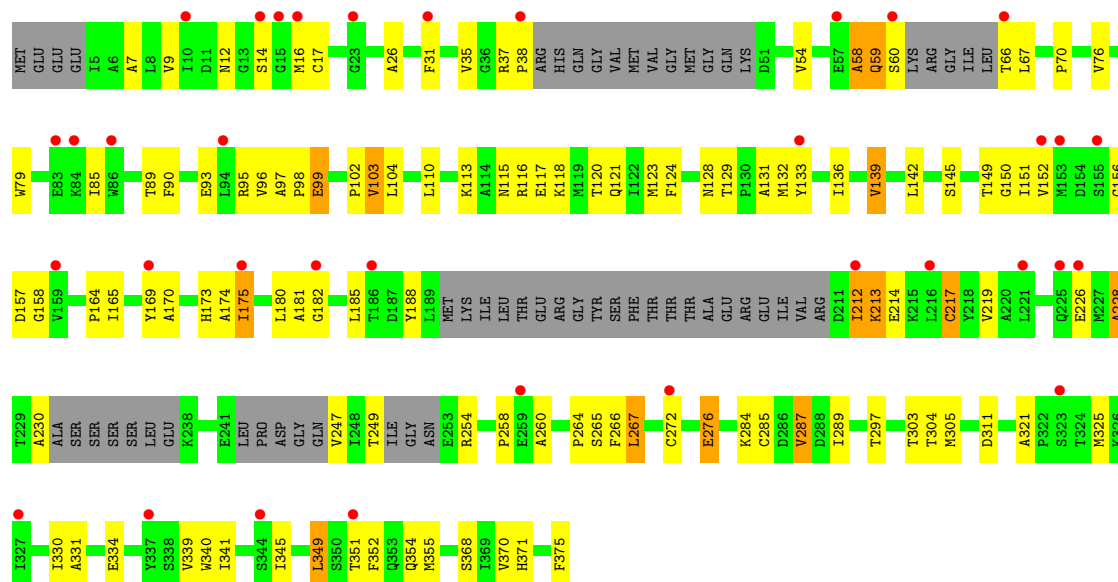


• Molecule 1: Actin gamma 1

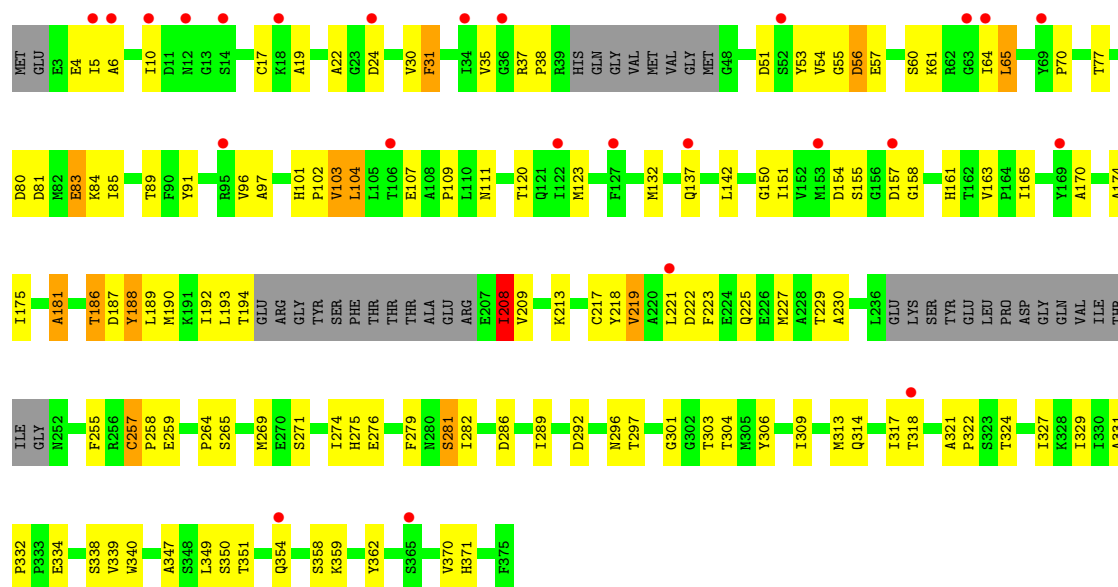




• Molecule 1: Actin gamma 1



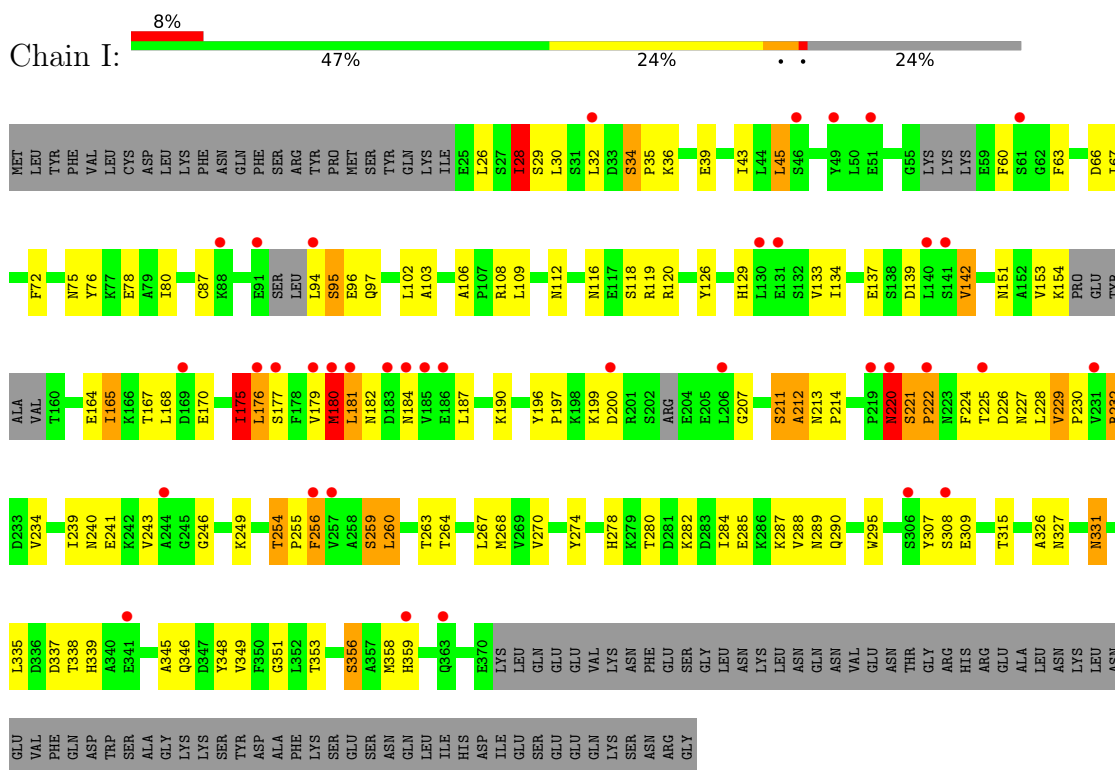
• Molecule 1: Actin gamma 1



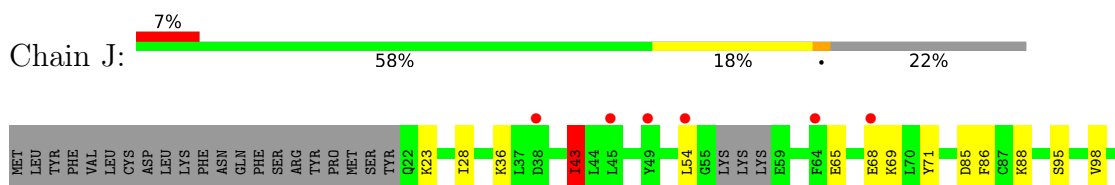
• Molecule 2: Type IV secretion protein Dot



- Molecule 2: Type IV secretion protein Dot



- Molecule 2: Type IV secretion protein Dot



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	110.58Å 110.58Å 407.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.10 – 3.42 62.10 – 3.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.10-3.42) 99.9 (62.10-3.42)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.287 , 0.298 0.290 , 0.292	Depositor DCC
R_{free} test set	3809 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.018 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	26804	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.30	6/2591 (0.2%)	1.49	57/3502 (1.6%)
1	B	1.39	7/2740 (0.3%)	1.47	67/3706 (1.8%)
1	C	1.64	25/2730 (0.9%)	1.47	62/3697 (1.7%)
1	D	1.65	28/2833 (1.0%)	1.46	64/3835 (1.7%)
1	E	1.56	12/2541 (0.5%)	1.38	42/3438 (1.2%)
1	F	1.60	18/2696 (0.7%)	1.40	50/3646 (1.4%)
2	H	1.68	31/2881 (1.1%)	1.41	59/3889 (1.5%)
2	I	1.62	22/2755 (0.8%)	1.48	56/3713 (1.5%)
2	J	1.26	17/2831 (0.6%)	1.19	29/3818 (0.8%)
2	K	1.02	6/2745 (0.2%)	0.96	15/3698 (0.4%)
All	All	1.49	172/27343 (0.6%)	1.38	501/36942 (1.4%)

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	ASN	CA-C	-8.63	1.44	1.53
2	I	274	TYR	CA-C	-8.08	1.42	1.52
1	D	111	ASN	CA-C	-8.05	1.43	1.52
2	I	175	ILE	CA-C	-7.97	1.42	1.52
2	H	257	VAL	CA-C	-7.77	1.42	1.52
2	H	240	ASN	CA-C	-7.71	1.43	1.52
2	I	221	SER	CA-C	-7.65	1.44	1.53
2	J	256	PHE	CA-C	-7.60	1.45	1.53
2	J	232	ARG	CA-C	-7.54	1.43	1.52
1	F	60	SER	CA-C	-7.48	1.43	1.52
1	F	281	SER	CA-C	-7.38	1.43	1.52
1	D	279	PHE	CA-C	-7.35	1.45	1.52
2	H	204	GLU	CA-C	-7.34	1.43	1.52
1	C	7	ALA	CA-C	-7.32	1.43	1.52
2	K	193	SER	CA-C	-7.30	1.43	1.52
2	H	68	GLU	CA-C	-7.21	1.43	1.52
2	I	34	SER	CA-C	-7.11	1.44	1.52
2	H	256	PHE	CA-C	-7.03	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	307	TYR	CA-C	-7.02	1.43	1.52
1	F	306	TYR	CA-C	-7.00	1.46	1.53
1	D	17	CYS	CA-C	-6.86	1.44	1.52
2	I	307	TYR	CA-C	-6.85	1.44	1.52
1	D	170	ALA	CA-C	-6.79	1.44	1.52
1	D	35	VAL	CA-C	-6.78	1.47	1.52
2	H	193	SER	CA-C	-6.78	1.44	1.52
2	J	139	ASP	CA-C	-6.74	1.44	1.52
1	E	17	CYS	CA-C	-6.74	1.44	1.52
2	H	75	ASN	CA-C	-6.65	1.45	1.53
1	C	139	VAL	CA-C	-6.58	1.44	1.52
2	K	199	LYS	CA-C	-6.51	1.44	1.52
1	F	332	PRO	CA-C	-6.50	1.47	1.52
1	D	164	PRO	CA-C	-6.47	1.46	1.52
1	C	147	ARG	CA-C	-6.44	1.44	1.52
1	B	281	SER	CA-C	-6.44	1.44	1.52
1	C	310	ALA	CA-C	-6.39	1.45	1.52
2	I	259	SER	CA-C	-6.38	1.46	1.53
2	J	261	SER	CA-C	-6.38	1.45	1.52
1	C	97	ALA	CA-C	-6.35	1.45	1.52
1	D	163	VAL	CA-C	-6.33	1.47	1.53
2	I	346	GLN	CA-C	-6.30	1.44	1.52
2	H	316	GLU	CA-C	-6.29	1.44	1.52
2	J	240	ASN	CA-C	-6.29	1.44	1.52
2	H	91	GLU	CA-C	-6.29	1.43	1.52
2	H	132	SER	CA-C	-6.26	1.44	1.52
1	C	259	GLU	CA-C	-6.22	1.44	1.52
1	E	287	VAL	CA-C	-6.22	1.44	1.52
2	I	240	ASN	CA-C	-6.22	1.45	1.52
2	H	335	LEU	CA-C	-6.21	1.45	1.52
1	F	17	CYS	CA-C	-6.20	1.45	1.52
1	E	181	ALA	CA-C	-6.19	1.44	1.52
1	D	344	SER	CA-C	-6.17	1.45	1.52
1	B	33	SER	CA-C	-6.16	1.46	1.53
1	F	154	ASP	CA-C	-6.14	1.45	1.52
2	I	232	ARG	CA-C	-6.12	1.46	1.53
1	B	362	TYR	CA-C	-6.07	1.45	1.52
1	A	18	LYS	CA-C	-5.99	1.45	1.52
1	F	54	VAL	CA-C	-5.99	1.45	1.52
2	J	309	GLU	CA-CB	-5.95	1.43	1.53
1	C	344	SER	CA-C	-5.95	1.45	1.52
2	H	48	LYS	CA-C	-5.94	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	96	VAL	CA-C	-5.94	1.45	1.52
1	E	7	ALA	CA-C	-5.92	1.45	1.52
2	J	221	SER	CA-C	-5.91	1.45	1.52
1	C	181	ALA	CA-C	-5.90	1.45	1.52
2	H	29	SER	CA-C	-5.89	1.44	1.52
2	J	43	ILE	CA-C	-5.87	1.45	1.52
2	H	119	ARG	CA-C	-5.85	1.45	1.52
1	F	170	ALA	CA-C	-5.84	1.45	1.53
2	I	327	ASN	CA-C	-5.83	1.46	1.53
1	E	97	ALA	CA-C	-5.74	1.46	1.52
2	H	216	ILE	CA-C	-5.73	1.48	1.52
2	J	280	THR	CA-C	-5.73	1.47	1.53
1	F	181	ALA	CA-CB	-5.73	1.46	1.53
2	H	38	ASP	CA-C	-5.72	1.46	1.53
1	D	290	ARG	CA-C	-5.66	1.45	1.52
2	I	28	ILE	CA-C	-5.66	1.45	1.52
2	J	198	LYS	CA-C	-5.66	1.46	1.53
1	D	7	ALA	CA-C	-5.65	1.45	1.53
2	H	258	ALA	N-CA	-5.65	1.38	1.45
2	I	246	GLY	CA-C	-5.64	1.46	1.52
2	I	165	ILE	CA-C	-5.62	1.46	1.52
1	A	19	ALA	CA-C	-5.62	1.45	1.52
2	H	332	TYR	CA-C	-5.61	1.47	1.53
1	D	33	SER	CA-C	-5.60	1.46	1.53
1	C	101	HIS	CA-C	-5.60	1.47	1.52
2	H	202	SER	CA-C	-5.59	1.45	1.53
2	H	261	SER	CA-C	-5.58	1.45	1.52
2	K	142	VAL	CA-C	-5.57	1.45	1.52
2	J	361	GLU	CA-C	-5.55	1.45	1.52
2	K	182	ASN	CA-C	-5.55	1.47	1.53
1	D	54	VAL	N-CA	-5.54	1.39	1.46
1	F	332	PRO	C-O	-5.54	1.20	1.24
2	H	243	VAL	CA-C	-5.54	1.46	1.52
1	C	276	GLU	CA-C	-5.53	1.45	1.52
2	K	139	ASP	CA-C	-5.52	1.45	1.53
1	D	154	ASP	CA-C	-5.50	1.46	1.53
1	C	359	LYS	CA-C	-5.50	1.45	1.52
1	D	304	THR	CA-C	-5.50	1.45	1.52
2	H	267	LEU	CA-C	-5.50	1.45	1.52
2	J	279	LYS	CA-C	-5.50	1.48	1.52
1	C	163	VAL	CA-CB	-5.49	1.49	1.54
1	B	54	VAL	CA-C	-5.49	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	326	ALA	CA-C	-5.48	1.46	1.52
2	I	168	LEU	CA-C	-5.46	1.45	1.52
1	C	181	ALA	CA-CB	-5.44	1.46	1.53
2	H	334	VAL	CA-C	-5.44	1.46	1.52
1	D	373	LYS	CA-C	-5.43	1.45	1.52
1	E	85	ILE	CA-C	-5.42	1.46	1.52
1	E	98	PRO	CA-C	-5.42	1.47	1.52
1	E	95	ARG	CA-C	-5.42	1.45	1.52
1	C	32	PRO	CA-C	-5.42	1.46	1.52
1	F	230	ALA	CA-C	-5.41	1.45	1.52
2	H	161	HIS	CA-C	-5.41	1.47	1.53
1	C	170	ALA	CA-C	-5.39	1.45	1.53
2	J	307	TYR	CA-C	-5.38	1.45	1.52
1	A	340	TRP	CA-C	-5.37	1.46	1.52
1	C	368	SER	CA-C	-5.37	1.46	1.53
1	C	105	LEU	CA-C	-5.36	1.46	1.52
1	D	72	GLU	CA-C	-5.35	1.46	1.52
2	I	254	THR	CA-C	-5.34	1.46	1.52
1	F	186	THR	CA-C	-5.33	1.45	1.53
2	I	108	ARG	CA-C	-5.33	1.45	1.52
1	C	27	PRO	CA-C	-5.33	1.46	1.52
1	B	304	THR	CA-C	-5.32	1.45	1.52
2	J	306	SER	CA-C	-5.32	1.46	1.52
2	J	226	ASP	CA-C	5.31	1.59	1.52
2	I	164	GLU	CA-C	-5.29	1.45	1.53
1	D	97	ALA	CA-C	-5.29	1.46	1.52
1	D	170	ALA	N-CA	-5.29	1.39	1.45
2	H	331	ASN	CA-C	-5.28	1.46	1.52
1	A	91	TYR	CA-C	-5.27	1.49	1.52
1	B	78	ASN	CA-C	-5.27	1.46	1.52
1	D	306	TYR	CA-C	-5.27	1.47	1.53
2	J	177	SER	CA-C	-5.24	1.45	1.52
1	C	334	GLU	CA-C	-5.24	1.46	1.53
1	F	111	ASN	CA-C	-5.22	1.47	1.53
2	H	122	TYR	CA-C	-5.22	1.46	1.52
1	A	223	PHE	CA-C	-5.22	1.46	1.52
1	D	247	VAL	N-CA	-5.21	1.40	1.46
1	F	6	ALA	CA-C	-5.20	1.46	1.53
1	D	350	SER	CA-C	-5.20	1.45	1.52
1	F	271	SER	CA-C	-5.20	1.46	1.52
1	A	78	ASN	CA-C	-5.18	1.46	1.52
1	E	170	ALA	CA-C	-5.18	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	139	VAL	CA-C	-5.17	1.46	1.52
2	I	224	PHE	N-CA	-5.17	1.39	1.46
2	I	139	ASP	CA-C	-5.17	1.46	1.52
1	D	108	ALA	CA-C	-5.17	1.46	1.52
1	D	170	ALA	CA-CB	-5.17	1.45	1.53
2	I	222	PRO	CA-C	-5.16	1.46	1.52
1	D	315	LYS	CA-C	-5.16	1.46	1.52
2	I	103	ALA	CA-C	-5.15	1.45	1.52
1	D	230	ALA	CA-C	-5.14	1.45	1.52
1	C	306	TYR	CA-C	-5.12	1.47	1.52
1	C	163	VAL	CA-C	-5.11	1.48	1.52
2	H	163	THR	CA-C	-5.11	1.46	1.52
1	D	360	GLN	CA-C	-5.11	1.46	1.52
2	H	342	PHE	CA-C	-5.10	1.46	1.52
1	C	161	HIS	CA-C	-5.09	1.46	1.52
2	J	182	ASN	CA-C	-5.08	1.46	1.52
1	F	362	TYR	CA-C	-5.07	1.46	1.52
1	C	326	LYS	CA-C	-5.07	1.46	1.52
1	F	358	SER	CA-C	-5.07	1.46	1.53
2	K	307	TYR	CA-C	-5.06	1.46	1.52
1	B	90	PHE	CA-C	-5.06	1.46	1.52
1	D	300	SER	CA-C	-5.04	1.46	1.52
1	D	161	HIS	CA-C	-5.03	1.46	1.52
1	E	145	SER	CA-C	-5.03	1.45	1.52
1	C	56	ASP	C-O	-5.03	1.18	1.24
1	F	38	PRO	N-CD	5.03	1.54	1.47
2	H	187	LEU	CA-C	-5.02	1.46	1.52
2	H	234	VAL	CA-C	-5.01	1.47	1.52

All (501) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	142	VAL	N-CA-C	-15.75	97.24	112.83
2	H	138	SER	N-CA-C	14.41	126.68	110.97
1	E	272	CYS	N-CA-C	14.18	126.45	111.14
1	E	157	ASP	N-CA-C	-14.04	95.65	112.92
2	J	257	VAL	N-CA-C	-13.94	98.93	112.17
1	C	221	LEU	N-CA-C	-13.63	97.14	114.04
1	A	229	THR	N-CA-C	-12.37	98.17	113.38
2	I	267	LEU	N-CA-C	-12.02	95.75	112.45
2	I	182	ASN	N-CA-C	-11.92	98.37	111.36
1	A	115	ASN	N-CA-C	-11.89	99.17	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	331	ALA	CA-C-N	-10.99	111.74	119.66
1	E	331	ALA	C-N-CA	-10.99	111.74	119.66
1	D	57	GLU	N-CA-C	-10.99	99.88	113.28
2	J	256	PHE	CB-CA-C	-10.84	101.16	116.34
2	I	164	GLU	N-CA-C	-10.79	95.99	110.55
1	D	98	PRO	N-CA-C	10.73	127.23	114.03
2	I	358	MET	N-CA-C	-10.66	99.80	113.12
1	E	304	THR	N-CA-C	-10.64	100.59	112.72
2	H	258	ALA	N-CA-C	-10.59	100.65	114.31
1	B	91	TYR	N-CA-C	10.18	122.46	111.36
1	C	139	VAL	N-CA-C	-10.05	100.37	110.62
1	B	229	THR	N-CA-C	-10.02	98.59	113.61
2	J	140	LEU	N-CA-C	-9.96	100.44	112.59
1	F	188	TYR	N-CA-C	-9.93	101.67	113.88
1	D	35	VAL	N-CA-C	-9.74	96.02	109.46
2	H	279	LYS	N-CA-C	-9.69	101.45	113.18
1	D	331	ALA	CA-C-N	-9.66	112.70	119.66
1	D	331	ALA	C-N-CA	-9.66	112.70	119.66
1	C	145	SER	N-CA-C	-9.65	101.01	113.17
1	F	65	LEU	N-CA-C	9.61	123.52	110.55
1	B	334	GLU	N-CA-C	-9.58	102.20	112.93
2	J	310	VAL	N-CA-C	-9.54	101.08	110.72
1	C	82	MET	N-CA-C	-9.43	101.90	113.50
2	H	85	ASP	N-CA-C	-9.39	102.33	113.88
1	D	351	THR	N-CA-C	-9.37	101.54	113.16
1	C	273	GLY	N-CA-C	9.22	124.30	112.68
2	I	249	LYS	N-CA-C	-9.19	101.97	113.55
1	F	157	ASP	N-CA-C	-9.11	101.69	113.17
1	A	359	LYS	N-CA-C	-9.09	100.77	112.23
1	A	196	ARG	N-CA-C	-9.08	101.90	113.16
2	K	181	LEU	N-CA-C	-9.08	96.43	109.96
1	A	331	ALA	CA-C-N	-9.01	111.10	120.38
1	A	331	ALA	C-N-CA	-9.01	111.10	120.38
1	C	85	ILE	N-CA-C	-8.99	101.45	110.62
2	I	29	SER	N-CA-C	-8.98	102.24	113.02
1	C	83	GLU	N-CA-C	-8.98	101.38	111.71
2	J	228	LEU	N-CA-C	-8.95	94.94	108.99
1	B	183	ARG	N-CA-C	-8.94	101.54	111.28
1	C	103	VAL	N-CA-C	8.92	120.73	107.80
1	D	182	GLY	N-CA-C	8.82	123.59	112.83
1	F	265	SER	N-CA-C	-8.81	102.44	113.01
1	A	250	ILE	N-CA-C	8.79	121.49	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	180	MET	N-CA-C	-8.79	101.67	111.07
1	D	274	ILE	N-CA-C	-8.78	101.13	113.07
1	A	85	ILE	N-CA-C	-8.78	101.67	110.62
1	D	103	VAL	N-CA-C	8.74	120.41	108.17
1	C	150	GLY	N-CA-C	8.69	122.64	110.74
2	I	134	ILE	N-CA-C	-8.68	100.63	113.39
1	C	260	ALA	N-CA-C	-8.67	101.80	112.38
2	I	356	SER	N-CA-C	-8.67	102.72	113.38
1	A	114	ALA	N-CA-C	-8.64	102.45	113.16
1	D	354	GLN	N-CA-C	-8.63	101.19	112.41
2	I	34	SER	CA-C-N	-8.62	110.88	120.45
2	I	34	SER	C-N-CA	-8.62	110.88	120.45
1	B	87	HIS	N-CA-C	-8.61	101.86	111.07
1	C	284	LYS	N-CA-C	-8.59	101.24	112.41
2	H	132	SER	N-CA-C	-8.58	101.87	111.82
1	A	249	THR	N-CA-C	-8.52	97.27	109.96
1	D	265	SER	N-CA-C	-8.51	102.88	113.18
1	C	163	VAL	CB-CA-C	-8.51	101.07	110.52
1	F	103	VAL	N-CA-C	8.49	120.06	108.17
2	J	259	SER	N-CA-C	8.49	122.85	111.30
2	I	151	ASN	N-CA-C	-8.49	98.73	111.81
2	I	75	ASN	N-CA-C	-8.46	100.30	110.44
1	E	213	LYS	N-CA-C	-8.38	100.89	112.12
2	I	78	GLU	N-CA-C	-8.34	102.19	111.28
2	I	170	GLU	N-CA-C	-8.33	101.98	112.90
2	I	256	PHE	N-CA-C	8.33	122.80	112.47
1	D	55	GLY	N-CA-C	8.29	126.44	111.02
1	B	103	VAL	N-CA-C	8.26	120.41	107.28
1	C	108	ALA	CA-C-N	-8.24	111.28	119.76
1	C	108	ALA	C-N-CA	-8.24	111.28	119.76
1	A	201	THR	N-CA-C	8.23	120.33	111.36
1	B	163	VAL	N-CA-C	8.21	116.97	107.77
1	F	209	VAL	N-CA-C	8.21	119.01	110.72
2	H	267	LEU	N-CA-C	-8.20	102.30	111.82
2	I	139	ASP	N-CA-C	-8.15	102.35	111.07
1	F	51	ASP	N-CA-C	-8.14	103.06	113.16
1	D	244	ASP	N-CA-C	-8.14	102.41	111.28
1	F	301	GLY	N-CA-C	8.11	122.14	112.33
1	A	313	MET	N-CA-C	-8.10	102.39	111.71
1	E	368	SER	N-CA-C	8.09	121.94	112.72
1	A	284	LYS	N-CA-C	-8.05	102.76	112.59
1	B	264	PRO	N-CA-C	-8.04	105.36	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	200	ASP	N-CA-C	8.00	123.08	113.16
1	E	116	ARG	N-CA-C	-7.99	103.75	113.97
1	D	116	ARG	N-CA-C	-7.98	103.37	113.43
1	A	224	GLU	N-CA-C	7.96	120.87	111.71
1	E	85	ILE	N-CA-C	-7.92	102.82	110.42
1	C	201	THR	N-CA-C	7.86	119.93	111.36
2	I	295	TRP	N-CA-C	-7.81	102.76	111.28
1	B	321	ALA	N-CA-C	7.80	122.67	109.09
2	I	80	ILE	N-CA-C	-7.78	102.86	110.72
1	A	227	MET	N-CA-C	-7.78	103.36	112.92
1	C	235	SER	N-CA-C	-7.72	104.09	113.97
2	H	163	THR	N-CA-C	-7.72	102.86	111.28
2	H	363	GLN	N-CA-C	-7.72	103.43	112.92
1	B	306	TYR	CA-C-N	-7.71	112.05	119.76
1	B	306	TYR	C-N-CA	-7.71	112.05	119.76
2	H	243	VAL	N-CA-C	-7.70	98.53	108.93
2	K	356	SER	N-CA-C	-7.67	103.53	113.12
2	H	48	LYS	N-CA-C	-7.65	102.94	111.82
2	I	353	THR	N-CA-C	7.64	119.69	111.36
2	J	225	THR	N-CA-C	-7.64	103.94	113.18
2	H	224	PHE	N-CA-C	-7.63	97.89	110.17
1	E	150	GLY	N-CA-C	7.62	120.83	110.69
2	I	241	GLU	N-CA-C	-7.62	103.71	113.16
1	E	217	CYS	N-CA-C	7.61	121.23	110.50
1	D	256	ARG	N-CA-C	-7.60	104.15	113.50
1	D	119	MET	N-CA-C	-7.59	103.28	112.54
1	C	159	VAL	N-CA-C	7.54	120.30	109.51
1	D	314	GLN	N-CA-C	-7.54	104.61	113.88
1	B	241	GLU	N-CA-C	7.53	120.61	109.24
1	B	181	ALA	N-CA-C	7.53	118.18	108.24
2	H	358	MET	N-CA-C	-7.52	103.69	113.17
1	A	72	GLU	N-CA-C	7.47	120.59	108.41
1	D	279	PHE	N-CA-C	-7.47	102.99	112.93
2	K	330	LEU	N-CA-C	7.45	121.39	109.24
2	J	239	ILE	CB-CA-C	-7.45	101.00	111.21
1	D	250	ILE	CB-CA-C	-7.45	100.20	110.77
1	D	152	VAL	N-CA-C	7.44	118.61	107.75
2	I	211	SER	N-CA-C	7.44	120.61	110.35
2	J	240	ASN	N-CA-C	-7.42	95.51	108.20
1	E	79	TRP	N-CA-C	7.38	119.40	111.36
1	D	108	ALA	CA-C-N	-7.37	112.19	119.78
1	D	108	ALA	C-N-CA	-7.37	112.19	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	171	ALA	N-CA-C	-7.36	104.04	113.16
1	A	247	VAL	N-CA-CB	7.35	124.00	111.50
1	A	139	VAL	N-CA-C	-7.32	103.16	110.62
2	J	279	LYS	N-CA-C	7.29	122.19	111.34
1	C	257	CYS	CA-C-N	-7.22	112.11	120.12
1	C	257	CYS	C-N-CA	-7.22	112.11	120.12
1	C	369	ILE	N-CA-C	-7.21	102.41	113.16
1	D	253	GLU	N-CA-C	-7.20	104.10	113.17
1	E	97	ALA	N-CA-C	-7.20	99.27	110.14
2	H	264	THR	N-CA-C	-7.20	103.47	111.82
2	H	285	GLU	N-CA-C	-7.20	103.52	111.36
2	I	351	GLY	N-CA-C	7.19	121.97	112.77
1	A	336	LYS	N-CA-C	-7.18	103.39	111.07
2	I	282	LYS	N-CA-C	7.17	119.18	111.36
1	B	252	ASN	N-CA-C	-7.15	104.55	113.20
1	A	372	ARG	N-CA-C	7.13	121.98	113.28
1	C	217	CYS	N-CA-C	7.13	120.05	110.35
1	B	362	TYR	N-CA-C	-7.07	103.65	111.36
1	B	121	GLN	N-CA-C	-7.07	103.51	111.14
2	I	60	PHE	N-CA-C	-7.05	104.68	113.28
2	H	184	ASN	N-CA-C	7.04	118.95	111.28
1	C	111	ASN	N-CA-C	-7.04	100.70	109.64
1	E	228	ALA	N-CA-C	7.03	118.74	111.14
2	H	195	ARG	N-CA-C	7.03	119.02	111.36
1	B	4	GLU	N-CA-C	-7.03	99.63	110.10
2	H	255	PRO	N-CA-C	7.03	123.52	113.47
2	K	104	GLU	N-CA-C	-7.02	104.34	113.12
1	C	100	GLU	N-CA-CB	-7.02	100.34	110.80
2	J	221	SER	CA-C-N	-7.01	112.75	119.76
2	J	221	SER	C-N-CA	-7.01	112.75	119.76
1	D	115	ASN	N-CA-C	-7.01	103.01	112.26
1	B	254	ARG	N-CA-C	6.99	118.55	111.07
1	F	331	ALA	CA-C-N	-6.97	114.64	119.66
1	F	331	ALA	C-N-CA	-6.97	114.64	119.66
1	C	97	ALA	N-CA-C	-6.96	100.89	109.65
1	F	208	ILE	N-CA-C	-6.95	103.71	110.72
2	I	339	HIS	N-CA-C	6.95	118.85	111.28
2	H	359	HIS	N-CA-C	-6.94	103.91	112.38
2	I	66	ASP	N-CA-C	-6.94	103.72	111.28
1	D	194	THR	N-CA-C	-6.87	104.71	113.23
2	I	224	PHE	N-CA-C	-6.87	100.11	110.28
2	H	361	GLU	N-CA-C	-6.87	103.90	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	55	GLY	N-CA-C	-6.83	103.65	111.85
1	A	71	ILE	N-CA-C	6.80	118.55	109.37
1	A	25	ASP	N-CA-C	-6.76	105.00	113.18
1	D	229	THR	N-CA-C	-6.76	104.65	113.17
2	I	212	ALA	N-CA-C	6.74	121.58	112.88
1	D	242	LEU	CA-C-O	-6.73	113.69	120.63
1	D	247	VAL	N-CA-C	-6.73	100.01	108.89
1	F	77	THR	N-CA-C	6.71	118.68	111.36
1	F	150	GLY	N-CA-C	6.71	119.91	110.38
1	D	82	MET	N-CA-C	-6.71	104.12	112.90
1	C	271	SER	N-CA-C	6.68	121.13	112.92
1	F	10	ILE	N-CA-C	6.66	117.22	107.37
2	H	133	VAL	N-CA-C	-6.64	104.29	110.53
1	A	253	GLU	N-CA-C	-6.63	101.59	111.81
1	C	101	HIS	CA-C-N	-6.62	112.83	119.99
1	C	101	HIS	C-N-CA	-6.62	112.83	119.99
1	C	111	ASN	CA-C-N	-6.62	112.97	119.78
1	C	111	ASN	C-N-CA	-6.62	112.97	119.78
1	F	4	GLU	N-CA-C	6.61	119.81	110.23
1	C	185	LEU	N-CA-C	6.58	118.54	111.36
1	F	306	TYR	CA-C-N	-6.58	112.72	119.83
1	F	306	TYR	C-N-CA	-6.58	112.72	119.83
1	F	83	GLU	N-CA-C	-6.57	104.19	111.36
2	H	130	LEU	N-CA-C	-6.56	105.24	113.18
1	E	54	VAL	N-CA-C	6.55	117.55	108.12
2	H	29	SER	N-CA-C	-6.54	104.40	112.38
1	E	145	SER	N-CA-C	-6.54	105.06	113.16
1	C	55	GLY	N-CA-C	6.53	121.82	112.82
2	I	87	CYS	N-CA-C	-6.53	104.95	113.17
1	E	174	ALA	N-CA-C	6.52	119.39	111.82
1	B	193	LEU	N-CA-C	-6.52	104.25	111.36
1	E	173	HIS	N-CA-C	6.52	118.47	111.36
2	H	339	HIS	N-CA-C	6.51	118.17	111.14
1	A	215	LYS	N-CA-C	6.50	120.83	112.12
1	F	60	SER	N-CA-C	-6.49	104.20	111.28
2	H	187	LEU	CA-C-N	-6.49	111.94	119.47
2	H	187	LEU	C-N-CA	-6.49	111.94	119.47
2	J	367	LYS	N-CA-C	-6.47	105.37	113.20
1	D	36	GLY	N-CA-C	6.47	121.29	110.56
2	I	220	ASN	N-CA-C	6.46	121.17	113.16
1	C	371	HIS	N-CA-C	-6.44	105.42	113.28
1	A	324	THR	N-CA-C	6.43	121.29	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	THR	N-CA-C	-6.42	105.40	112.72
1	F	271	SER	N-CA-C	-6.42	100.36	108.45
1	C	266	PHE	N-CA-C	-6.41	104.38	111.36
1	F	279	PHE	N-CA-C	-6.38	104.41	111.36
2	K	142	VAL	CB-CA-C	-6.38	103.53	112.14
1	C	167	GLU	N-CA-C	6.38	120.35	111.74
2	I	243	VAL	N-CA-C	-6.37	98.32	107.37
1	E	12	ASN	N-CA-C	-6.37	99.50	109.25
2	H	211	SER	N-CA-C	6.36	118.74	109.07
1	D	10	ILE	N-CA-C	6.35	118.17	107.18
1	E	97	ALA	CA-C-N	-6.35	114.36	120.83
1	E	97	ALA	C-N-CA	-6.35	114.36	120.83
2	J	220	ASN	N-CA-C	6.35	119.22	107.99
1	B	257	CYS	CA-C-N	-6.34	113.21	120.89
1	B	257	CYS	C-N-CA	-6.34	113.21	120.89
1	F	257	CYS	CA-C-N	-6.34	113.28	119.87
1	F	257	CYS	C-N-CA	-6.34	113.28	119.87
1	F	55	GLY	N-CA-C	6.32	122.77	111.02
2	J	28	ILE	N-CA-C	-6.32	103.72	112.50
1	C	242	LEU	CA-C-N	-6.29	112.43	118.97
1	C	242	LEU	C-N-CA	-6.29	112.43	118.97
2	J	368	ASN	N-CA-C	-6.29	104.92	112.59
1	A	369	ILE	N-CA-C	-6.29	104.46	113.07
1	D	251	GLY	CA-C-O	-6.28	115.47	121.19
1	B	150	GLY	N-CA-C	6.28	119.04	110.69
2	H	80	ILE	N-CA-C	-6.27	104.40	110.42
1	D	184	ASP	N-CA-C	-6.25	104.76	112.38
1	F	321	ALA	CA-C-N	-6.25	113.23	119.92
1	F	321	ALA	C-N-CA	-6.25	113.23	119.92
2	I	106	ALA	CA-C-N	-6.25	112.57	119.19
2	I	106	ALA	C-N-CA	-6.25	112.57	119.19
1	B	196	ARG	N-CA-C	-6.23	104.84	112.88
2	H	331	ASN	N-CA-C	-6.23	96.96	107.99
2	J	259	SER	CB-CA-C	-6.23	102.61	111.95
1	D	195	GLU	N-CA-C	-6.22	104.58	111.36
1	D	251	GLY	N-CA-C	-6.21	100.17	110.80
2	H	23	LYS	N-CA-C	-6.21	105.64	113.72
1	F	163	VAL	CB-CA-C	-6.21	103.63	110.52
1	A	146	GLY	N-CA-C	-6.20	106.39	115.63
1	B	290	ARG	N-CA-C	6.20	118.83	111.71
1	F	53	TYR	N-CA-C	-6.20	98.31	108.41
2	I	35	PRO	N-CA-C	-6.19	106.61	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	MET	N-CA-C	-6.19	106.00	112.93
2	H	183	ASP	N-CA-C	-6.18	104.84	112.38
1	F	97	ALA	N-CA-C	-6.17	102.01	109.72
1	C	132	MET	N-CA-C	6.17	118.67	108.99
1	A	111	ASN	N-CA-C	-6.16	102.31	110.07
1	E	339	VAL	N-CA-C	-6.15	104.51	110.72
1	D	242	LEU	N-CA-C	-6.15	102.39	110.39
2	K	58	LYS	N-CA-C	-6.14	105.54	113.16
2	J	226	ASP	CA-C-O	6.13	127.03	119.97
1	B	314	GLN	N-CA-C	6.13	117.65	110.97
1	E	58	ALA	N-CA-C	-6.12	105.74	112.72
2	H	64	PHE	N-CA-C	-6.11	105.59	113.16
2	I	137	GLU	N-CA-C	-6.09	94.95	107.67
1	A	230	ALA	N-CA-C	-6.07	104.67	111.28
1	C	233	SER	N-CA-C	6.07	120.96	113.50
1	F	259	GLU	N-CA-C	-6.06	105.64	113.16
2	H	106	ALA	CA-C-N	-6.06	112.32	119.05
2	H	106	ALA	C-N-CA	-6.06	112.32	119.05
2	J	207	GLY	N-CA-C	6.06	118.90	111.45
1	F	217	CYS	N-CA-C	6.06	119.04	110.50
1	A	345	ILE	N-CA-C	-6.06	103.93	110.23
1	C	10	ILE	N-CA-C	6.04	115.43	106.85
2	I	207	GLY	N-CA-C	6.04	118.02	110.29
2	K	305	HIS	N-CA-C	6.04	117.07	108.74
1	C	272	CYS	N-CA-C	6.03	125.34	113.29
2	I	214	PRO	N-CA-C	6.01	124.85	112.47
1	A	92	ASN	N-CA-C	6.01	117.50	111.07
1	E	265	SER	N-CA-C	-6.00	106.01	113.15
1	C	306	TYR	N-CA-C	-5.99	102.10	109.65
1	B	132	MET	N-CA-C	5.96	118.76	109.52
2	H	191	ALA	N-CA-C	5.96	117.85	111.36
1	B	240	TYR	N-CA-C	5.95	118.82	108.76
1	B	93	GLU	N-CA-C	-5.95	106.64	114.31
2	H	214	PRO	N-CA-C	5.95	124.72	112.47
1	F	56	ASP	N-CA-C	5.94	118.54	111.71
1	F	229	THR	N-CA-C	-5.94	104.80	111.28
1	B	256	ARG	N-CA-C	-5.94	104.81	111.28
2	H	65	GLU	N-CA-C	-5.93	106.58	113.88
1	B	304	THR	N-CA-C	-5.93	105.23	112.88
1	A	112	PRO	N-CA-C	-5.92	101.91	111.03
1	A	111	ASN	CA-C-N	-5.92	113.44	119.83
1	A	111	ASN	C-N-CA	-5.92	113.44	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	182	GLY	N-CA-C	5.92	120.05	112.83
1	B	259	GLU	N-CA-C	-5.91	105.92	113.01
1	E	321	ALA	CA-C-N	-5.90	113.61	119.92
1	E	321	ALA	C-N-CA	-5.90	113.61	119.92
1	E	128	ASN	N-CA-C	5.89	119.77	111.52
1	B	212	ILE	N-CA-C	5.88	118.09	108.97
1	F	91	TYR	N-CA-C	5.88	117.77	111.36
1	D	97	ALA	N-CA-C	-5.88	99.34	109.15
1	A	204	ALA	N-CA-C	-5.87	104.88	111.28
1	D	76	VAL	N-CA-C	5.86	116.83	107.98
1	F	223	PHE	N-CA-C	5.86	117.36	110.97
1	A	306	TYR	CA-C-N	-5.84	113.75	119.76
1	A	306	TYR	C-N-CA	-5.84	113.75	119.76
1	E	76	VAL	N-CA-C	5.83	116.07	107.15
1	D	348	SER	N-CA-C	-5.82	106.34	113.50
1	B	331	ALA	CA-C-N	-5.81	114.39	120.38
1	B	331	ALA	C-N-CA	-5.81	114.39	120.38
1	A	7	ALA	N-CA-C	-5.80	101.61	110.14
2	I	97	GLN	N-CA-C	-5.80	104.64	110.97
1	A	332	PRO	CA-C-N	-5.80	113.70	119.56
1	A	332	PRO	C-N-CA	-5.80	113.70	119.56
1	D	298	VAL	N-CA-C	5.80	118.19	109.20
1	D	306	TYR	CA-C-N	-5.79	113.80	119.76
1	D	306	TYR	C-N-CA	-5.79	113.80	119.76
1	D	203	THR	N-CA-C	-5.78	106.07	113.01
1	F	274	ILE	N-CA-C	-5.78	103.95	112.04
1	C	56	ASP	N-CA-C	-5.78	104.89	111.07
1	B	277	THR	N-CA-C	-5.78	104.36	111.75
2	K	329	LYS	N-CA-C	-5.78	99.49	108.90
2	K	291	ILE	CB-CA-C	-5.77	104.46	112.02
1	E	349	LEU	N-CA-C	5.77	119.05	110.52
1	C	287	VAL	N-CA-C	-5.76	103.85	111.05
1	C	199	SER	N-CA-C	5.76	118.86	109.59
1	D	92	ASN	N-CA-C	5.75	117.62	111.36
1	A	357	ILE	N-CA-C	5.73	116.12	107.75
1	F	186	THR	N-CA-C	-5.73	101.98	110.46
1	D	91	TYR	N-CA-C	5.73	118.39	111.40
1	B	194	THR	N-CA-C	-5.73	106.14	113.01
2	I	226	ASP	N-CA-C	-5.71	105.05	111.28
2	K	184	ASN	N-CA-C	5.71	117.50	111.28
1	B	192	ILE	N-CA-C	5.70	118.21	111.09
1	C	306	TYR	CA-C-N	-5.68	114.08	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	TYR	C-N-CA	-5.68	114.08	119.76
1	B	100	GLU	N-CA-C	5.67	117.54	111.36
2	H	334	VAL	CB-CA-C	-5.67	104.16	111.53
1	A	361	GLU	N-CA-C	-5.66	105.19	111.36
2	I	264	THR	N-CA-C	-5.66	105.49	112.90
1	D	80	ASP	N-CA-C	-5.65	105.48	112.38
1	C	211	ASP	N-CA-C	-5.65	105.12	111.28
1	A	345	ILE	N-CA-CB	5.65	116.55	110.62
1	D	352	PHE	N-CA-C	-5.65	106.38	113.72
1	C	330	ILE	N-CA-C	5.65	115.99	107.80
1	A	158	GLY	N-CA-C	5.64	119.31	112.49
1	E	311	ASP	N-CA-C	-5.64	105.21	111.36
2	I	164	GLU	CA-C-N	-5.64	115.83	123.10
2	I	164	GLU	C-N-CA	-5.64	115.83	123.10
1	B	97	ALA	CA-C-N	-5.63	113.96	120.04
1	B	97	ALA	C-N-CA	-5.63	113.96	120.04
2	H	369	LYS	N-CA-C	-5.63	106.46	113.55
2	H	163	THR	CA-C-N	-5.62	114.08	122.74
2	H	163	THR	C-N-CA	-5.62	114.08	122.74
2	I	260	LEU	N-CA-C	-5.62	100.52	109.07
2	H	327	ASN	N-CA-C	5.62	119.14	111.39
1	C	203	THR	N-CA-C	-5.62	105.06	111.07
1	B	361	GLU	N-CA-C	-5.61	105.17	111.28
2	H	60	PHE	N-CA-C	-5.61	106.33	112.72
1	E	276	GLU	N-CA-C	-5.60	106.49	113.38
1	E	115	ASN	N-CA-C	-5.59	106.04	112.92
1	B	266	PHE	N-CA-C	-5.59	105.28	111.71
1	E	284	LYS	N-CA-C	-5.58	106.36	112.72
1	E	375	PHE	CB-CA-C	-5.58	99.51	110.10
1	D	264	PRO	N-CA-C	-5.57	108.89	114.68
1	A	103	VAL	N-CA-C	5.57	116.14	108.12
1	D	266	PHE	N-CA-C	-5.57	104.85	111.03
2	H	161	HIS	N-CA-C	5.57	118.95	108.65
1	B	270	GLU	N-CA-C	-5.56	106.26	113.16
2	J	222	PRO	N-CA-C	-5.55	102.48	111.19
2	H	212	ALA	N-CA-C	5.55	120.11	113.23
1	B	85	ILE	N-CA-C	-5.54	105.54	113.07
1	F	338	SER	N-CA-C	5.53	118.07	111.71
1	C	184	ASP	N-CA-C	-5.53	105.26	111.28
2	H	216	ILE	CB-CA-C	-5.53	107.03	113.22
1	F	321	ALA	N-CA-C	5.52	117.86	109.41
1	C	77	THR	N-CA-C	5.52	117.37	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	VAL	N-CA-C	-5.51	105.47	110.82
1	A	321	ALA	N-CA-C	5.51	118.80	109.87
1	C	201	THR	CB-CA-C	-5.51	101.48	110.85
1	B	190	MET	CB-CA-C	-5.51	102.23	110.88
1	B	101	HIS	N-CA-C	5.50	118.22	109.64
2	H	316	GLU	CA-C-N	-5.49	113.53	119.24
2	H	316	GLU	C-N-CA	-5.49	113.53	119.24
2	J	230	PRO	N-CA-C	5.49	119.70	111.14
2	H	179	VAL	N-CA-C	-5.49	105.87	113.00
2	H	346	GLN	N-CA-C	-5.49	105.40	111.71
1	F	371	HIS	N-CA-C	-5.48	105.39	111.36
2	H	261	SER	N-CA-C	5.47	117.39	108.63
1	D	163	VAL	N-CA-C	5.47	113.97	107.73
1	D	313	MET	N-CA-C	-5.46	106.65	113.15
2	I	118	SER	N-CA-C	-5.46	105.88	112.54
1	B	195	GLU	N-CA-C	-5.46	106.21	112.92
1	A	266	PHE	N-CA-C	-5.44	105.25	111.07
1	C	23	GLY	N-CA-C	-5.44	107.52	114.37
1	F	31	PHE	CA-C-N	-5.43	114.17	119.76
1	F	31	PHE	C-N-CA	-5.43	114.17	119.76
1	A	259	GLU	N-CA-C	-5.43	106.16	112.89
1	E	103	VAL	N-CA-C	5.43	117.38	108.97
1	E	90	PHE	N-CA-C	5.41	116.87	110.97
1	F	281	SER	N-CA-C	-5.41	105.28	111.07
1	B	142	LEU	N-CA-C	-5.39	105.44	112.23
1	A	172	PRO	N-CA-C	5.37	120.90	113.65
2	J	124	THR	N-CA-C	-5.37	105.59	111.82
1	B	186	THR	N-CA-C	-5.37	105.43	111.28
2	H	33	ASP	CB-CA-C	-5.37	102.32	111.02
2	J	309	GLU	N-CA-C	5.36	119.88	113.23
1	B	309	ILE	N-CA-C	-5.35	104.55	112.04
1	E	26	ALA	N-CA-C	5.35	113.03	108.22
1	A	68	LYS	N-CA-C	5.34	117.10	108.34
1	F	19	ALA	N-CA-C	5.34	117.31	109.24
1	B	348	SER	N-CA-C	-5.34	105.45	112.72
2	H	105	VAL	N-CA-C	5.33	117.76	111.09
1	E	321	ALA	N-CA-C	5.32	118.38	110.39
1	D	360	GLN	N-CA-C	-5.32	105.48	111.28
1	C	314	GLN	N-CA-C	-5.32	105.40	111.14
1	E	212	ILE	CB-CA-C	-5.32	106.62	112.68
2	K	147	ARG	N-CA-C	-5.31	105.60	111.71
2	K	297	SER	N-CA-C	5.31	117.15	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	349	LEU	N-CA-C	5.31	118.76	110.32
1	C	298	VAL	N-CA-C	5.31	115.74	107.99
1	D	216	LEU	N-CA-C	5.30	117.87	111.40
1	B	292	ASP	N-CA-C	-5.30	105.40	111.07
2	H	196	TYR	CA-C-N	-5.30	114.63	119.82
2	H	196	TYR	C-N-CA	-5.30	114.63	119.82
1	C	173	HIS	N-CA-C	-5.29	106.87	113.38
2	I	95	SER	N-CA-C	-5.29	100.69	108.99
1	A	83	GLU	N-CA-C	-5.29	105.63	111.71
1	D	187	ASP	N-CA-C	5.29	117.79	111.71
1	D	321	ALA	CA-C-N	-5.28	114.27	119.92
1	D	321	ALA	C-N-CA	-5.28	114.27	119.92
1	C	54	VAL	CB-CA-C	-5.27	102.64	111.29
2	K	302	GLU	N-CA-C	-5.26	106.64	113.16
1	D	211	ASP	N-CA-C	-5.25	105.55	111.28
1	B	369	ILE	N-CA-C	-5.24	106.19	113.00
1	B	330	ILE	N-CA-C	5.24	115.13	107.37
1	B	303	THR	N-CA-C	-5.24	106.86	113.20
1	D	32	PRO	N-CA-C	5.24	119.41	111.19
1	F	54	VAL	CB-CA-C	-5.24	102.82	110.62
2	H	158	ALA	N-CA-C	5.22	117.61	110.24
2	I	200	ASP	N-CA-C	5.22	120.30	112.94
1	C	100	GLU	N-CA-C	5.22	121.44	113.61
2	H	194	GLU	N-CA-C	-5.21	106.07	112.90
1	D	100	GLU	N-CA-C	-5.21	107.94	114.56
1	D	100	GLU	N-CA-CB	5.20	117.92	111.00
2	I	338	THR	N-CA-C	-5.20	106.98	113.38
2	I	268	MET	N-CA-C	5.20	116.94	111.28
1	F	354	GLN	N-CA-C	-5.19	107.61	114.04
1	F	22	ALA	N-CA-C	5.19	117.19	109.25
2	H	69	LYS	N-CA-C	-5.18	105.06	111.33
2	I	239	ILE	N-CA-C	5.18	115.42	108.17
2	I	225	THR	N-CA-C	-5.18	106.94	113.20
2	I	259	SER	CB-CA-C	-5.17	107.93	114.40
1	B	129	THR	CA-C-N	-5.15	113.40	119.84
1	B	129	THR	C-N-CA	-5.15	113.40	119.84
1	B	272	CYS	N-CA-C	5.15	117.76	110.50
1	D	94	LEU	N-CA-C	-5.14	106.85	113.23
1	A	202	THR	N-CA-C	5.14	117.16	110.53
1	D	286	ASP	N-CA-C	5.13	117.30	110.53
1	B	59	GLN	N-CA-C	-5.13	106.12	112.38
2	I	26	LEU	N-CA-C	-5.13	106.28	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ILE	N-CA-C	-5.12	104.51	111.89
1	B	366	GLY	CA-C-N	-5.12	114.43	120.12
1	B	366	GLY	C-N-CA	-5.12	114.43	120.12
1	E	31	PHE	N-CA-C	5.12	116.53	108.23
1	C	338	SER	N-CA-C	5.11	116.93	111.36
1	A	198	TYR	N-CA-C	-5.11	103.30	110.50
2	H	235	PRO	N-CA-C	5.11	119.50	111.38
1	E	156	GLY	N-CA-C	-5.10	101.92	111.66
1	D	303	THR	N-CA-C	-5.10	107.22	112.93
1	B	289	ILE	N-CA-C	5.08	119.56	112.50
2	J	308	SER	CA-C-N	-5.08	112.72	121.66
2	J	308	SER	C-N-CA	-5.08	112.72	121.66
1	B	90	PHE	CB-CA-C	-5.07	102.88	110.90
2	I	229	VAL	CA-C-N	-5.07	115.01	120.03
2	I	229	VAL	C-N-CA	-5.07	115.01	120.03
2	J	43	ILE	CB-CA-C	-5.07	105.48	111.97
2	H	53	SER	N-CA-C	-5.07	105.83	111.36
1	B	155	SER	CB-CA-C	-5.05	104.87	112.09
1	B	316	GLU	N-CA-C	5.05	116.59	111.14
1	F	174	ALA	N-CA-C	5.05	119.39	112.88
1	C	359	LYS	N-CA-C	-5.04	105.97	111.82
1	C	339	VAL	N-CA-C	-5.04	105.48	110.62
1	A	177	ARG	N-CA-C	5.04	116.85	109.24
1	D	230	ALA	N-CA-C	-5.03	107.19	113.38
2	J	36	LYS	N-CA-C	5.02	119.10	112.92
1	F	64	ILE	CB-CA-C	-5.02	103.06	111.29
1	B	163	VAL	CB-CA-C	-5.01	105.01	110.78
2	J	264	THR	N-CA-C	-5.01	107.02	113.23
1	A	142	LEU	N-CA-C	-5.00	105.91	111.36

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	2538	0	2511	70	0
1	B	2683	0	2645	111	0
1	C	2673	0	2626	57	0
1	D	2774	0	2746	64	0
1	E	2488	0	2443	55	0
1	F	2641	0	2618	56	0
2	H	2826	0	2816	40	0
2	I	2707	0	2686	61	0
2	J	2780	0	2779	49	0
2	K	2694	0	2696	39	0
All	All	26804	0	26566	598	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 11.

All (598) 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)
2:H:157:TYR:CD2	2:H:180:MET:HE3	1.47	1.46
1:B:105:LEU:HD21	1:B:123:MET:CE	1.69	1.21
1:B:105:LEU:CD2	1:B:123:MET:HE1	1.71	1.20
1:B:143:TYR:CD2	1:B:346:LEU:HD11	1.77	1.19
2:H:157:TYR:CD2	2:H:180:MET:CE	2.26	1.18
2:H:157:TYR:HD2	2:H:180:MET:CE	1.57	1.17
2:I:176:LEU:HD23	2:I:177:SER:N	1.57	1.17
1:A:208:ILE:CG2	1:A:247:VAL:HG21	1.79	1.13
1:C:202:THR:HG22	1:C:203:THR:H	1.07	1.12
1:A:34:ILE:HG21	1:A:67:LEU:HD22	1.31	1.12
1:F:35:VAL:HG12	1:F:37:ARG:NH2	1.67	1.06
1:B:192:ILE:HD12	1:B:253:GLU:HG2	1.30	1.06
1:F:35:VAL:HG12	1:F:37:ARG:HH21	0.93	1.06
1:A:208:ILE:HG23	1:A:247:VAL:CG2	1.85	1.04
1:B:192:ILE:HD12	1:B:253:GLU:CG	1.87	1.04
1:E:212:ILE:HG23	1:E:212:ILE:O	1.61	1.01
1:F:35:VAL:CG1	1:F:37:ARG:HH21	1.74	0.99
1:F:35:VAL:CG1	1:F:37:ARG:NH2	2.25	0.98
1:A:208:ILE:HG23	1:A:247:VAL:HG21	1.40	0.98
1:B:143:TYR:CE2	1:B:346:LEU:HD11	1.98	0.98
1:B:192:ILE:HD12	1:B:253:GLU:HB3	1.44	0.97
1:B:192:ILE:HD12	1:B:253:GLU:CB	1.94	0.95
1:C:202:THR:HG22	1:C:203:THR:N	1.73	0.95
1:C:202:THR:CG2	1:C:203:THR:H	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:SER:HB3	1:C:303:THR:HB	1.50	0.93
2:I:176:LEU:HD23	2:I:177:SER:CA	2.01	0.91
1:B:155:SER:OG	1:B:304:THR:HG23	1.70	0.90
1:B:192:ILE:CD1	1:B:253:GLU:HB3	2.03	0.88
1:B:143:TYR:HD2	1:B:346:LEU:HD11	1.38	0.87
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.56	0.87
2:H:157:TYR:CE2	2:H:180:MET:HE3	2.09	0.87
2:J:355:GLN:O	2:J:359:HIS:CG	2.27	0.87
1:A:208:ILE:CG2	1:A:247:VAL:CG2	2.50	0.86
1:C:186:THR:HG23	1:C:209:VAL:HG23	1.56	0.86
1:A:34:ILE:HG21	1:A:67:LEU:CD2	2.07	0.85
1:B:250:ILE:HG22	1:B:254:ARG:CG	2.09	0.83
1:B:188:TYR:CZ	1:B:266:PHE:HB3	2.14	0.83
2:I:176:LEU:CD2	2:I:177:SER:N	2.40	0.83
1:B:120:THR:HG22	1:B:362:TYR:CE2	2.14	0.82
1:A:34:ILE:CG2	1:A:67:LEU:HD22	2.10	0.81
1:D:5:ILE:CG2	1:D:101:HIS:ND1	2.44	0.81
2:I:176:LEU:HD23	2:I:176:LEU:C	2.06	0.80
1:F:155:SER:HB3	1:F:303:THR:HB	1.63	0.80
1:D:139:VAL:HA	1:D:165:ILE:HD13	1.64	0.79
1:A:208:ILE:HG21	1:A:247:VAL:HG21	1.62	0.78
1:E:285:CYS:HB3	1:E:289:ILE:HD11	1.65	0.78
2:I:43:ILE:HD11	2:I:76:TYR:HB3	1.65	0.78
1:D:158:GLY:O	1:D:159:VAL:HG13	1.82	0.78
1:E:260:ALA:HB1	1:E:267:LEU:HD11	1.65	0.78
2:H:157:TYR:HD2	2:H:180:MET:HE3	0.99	0.78
2:K:130:LEU:HD13	2:K:335:LEU:HD11	1.65	0.78
1:A:208:ILE:HG23	1:A:247:VAL:HG23	1.64	0.77
1:B:250:ILE:HG22	1:B:254:ARG:HG3	1.64	0.77
2:H:157:TYR:CE2	2:H:180:MET:CE	2.66	0.77
1:B:119:MET:C	1:B:132:MET:HE1	2.09	0.77
1:C:31:PHE:HB2	1:C:56:ASP:HA	1.67	0.76
1:B:192:ILE:CD1	1:B:253:GLU:HG2	2.15	0.76
1:B:107:GLU:HB3	1:B:134:VAL:HG12	1.66	0.76
2:J:196:TYR:HD1	2:J:260:LEU:CD2	1.99	0.76
1:B:223:PHE:CD1	1:B:255:PHE:CD1	2.74	0.76
1:B:120:THR:HA	1:B:132:MET:SD	2.25	0.75
1:D:5:ILE:HG21	1:D:101:HIS:ND1	2.01	0.75
1:C:158:GLY:O	1:C:181:ALA:HB2	1.87	0.74
1:E:9:VAL:HG13	1:E:340:TRP:NE1	2.01	0.74
2:J:202:SER:HB3	2:J:238:ALA:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG21	1:A:100:GLU:O	1.87	0.73
1:B:250:ILE:CG2	1:B:254:ARG:HG2	2.20	0.72
1:D:164:PRO:HG3	1:D:174:ALA:HB3	1.70	0.72
2:J:196:TYR:HD1	2:J:260:LEU:HD21	1.53	0.72
1:B:223:PHE:CE1	1:B:255:PHE:CE1	2.77	0.72
1:B:285:CYS:HB3	1:B:289:ILE:HD11	1.73	0.71
1:B:24:ASP:HB2	1:B:340:TRP:HH2	1.56	0.71
2:I:28:ILE:HG22	2:I:32:LEU:CD1	2.21	0.71
1:E:212:ILE:O	1:E:212:ILE:CG2	2.34	0.70
1:A:120:THR:HA	1:A:132:MET:SD	2.31	0.70
2:J:196:TYR:CD1	2:J:260:LEU:CD2	2.73	0.70
2:J:355:GLN:O	2:J:359:HIS:CD2	2.44	0.70
2:I:153:VAL:HB	2:I:180:MET:HG3	1.72	0.69
1:F:35:VAL:HG11	1:F:37:ARG:NH2	2.08	0.69
1:B:223:PHE:CD1	1:B:255:PHE:CE1	2.80	0.69
2:J:355:GLN:O	2:J:359:HIS:CE1	2.46	0.68
1:A:34:ILE:CG2	1:A:67:LEU:CD2	2.71	0.68
1:B:223:PHE:CE1	1:B:255:PHE:HE1	2.11	0.68
1:B:188:TYR:CE1	1:B:266:PHE:O	2.46	0.68
1:B:120:THR:HG22	1:B:362:TYR:HE2	1.59	0.68
1:B:188:TYR:OH	1:B:266:PHE:HB3	1.94	0.67
1:B:119:MET:CB	1:B:132:MET:HE1	2.25	0.67
1:D:105:LEU:HB2	1:D:134:VAL:HG12	1.76	0.67
2:I:28:ILE:HG22	2:I:32:LEU:HD13	1.76	0.67
1:D:158:GLY:O	1:D:159:VAL:CG1	2.43	0.67
1:F:158:GLY:O	1:F:181:ALA:HB2	1.94	0.67
2:I:28:ILE:O	2:I:32:LEU:HD13	1.94	0.67
1:A:189:LEU:HD12	1:A:192:ILE:HD11	1.77	0.67
1:C:159:VAL:HG11	1:C:177:ARG:NH1	2.09	0.66
2:J:164:GLU:HB3	2:J:166:LYS:HE3	1.77	0.66
1:B:250:ILE:CG2	1:B:254:ARG:CG	2.73	0.66
1:C:16:MET:HE2	1:C:32:PRO:HD3	1.77	0.66
1:B:250:ILE:HG21	1:B:254:ARG:HG2	1.76	0.66
1:F:104:LEU:HD12	1:F:347:ALA:HB2	1.77	0.65
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.79	0.64
1:E:164:PRO:HD2	1:E:175:ILE:HG22	1.79	0.64
1:B:151:ILE:HG23	1:B:297:THR:HA	1.78	0.64
1:B:153:MET:HG2	1:B:162:THR:HG22	1.77	0.64
1:A:192:ILE:HD12	1:A:253:GLU:HB3	1.80	0.64
1:C:204:ALA:O	1:C:205:GLU:C	2.41	0.64
2:J:147:ARG:HH11	2:J:159:VAL:HG12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:355:GLN:O	2:J:359:HIS:ND1	2.30	0.64
1:B:120:THR:N	1:B:132:MET:HE1	2.13	0.63
1:F:303:THR:O	1:F:303:THR:HG22	1.99	0.63
1:B:215:LYS:O	1:B:215:LYS:HG2	1.97	0.63
1:E:133:TYR:HE2	1:E:355:MET:HE3	1.63	0.62
1:F:80:ASP:O	1:F:83:GLU:HG3	1.99	0.62
1:A:113:LYS:HA	1:A:116:ARG:HG3	1.81	0.62
1:F:81:ASP:HA	1:F:84:LYS:HD2	1.81	0.62
1:B:50:LYS:N	1:B:53:TYR:HH	1.98	0.62
1:B:223:PHE:CD1	1:B:255:PHE:HD1	2.16	0.62
1:B:223:PHE:HD1	1:B:255:PHE:CD1	2.17	0.62
1:C:303:THR:HG22	1:C:303:THR:O	2.00	0.62
2:I:142:VAL:HG21	2:I:290:GLN:HB3	1.82	0.61
1:B:140:LEU:HD22	1:B:346:LEU:HD12	1.82	0.61
1:B:182:GLY:HA2	1:B:185:LEU:HD12	1.81	0.61
1:C:21:PHE:HB2	1:C:24:ASP:OD2	2.01	0.61
1:B:223:PHE:HD1	1:B:255:PHE:HD1	1.49	0.60
2:H:201:ARG:HA	2:H:258:ALA:HB1	1.83	0.60
2:I:176:LEU:O	2:I:180:MET:HB2	2.01	0.60
1:F:189:LEU:HA	1:F:192:ILE:HG12	1.83	0.59
2:J:196:TYR:CD1	2:J:260:LEU:HD22	2.37	0.59
1:F:120:THR:HA	1:F:132:MET:SD	2.42	0.59
1:A:72:GLU:OE2	1:A:73:HIS:HD2	1.85	0.59
1:F:24:ASP:HB2	1:F:340:TRP:HH2	1.66	0.59
1:C:202:THR:CG2	1:C:203:THR:N	2.44	0.59
1:A:72:GLU:OE2	1:A:73:HIS:CD2	2.56	0.58
1:C:186:THR:CG2	1:C:209:VAL:HG23	2.30	0.58
1:A:227:MET:HG2	1:C:324:THR:HG21	1.85	0.58
1:D:21:PHE:O	1:D:22:ALA:C	2.47	0.58
1:D:219:VAL:HG22	1:D:258:PRO:HB3	1.85	0.58
2:H:212:ALA:HB1	2:H:228:LEU:HD22	1.84	0.58
2:J:200:ASP:HB3	2:J:239:ILE:HG23	1.85	0.58
1:C:136:ILE:HG22	1:C:138:ALA:H	1.67	0.58
2:K:149:SER:HA	2:K:277:LYS:NZ	2.18	0.58
1:A:160:THR:HG22	1:A:180:LEU:O	2.04	0.57
1:F:158:GLY:O	1:F:181:ALA:CB	2.52	0.57
2:I:260:LEU:HA	2:I:309:GLU:HG2	1.85	0.57
2:K:156:GLU:OE1	2:K:156:GLU:N	2.36	0.57
2:I:177:SER:HB2	2:I:263:THR:HB	1.86	0.57
2:K:147:ARG:HH12	2:K:160:THR:HA	1.69	0.57
1:B:119:MET:HB3	1:B:132:MET:CE	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:229:VAL:HB	2:J:230:PRO:HD2	1.86	0.57
2:K:259:SER:OG	2:K:260:LEU:N	2.38	0.57
1:E:264:PRO:C	1:E:266:PHE:H	2.13	0.57
1:A:176:LEU:HD11	1:A:284:LYS:HZ1	1.69	0.56
2:J:54:LEU:HD11	2:J:86:PHE:HE1	1.70	0.56
1:B:192:ILE:HA	1:B:195:GLU:HB2	1.86	0.56
1:D:156:GLY:O	1:D:181:ALA:HB1	2.05	0.56
1:B:120:THR:HG22	1:B:362:TYR:CD2	2.39	0.56
1:D:151:ILE:HG21	1:D:282:ILE:HD11	1.87	0.56
1:B:189:LEU:CD1	1:B:192:ILE:HD11	2.34	0.56
1:D:155:SER:OG	1:D:160:THR:HG23	2.06	0.56
1:A:35:VAL:CG2	1:A:85:ILE:CD1	2.84	0.55
1:E:9:VAL:CG1	1:E:340:TRP:NE1	2.70	0.55
2:K:273:ASP:OD2	2:K:277:LYS:NZ	2.37	0.55
1:D:12:ASN:HB3	1:D:82:MET:HE1	1.88	0.55
1:F:189:LEU:O	1:F:193:LEU:HB2	2.06	0.55
1:C:139:VAL:HA	1:C:165:ILE:HD13	1.88	0.55
1:A:164:PRO:HG2	1:A:174:ALA:HB3	1.89	0.55
1:F:155:SER:CB	1:F:303:THR:HB	2.36	0.55
2:K:268:MET:HG3	2:K:319:LEU:HD13	1.87	0.55
2:I:221:SER:O	2:I:222:PRO:C	2.49	0.55
2:H:157:TYR:CE2	2:H:180:MET:HE1	2.41	0.54
2:K:275:ILE:HA	2:K:284:ILE:HD11	1.89	0.54
1:D:5:ILE:CG2	1:D:101:HIS:CE1	2.91	0.54
1:D:91:TYR:O	1:D:95:ARG:HA	2.07	0.54
1:E:180:LEU:HD11	1:E:267:LEU:HD13	1.90	0.54
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.88	0.54
2:H:28:ILE:HA	2:H:31:SER:HB2	1.88	0.54
1:B:73:HIS:HB3	1:B:177:ARG:HH22	1.71	0.54
1:C:137:GLN:HG2	1:C:339:VAL:HG11	1.90	0.54
1:D:136:ILE:HB	1:D:139:VAL:HG23	1.89	0.54
2:I:187:LEU:HD23	2:I:190:LYS:HD2	1.90	0.54
1:D:145:SER:HB2	1:D:147:ARG:HH11	1.71	0.54
1:E:59:GLN:O	1:E:60:SER:C	2.50	0.54
1:C:259:GLU:C	1:C:261:LEU:N	2.57	0.53
1:D:158:GLY:C	1:D:159:VAL:HG13	2.32	0.53
1:D:155:SER:HB3	1:D:303:THR:OG1	2.07	0.53
1:E:185:LEU:O	1:E:188:TYR:HB3	2.08	0.53
1:F:109:PRO:HB3	1:F:175:ILE:HD13	1.89	0.53
1:B:223:PHE:CE1	1:B:255:PHE:CD1	2.97	0.53
1:B:105:LEU:HD11	1:B:123:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:MET:HB3	1:B:132:MET:HE1	1.91	0.53
2:K:141:SER:HB3	2:K:144:ASN:HB2	1.91	0.53
1:B:155:SER:HB2	1:B:303:THR:HB	1.90	0.53
1:B:213:LYS:HD3	1:B:240:TYR:CD2	2.44	0.53
1:B:119:MET:CB	1:B:132:MET:CE	2.87	0.53
1:B:194:THR:HG22	1:B:194:THR:O	2.09	0.53
1:D:242:LEU:HD13	1:D:246:GLN:HB3	1.90	0.53
1:B:312:ARG:O	1:B:313:MET:C	2.49	0.53
1:C:155:SER:CB	1:C:303:THR:HB	2.32	0.52
1:B:188:TYR:CG	1:B:267:LEU:HD11	2.44	0.52
1:D:242:LEU:O	1:D:245:GLY:N	2.38	0.52
1:E:103:VAL:HG11	1:E:123:MET:SD	2.50	0.52
1:E:118:LYS:HA	1:E:121:GLN:HG2	1.90	0.52
2:I:175:ILE:O	2:I:176:LEU:C	2.50	0.52
1:A:178:LEU:HD11	1:A:271:SER:HB3	1.90	0.52
2:J:65:GLU:O	2:J:69:LYS:HG3	2.10	0.52
1:A:133:TYR:CE2	1:A:355:MET:HG3	2.44	0.52
1:A:357:ILE:HD11	1:A:374:CYS:SG	2.50	0.52
1:E:133:TYR:CE2	1:E:355:MET:HE3	2.45	0.52
1:A:72:GLU:O	1:A:73:HIS:C	2.52	0.52
1:B:11:ASP:HA	1:B:106:THR:OG1	2.10	0.52
1:B:345:ILE:O	1:B:349:LEU:HG	2.10	0.52
1:D:159:VAL:CG2	1:D:161:HIS:NE2	2.73	0.52
1:F:70:PRO:HG3	1:F:85:ILE:HD11	1.91	0.52
1:B:91:TYR:O	1:B:95:ARG:HA	2.10	0.52
1:B:185:LEU:HD23	1:B:260:ALA:HB3	1.92	0.52
1:B:360:GLN:HA	1:B:363:ASP:HB2	1.92	0.52
1:E:120:THR:HG21	1:E:370:VAL:HB	1.92	0.52
1:B:163:VAL:HG13	1:B:175:ILE:HG12	1.91	0.52
1:E:352:PHE:C	1:E:354:GLN:H	2.18	0.52
1:D:35:VAL:HG12	1:D:68:LYS:HB2	1.91	0.52
1:C:242:LEU:HD12	1:C:246:GLN:HB3	1.93	0.51
1:D:113:LYS:H	1:D:113:LYS:HD2	1.75	0.51
1:E:351:THR:HG22	2:K:30:LEU:HD13	1.92	0.51
1:B:189:LEU:HD12	1:B:192:ILE:CD1	2.35	0.51
1:D:193:LEU:HD21	1:D:250:ILE:HG23	1.91	0.51
1:B:185:LEU:HD21	1:B:261:LEU:HG	1.92	0.51
1:F:189:LEU:HD12	1:F:192:ILE:HD11	1.92	0.51
1:A:20:GLY:HA2	1:A:28:ARG:H	1.76	0.51
1:B:105:LEU:HD11	1:B:123:MET:HE3	1.93	0.51
1:B:192:ILE:HD11	1:B:253:GLU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:MET:HE2	1:C:134:VAL:HG23	1.92	0.51
1:A:104:LEU:HD12	1:A:133:TYR:HB3	1.93	0.51
1:A:273:GLY:C	1:A:275:HIS:N	2.67	0.51
1:C:275:HIS:CD2	1:C:276:GLU:HG3	2.46	0.51
1:D:5:ILE:HG21	1:D:101:HIS:CE1	2.45	0.51
2:J:146:LEU:O	2:J:150:TYR:N	2.43	0.51
2:J:260:LEU:HA	2:J:309:GLU:OE2	2.11	0.51
2:K:212:ALA:O	2:K:229:VAL:HG22	2.10	0.51
1:A:35:VAL:HG23	1:A:85:ILE:CD1	2.41	0.51
1:A:300:SER:HA	1:A:335:ARG:HB2	1.93	0.51
1:B:333:PRO:C	1:B:335:ARG:H	2.18	0.51
2:I:120:ARG:HH22	2:I:256:PHE:HB3	1.76	0.51
2:K:120:ARG:NH1	2:K:217:MET:HG2	2.25	0.51
1:E:264:PRO:C	1:E:266:PHE:N	2.68	0.51
2:I:254:THR:HG21	2:I:308:SER:HB2	1.92	0.50
1:B:105:LEU:HD21	1:B:123:MET:HE1	0.76	0.50
2:H:360:HIS:HA	2:H:363:GLN:HB2	1.94	0.50
2:I:180:MET:HB3	2:I:181:LEU:HD23	1.92	0.50
2:J:259:SER:HB2	2:J:305:HIS:CG	2.47	0.50
1:A:23:GLY:H	1:A:344:SER:HB2	1.76	0.50
1:D:263:GLN:C	1:D:265:SER:H	2.19	0.50
2:H:260:LEU:HA	2:H:309:GLU:HG2	1.93	0.50
2:J:68:GLU:HG2	2:J:342:PHE:CD1	2.46	0.50
1:C:259:GLU:C	1:C:261:LEU:H	2.19	0.50
1:F:218:TYR:O	1:F:255:PHE:HA	2.11	0.50
2:I:180:MET:HE3	2:I:180:MET:HA	1.93	0.50
1:C:186:THR:HG23	1:C:209:VAL:CG2	2.35	0.50
1:C:189:LEU:HD23	1:C:209:VAL:HB	1.92	0.50
2:I:232:ARG:HE	2:I:234:VAL:HG22	1.77	0.50
1:B:136:ILE:HG22	1:B:138:ALA:H	1.76	0.50
1:A:170:ALA:H	1:A:375:PHE:HZ	1.57	0.49
1:A:299:LEU:HD13	1:A:309:ILE:HG23	1.94	0.49
1:B:213:LYS:HD2	1:B:250:ILE:HG12	1.94	0.49
1:B:265:SER:C	1:B:268:GLY:H	2.19	0.49
1:F:5:ILE:HD12	1:F:102:PRO:HD3	1.93	0.49
1:A:312:ARG:O	1:A:313:MET:C	2.52	0.49
1:D:99:GLU:OE1	1:D:99:GLU:N	2.42	0.49
2:J:259:SER:O	2:J:309:GLU:HB3	2.12	0.49
2:J:256:PHE:HB2	2:J:258:ALA:H	1.76	0.49
2:H:212:ALA:O	2:H:229:VAL:HG22	2.13	0.49
2:I:129:HIS:CD2	2:I:335:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:TYR:CE1	1:C:248:ILE:HG12	2.48	0.49
2:K:199:LYS:HE2	2:K:259:SER:OG	2.12	0.49
2:K:361:GLU:HG2	2:K:362:LEU:N	2.27	0.49
1:C:10:ILE:HD12	1:C:89:THR:HG21	1.94	0.49
1:A:18:LYS:HE2	1:A:337:TYR:HD1	1.76	0.49
1:D:212:ILE:HG23	1:D:216:LEU:HD12	1.94	0.49
1:E:303:THR:C	1:E:305:MET:H	2.21	0.49
1:F:5:ILE:O	1:F:5:ILE:HG13	2.13	0.49
2:K:281:ASP:OD2	2:K:287:LYS:NZ	2.30	0.49
1:A:185:LEU:HD11	1:A:261:LEU:HG	1.95	0.49
1:D:70:PRO:HB3	1:D:81:ASP:OD1	2.13	0.49
1:E:89:THR:HA	1:E:93:GLU:HB2	1.95	0.48
1:C:120:THR:HA	1:C:132:MET:SD	2.53	0.48
1:C:153:MET:HG2	1:C:162:THR:HG22	1.95	0.48
1:F:264:PRO:HB2	1:F:269:MET:HB2	1.95	0.48
2:I:176:LEU:HD23	2:I:177:SER:CB	2.42	0.48
1:A:20:GLY:CA	1:A:28:ARG:H	2.26	0.48
2:I:232:ARG:H	2:I:232:ARG:HG2	1.29	0.48
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.94	0.48
1:F:313:MET:O	1:F:317:ILE:HG22	2.13	0.48
2:J:259:SER:HB2	2:J:305:HIS:ND1	2.28	0.48
2:K:172:LYS:HA	2:K:175:ILE:HG22	1.96	0.48
2:K:358:MET:HA	2:K:361:GLU:OE1	2.13	0.48
1:B:276:GLU:O	1:B:277:THR:C	2.52	0.48
1:F:186:THR:C	1:F:188:TYR:H	2.21	0.48
1:C:212:ILE:HG23	1:C:216:LEU:HD12	1.94	0.48
2:J:229:VAL:HB	2:J:230:PRO:CD	2.44	0.48
1:D:12:ASN:HD21	1:D:86:TRP:HE1	1.60	0.48
2:H:358:MET:C	2:H:360:HIS:N	2.66	0.48
2:J:43:ILE:HD12	2:J:71:TYR:HD1	1.78	0.48
2:I:256:PHE:O	2:I:256:PHE:CD2	2.67	0.47
2:I:345:ALA:O	2:I:349:VAL:HG23	2.14	0.47
2:I:32:LEU:HD12	2:I:45:LEU:HD23	1.96	0.47
2:J:85:ASP:OD1	2:J:88:LYS:NZ	2.47	0.47
1:D:105:LEU:HD11	1:D:123:MET:SD	2.54	0.47
2:K:278:HIS:O	2:K:284:ILE:HD12	2.15	0.47
2:K:284:ILE:HA	2:K:287:LYS:HB2	1.95	0.47
1:A:124:PHE:O	1:A:128:ASN:HA	2.15	0.47
2:I:220:ASN:O	2:I:221:SER:C	2.56	0.47
1:E:37:ARG:O	1:E:38:PRO:C	2.56	0.47
1:A:109:PRO:HG2	1:A:163:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:TYR:O	1:D:192:ILE:HG12	2.14	0.47
1:E:58:ALA:O	1:E:67:LEU:HD21	2.15	0.47
1:F:222:ASP:HB3	1:F:225:GLN:HB3	1.95	0.47
1:F:314:GLN:HG2	1:F:329:ILE:HG13	1.97	0.47
2:I:184:ASN:H	2:I:187:LEU:HG	1.80	0.47
2:H:68:GLU:O	2:H:69:LYS:C	2.55	0.47
2:K:120:ARG:HH11	2:K:217:MET:HG2	1.80	0.47
1:B:143:TYR:CE2	1:B:346:LEU:CD1	2.84	0.47
1:B:251:GLY:C	1:B:253:GLU:H	2.20	0.47
1:D:12:ASN:ND2	1:D:86:TRP:HE1	2.13	0.47
2:J:129:HIS:CE1	2:J:335:LEU:HD13	2.50	0.47
2:J:260:LEU:HA	2:J:309:GLU:CD	2.40	0.47
1:B:192:ILE:HB	1:B:253:GLU:HG2	1.97	0.46
1:B:275:HIS:HA	1:B:313:MET:SD	2.56	0.46
1:F:186:THR:O	1:F:187:ASP:HB2	2.15	0.46
2:H:150:TYR:CD2	2:H:159:VAL:HG22	2.51	0.46
1:A:190:MET:HG2	1:A:209:VAL:HG11	1.97	0.46
1:B:143:TYR:CD2	1:B:346:LEU:CD1	2.73	0.46
2:I:119:ARG:HG2	2:I:255:PRO:HD3	1.97	0.46
1:B:120:THR:CG2	1:B:362:TYR:CD2	2.99	0.46
1:D:287:VAL:HG12	1:D:287:VAL:O	2.15	0.46
2:I:126:TYR:OH	2:I:335:LEU:HB2	2.14	0.46
2:J:212:ALA:HB1	2:J:228:LEU:HD23	1.97	0.46
1:A:16:MET:HE1	1:A:336:LYS:NZ	2.31	0.46
1:C:251:GLY:C	1:C:253:GLU:H	2.23	0.46
1:D:194:THR:HA	1:D:198:TYR:O	2.14	0.46
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.97	0.46
2:J:247:TYR:CD2	2:J:258:ALA:HB1	2.50	0.46
1:A:332:PRO:HD2	1:A:335:ARG:HB3	1.97	0.46
1:B:153:MET:HE3	1:B:153:MET:HB3	1.85	0.46
1:B:98:PRO:HB2	1:B:129:THR:HG22	1.97	0.46
1:C:192:ILE:HG13	1:C:253:GLU:HG2	1.98	0.46
1:F:103:VAL:HG21	1:F:123:MET:HE3	1.97	0.46
2:H:28:ILE:C	2:H:30:LEU:N	2.70	0.46
2:I:34:SER:C	2:I:36:LYS:N	2.73	0.46
2:I:63:PHE:O	2:I:67:ILE:HG12	2.15	0.46
2:I:356:SER:HA	2:I:359:HIS:HB3	1.98	0.46
1:E:16:MET:HB3	1:E:16:MET:HE3	1.71	0.46
1:E:151:ILE:HG23	1:E:297:THR:HG23	1.98	0.46
2:I:112:ASN:O	2:I:116:ASN:HB2	2.16	0.46
2:I:176:LEU:CD2	2:I:177:SER:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:O	1:B:346:LEU:HG	2.15	0.46
1:C:108:ALA:O	1:C:109:PRO:C	2.57	0.46
1:D:137:GLN:HA	1:D:339:VAL:HG13	1.98	0.46
2:H:117:GLU:HA	2:H:120:ARG:HG3	1.98	0.46
2:H:130:LEU:O	2:H:134:ILE:HG12	2.16	0.46
2:J:330:LEU:HD23	2:J:330:LEU:HA	1.78	0.46
1:A:111:ASN:O	1:A:112:PRO:C	2.55	0.45
1:D:152:VAL:HG22	1:D:298:VAL:HG22	1.96	0.45
1:C:12:ASN:HD21	1:C:86:TRP:HE1	1.62	0.45
1:E:228:ALA:C	1:E:230:ALA:H	2.24	0.45
2:I:94:LEU:HB3	2:I:95:SER:H	1.38	0.45
2:I:165:ILE:O	2:I:167:THR:N	2.48	0.45
1:A:272:CYS:HB3	1:A:276:GLU:HB2	1.98	0.45
1:C:54:VAL:HG21	1:C:84:LYS:HB3	1.98	0.45
1:C:208:ILE:HG22	1:C:208:ILE:O	2.15	0.45
2:I:153:VAL:O	2:I:154:LYS:C	2.59	0.45
1:A:72:GLU:C	1:A:74:GLY:N	2.71	0.45
1:A:112:PRO:O	1:A:115:ASN:HB2	2.16	0.45
1:B:114:ALA:O	1:B:118:LYS:N	2.46	0.45
1:D:166:TYR:O	1:D:167:GLU:C	2.59	0.45
1:E:120:THR:O	1:E:124:PHE:HB2	2.16	0.45
2:K:140:LEU:HD13	2:K:140:LEU:HA	1.82	0.45
1:B:16:MET:HE3	1:B:16:MET:HB2	1.87	0.45
1:E:9:VAL:CG1	1:E:340:TRP:CE2	3.00	0.45
1:E:117:GLU:HG3	1:E:371:HIS:CE1	2.52	0.45
1:E:217:CYS:SG	1:E:254:ARG:HA	2.57	0.45
1:F:151:ILE:HG23	1:F:297:THR:HG23	1.99	0.45
1:F:227:MET:HE3	1:F:227:MET:HB3	1.74	0.45
2:I:284:ILE:HG12	2:I:288:VAL:HG23	1.98	0.45
2:J:130:LEU:HD23	2:J:297:SER:HB3	1.99	0.45
1:B:163:VAL:HG22	1:B:175:ILE:HG23	1.98	0.45
2:J:356:SER:O	2:J:359:HIS:HB2	2.17	0.45
2:K:268:MET:HE1	2:K:323:PHE:HZ	1.81	0.45
1:B:276:GLU:C	1:B:278:THR:N	2.71	0.45
1:E:352:PHE:C	1:E:354:GLN:N	2.74	0.45
2:I:285:GLU:O	2:I:289:ASN:HB2	2.17	0.45
1:A:84:LYS:O	1:A:85:ILE:C	2.57	0.45
1:A:350:SER:O	1:A:353:GLN:HB2	2.17	0.45
1:B:360:GLN:O	1:B:361:GLU:C	2.56	0.45
1:E:228:ALA:C	1:E:230:ALA:N	2.75	0.45
2:I:32:LEU:HD21	2:I:102:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:285:GLU:HG3	2:K:328:ILE:HG23	1.99	0.45
1:A:143:TYR:HD1	1:A:143:TYR:HA	1.71	0.45
1:D:159:VAL:HG21	1:D:161:HIS:NE2	2.32	0.45
2:J:209:THR:OG1	2:J:236:LYS:HG2	2.17	0.45
1:A:114:ALA:C	1:A:116:ARG:H	2.25	0.45
1:B:87:HIS:O	1:B:91:TYR:HB2	2.17	0.45
1:D:242:LEU:HD11	1:D:248:ILE:HD11	1.99	0.45
1:F:208:ILE:H	1:F:208:ILE:HG12	1.56	0.45
2:H:132:SER:HA	2:H:135:LYS:HB2	1.98	0.45
2:I:199:LYS:HE3	2:I:259:SER:HB2	1.98	0.45
2:J:239:ILE:HG13	2:J:257:VAL:HG12	1.99	0.45
1:B:335:ARG:HA	1:B:338:SER:HB3	1.99	0.44
1:D:73:HIS:HB3	1:D:177:ARG:NH2	2.32	0.44
1:D:335:ARG:H	1:D:335:ARG:HG2	1.59	0.44
2:H:213:ASN:HA	2:H:214:PRO:HD3	1.87	0.44
1:A:6:ALA:O	1:A:102:PRO:HD2	2.17	0.44
1:C:189:LEU:HA	1:C:192:ILE:HG12	1.99	0.44
1:D:275:HIS:H	1:D:275:HIS:CD2	2.34	0.44
1:D:113:LYS:HD2	1:D:113:LYS:N	2.31	0.44
1:E:142:LEU:HD13	1:E:152:VAL:HG22	1.98	0.44
2:H:200:ASP:OD1	2:H:200:ASP:N	2.51	0.44
2:J:54:LEU:HD11	2:J:86:PHE:CE1	2.49	0.44
1:B:136:ILE:HB	1:B:139:VAL:HG23	2.00	0.44
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.88	0.44
1:D:159:VAL:HG23	1:D:161:HIS:NE2	2.32	0.44
2:J:196:TYR:N	2:J:197:PRO:HD2	2.32	0.44
2:I:28:ILE:C	2:I:30:LEU:H	2.25	0.44
1:E:9:VAL:HG13	1:E:9:VAL:O	2.18	0.44
1:F:189:LEU:HG	1:F:193:LEU:HD12	1.99	0.44
2:H:196:TYR:O	2:H:199:LYS:HG3	2.18	0.44
1:D:73:HIS:HA	1:D:159:VAL:HG13	1.99	0.44
1:E:99:GLU:H	1:E:99:GLU:HG2	1.50	0.44
1:E:113:LYS:HB3	1:E:113:LYS:HE3	1.78	0.44
2:H:28:ILE:HG22	2:H:32:LEU:HG	2.00	0.44
2:I:212:ALA:C	2:I:229:VAL:HG22	2.43	0.44
1:B:83:GLU:HG2	1:B:122:ILE:HD13	2.00	0.44
1:B:180:LEU:HD21	1:B:261:LEU:HA	1.98	0.44
1:D:37:ARG:HB2	1:D:37:ARG:NH1	2.32	0.44
1:E:136:ILE:HB	1:E:139:VAL:HG23	1.99	0.44
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.00	0.43
1:B:189:LEU:HD13	1:B:257:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:HIS:CD2	1:F:276:GLU:HG3	2.53	0.43
2:H:121:LEU:O	2:H:122:TYR:C	2.60	0.43
1:A:127:PHE:O	1:A:128:ASN:C	2.60	0.43
1:A:192:ILE:HB	1:A:253:GLU:HG2	1.99	0.43
1:C:281:SER:C	1:C:283:MET:N	2.74	0.43
1:C:341:ILE:O	1:C:345:ILE:HG13	2.17	0.43
2:I:213:ASN:HD21	2:I:227:ASN:HB3	1.82	0.43
1:A:124:PHE:CE2	1:A:132:MET:HG2	2.54	0.43
1:C:148:THR:OG1	2:I:359:HIS:ND1	2.42	0.43
1:E:305:MET:HE3	1:E:305:MET:HB3	1.95	0.43
1:B:119:MET:HB2	1:B:132:MET:HE1	2.01	0.43
1:F:213:LYS:HE2	1:F:213:LYS:HB3	1.88	0.43
1:D:163:VAL:HG13	1:D:175:ILE:HG12	2.01	0.43
2:I:278:HIS:C	2:I:280:THR:N	2.75	0.43
2:K:144:ASN:O	2:K:147:ARG:HB3	2.19	0.43
2:K:353:THR:O	2:K:357:ALA:N	2.44	0.43
1:A:78:ASN:HD22	1:A:78:ASN:HA	1.59	0.43
1:A:164:PRO:HG2	1:A:174:ALA:CB	2.47	0.43
1:C:171:LEU:O	1:C:175:ILE:HG13	2.18	0.43
2:K:155:PRO:O	2:K:158:ALA:HB2	2.19	0.43
1:D:39:ARG:H	1:D:65:LEU:N	2.17	0.43
1:E:345:ILE:O	1:E:349:LEU:HG	2.18	0.43
1:F:5:ILE:CD1	1:F:102:PRO:HD3	2.48	0.43
2:I:331:ASN:HD22	2:I:331:ASN:HA	1.53	0.43
2:J:101:ARG:O	2:J:105:VAL:HG23	2.19	0.43
1:B:154:ASP:O	1:B:160:THR:HA	2.19	0.43
1:D:189:LEU:HD23	1:D:209:VAL:HG13	2.00	0.43
2:I:196:TYR:O	2:I:199:LYS:HG3	2.19	0.43
1:C:193:LEU:HD21	1:C:250:ILE:HG23	2.01	0.43
1:C:261:LEU:O	1:C:273:GLY:HA2	2.19	0.43
2:H:121:LEU:O	2:H:125:LEU:HG	2.19	0.43
2:H:176:LEU:HD23	2:H:299:TYR:CE1	2.53	0.43
1:A:344:SER:O	1:A:345:ILE:C	2.60	0.43
1:B:274:ILE:HG13	1:B:313:MET:HE1	2.01	0.43
1:C:26:ALA:O	1:C:27:PRO:C	2.60	0.43
1:F:313:MET:O	1:F:314:GLN:C	2.61	0.43
2:K:123:GLU:HB3	2:K:300:ILE:HG21	2.00	0.43
2:K:356:SER:O	2:K:359:HIS:ND1	2.52	0.43
1:D:11:ASP:HA	1:D:106:THR:OG1	2.19	0.42
1:F:96:VAL:HB	1:F:101:HIS:CE1	2.53	0.42
2:H:63:PHE:HE2	2:H:83:ILE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:256:PHE:HB3	2:J:257:VAL:H	1.30	0.42
1:B:283:MET:HE3	1:B:283:MET:HB3	1.85	0.42
1:E:132:MET:HB2	1:E:132:MET:HE3	1.53	0.42
1:B:251:GLY:C	1:B:253:GLU:N	2.73	0.42
2:H:358:MET:C	2:H:360:HIS:H	2.28	0.42
2:K:175:ILE:HD11	2:K:291:ILE:HG23	2.01	0.42
1:C:259:GLU:O	1:C:260:ALA:C	2.60	0.42
1:E:219:VAL:HG22	1:E:258:PRO:CB	2.50	0.42
1:F:37:ARG:HH22	1:F:81:ASP:CG	2.28	0.42
2:J:43:ILE:HD12	2:J:71:TYR:CD1	2.54	0.42
2:K:202:SER:HB2	2:K:240:ASN:HB2	2.01	0.42
2:K:214:PRO:HB2	2:K:301:LYS:O	2.20	0.42
2:H:316:GLU:O	2:H:317:PRO:C	2.58	0.42
2:I:72:PHE:HA	2:I:119:ARG:HH12	1.83	0.42
2:K:200:ASP:OD1	2:K:247:TYR:HB3	2.19	0.42
1:D:287:VAL:O	1:D:287:VAL:CG1	2.68	0.42
1:E:120:THR:CG2	1:E:370:VAL:HB	2.49	0.42
1:E:354:GLN:HE21	1:E:354:GLN:HB2	1.70	0.42
1:F:292:ASP:O	1:F:296:ASN:HB2	2.19	0.42
2:I:176:LEU:HG	2:I:270:VAL:HG21	2.02	0.42
2:K:77:LYS:HG3	2:K:81:GLU:OE2	2.20	0.42
1:B:193:LEU:C	1:B:195:GLU:H	2.27	0.42
1:B:213:LYS:C	1:B:215:LYS:H	2.28	0.42
1:B:305:MET:HE3	1:B:305:MET:HB3	1.85	0.42
1:C:305:MET:HE3	1:C:305:MET:HB3	1.79	0.42
1:F:286:ASP:O	1:F:289:ILE:HG12	2.20	0.42
1:F:303:THR:O	1:F:303:THR:CG2	2.66	0.42
2:I:212:ALA:O	2:I:229:VAL:HG22	2.19	0.42
2:J:23:LYS:HE3	2:J:23:LYS:HB3	1.91	0.42
1:B:255:PHE:O	1:B:259:GLU:HB2	2.19	0.42
1:B:260:ALA:HB1	1:B:267:LEU:HD13	2.02	0.42
1:C:251:GLY:O	1:C:252:ASN:HB2	2.20	0.42
1:C:313:MET:HE2	1:C:313:MET:HB3	1.87	0.42
1:F:317:ILE:HG21	1:F:329:ILE:HD11	2.02	0.42
2:I:34:SER:C	2:I:36:LYS:H	2.26	0.42
2:J:259:SER:HB2	2:J:305:HIS:CB	2.49	0.42
2:K:217:MET:HE1	2:K:236:LYS:HA	2.02	0.42
1:C:286:ASP:O	1:C:290:ARG:HG3	2.20	0.42
1:E:14:SER:CB	1:E:158:GLY:HA3	2.50	0.42
1:F:219:VAL:HG12	1:F:258:PRO:HB3	2.02	0.42
2:I:32:LEU:CD1	2:I:45:LEU:HD23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:95:SER:OG	2:J:98:VAL:HG23	2.20	0.42
2:K:364:GLU:O	2:K:368:ASN:N	2.53	0.42
1:E:355:MET:HG3	2:K:358:MET:SD	2.60	0.41
1:F:281:SER:OG	1:F:282:ILE:N	2.53	0.41
2:J:296:ILE:HG12	2:J:310:VAL:HG11	2.02	0.41
1:D:70:PRO:HG2	1:D:85:ILE:HD11	2.02	0.41
1:D:305:MET:HE3	1:D:305:MET:HB3	1.74	0.41
1:F:339:VAL:HG13	1:F:340:TRP:N	2.36	0.41
2:I:39:GLU:HA	2:I:109:LEU:HD13	2.01	0.41
1:A:34:ILE:HG22	1:A:67:LEU:HD23	2.03	0.41
1:C:262:PHE:HE2	1:C:313:MET:HG3	1.85	0.41
2:H:356:SER:HA	2:H:359:HIS:HB2	2.02	0.41
2:J:247:TYR:CE2	2:J:258:ALA:HB1	2.55	0.41
1:A:191:LYS:O	1:A:194:THR:HB	2.20	0.41
1:D:8:LEU:HD13	1:D:90:PHE:HE1	1.85	0.41
1:E:213:LYS:HE3	1:E:214:GLU:OE1	2.19	0.41
1:F:190:MET:O	1:F:194:THR:HG23	2.21	0.41
2:H:256:PHE:O	2:H:256:PHE:CG	2.73	0.41
1:A:171:LEU:O	1:A:175:ILE:HG13	2.20	0.41
1:E:35:VAL:HG23	1:E:70:PRO:HD3	2.03	0.41
1:F:61:LYS:HB2	1:F:65:LEU:HG	2.03	0.41
2:I:176:LEU:CD2	2:I:177:SER:CB	2.98	0.41
2:K:268:MET:HE3	2:K:314:LEU:CD2	2.51	0.41
1:A:103:VAL:O	1:A:132:MET:HA	2.21	0.41
1:A:166:TYR:C	1:A:168:GLY:N	2.77	0.41
1:C:303:THR:O	1:C:303:THR:CG2	2.68	0.41
1:D:136:ILE:HG22	1:D:138:ALA:H	1.84	0.41
1:D:163:VAL:HG22	1:D:175:ILE:HG23	2.01	0.41
1:E:175:ILE:O	1:E:175:ILE:HG13	2.21	0.41
1:F:142:LEU:HD22	1:F:165:ILE:HD12	2.02	0.41
1:F:155:SER:HB2	1:F:304:THR:HG23	2.03	0.41
2:H:67:ILE:HG23	2:H:79:ALA:HB1	2.01	0.41
2:K:180:MET:O	2:K:181:LEU:C	2.60	0.41
1:A:132:MET:HB2	1:A:132:MET:HE3	1.57	0.41
1:F:107:GLU:O	1:F:137:GLN:HG3	2.20	0.41
2:H:88:LYS:HA	2:H:91:GLU:HG3	2.02	0.41
2:H:366:PHE:C	2:H:368:ASN:H	2.28	0.41
1:D:87:HIS:O	1:D:91:TYR:N	2.50	0.41
1:E:9:VAL:HG13	1:E:340:TRP:HE1	1.84	0.41
1:E:287:VAL:H	1:E:287:VAL:HG23	1.65	0.41
2:H:187:LEU:O	2:H:188:PRO:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:221:SER:HB3	2:I:348:TYR:OH	2.21	0.41
1:B:213:LYS:H	1:B:213:LYS:HG2	1.17	0.41
1:B:256:ARG:HE	1:B:256:ARG:HB3	1.77	0.41
1:B:368:SER:C	1:B:370:VAL:N	2.79	0.41
1:C:155:SER:O	1:C:301:GLY:HA3	2.21	0.41
1:C:278:THR:O	1:C:282:ILE:HG13	2.21	0.41
1:E:341:ILE:O	1:E:345:ILE:HG13	2.21	0.41
2:H:342:PHE:O	2:H:346:GLN:HG3	2.20	0.41
2:I:142:VAL:HB	2:I:287:LYS:HB3	2.02	0.41
2:I:228:LEU:HA	2:I:228:LEU:HD23	1.78	0.41
2:J:255:PRO:O	2:J:256:PHE:HB2	2.20	0.41
2:J:309:GLU:O	2:J:310:VAL:C	2.60	0.41
1:A:193:LEU:C	1:A:195:GLU:N	2.78	0.41
1:B:193:LEU:C	1:B:195:GLU:N	2.76	0.41
1:C:12:ASN:HD21	1:C:86:TRP:NE1	2.17	0.41
2:J:129:HIS:O	2:J:133:VAL:HG23	2.20	0.41
1:D:227:MET:HB3	1:D:227:MET:HE3	1.86	0.40
2:K:268:MET:HG3	2:K:319:LEU:HD22	2.03	0.40
1:B:32:PRO:HB2	1:B:34:ILE:HG12	2.03	0.40
1:E:37:ARG:HB3	1:E:38:PRO:HD2	2.03	0.40
1:E:110:LEU:HB2	1:E:175:ILE:HD11	2.02	0.40
1:C:111:ASN:O	1:C:112:PRO:C	2.57	0.40
1:D:241:GLU:CD	1:D:241:GLU:C	2.90	0.40
1:D:350:SER:HA	1:D:353:GLN:HG2	2.04	0.40
1:F:165:ILE:HD13	1:F:165:ILE:HG21	1.77	0.40
2:J:337:ASP:OD1	2:J:339:HIS:ND1	2.53	0.40
1:A:161:HIS:CD2	1:A:177:ARG:HB3	2.56	0.40
1:A:191:LYS:HE2	1:A:191:LYS:HB2	1.89	0.40
1:A:276:GLU:C	1:A:278:THR:N	2.78	0.40
1:B:89:THR:O	1:B:94:LEU:HB2	2.20	0.40
1:B:118:LYS:HD2	1:B:118:LYS:HA	1.90	0.40
1:C:186:THR:CG2	1:C:209:VAL:CG2	2.96	0.40
1:D:151:ILE:HD13	1:D:282:ILE:HG13	2.03	0.40
2:I:28:ILE:HG22	2:I:32:LEU:HD11	2.01	0.40
1:E:113:LYS:H	1:E:113:LYS:HG2	1.69	0.40
1:F:31:PHE:HZ	1:F:89:THR:OG1	2.05	0.40
1:F:109:PRO:HD2	1:F:161:HIS:CD2	2.56	0.40
2:H:162:GLU:O	2:H:163:THR:C	2.65	0.40
2:H:245:GLY:O	2:H:246:GLY:C	2.61	0.40
2:H:349:VAL:O	2:H:350:PHE:C	2.64	0.40
2:J:102:LEU:C	2:J:104:GLU:H	2.29	0.40

There are no symmetry-related clashes.

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	310/375 (83%)	292 (94%)	17 (6%)	1 (0%)	36	65
1	B	335/375 (89%)	323 (96%)	12 (4%)	0	100	100
1	C	332/375 (88%)	316 (95%)	16 (5%)	0	100	100
1	D	346/375 (92%)	328 (95%)	18 (5%)	0	100	100
1	E	304/375 (81%)	283 (93%)	21 (7%)	0	100	100
1	F	330/375 (88%)	318 (96%)	12 (4%)	0	100	100
2	H	344/441 (78%)	321 (93%)	23 (7%)	0	100	100
2	I	325/441 (74%)	301 (93%)	24 (7%)	0	100	100
2	J	337/441 (76%)	315 (94%)	21 (6%)	1 (0%)	36	65
2	K	321/441 (73%)	305 (95%)	16 (5%)	0	100	100
All	All	3284/4014 (82%)	3102 (94%)	180 (6%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
2	J	214	PRO

5.3.2 Protein sidechains [i](#)

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	275/318 (86%)	255 (93%)	20 (7%)	13	37
1	B	289/318 (91%)	268 (93%)	21 (7%)	13	37
1	C	292/318 (92%)	278 (95%)	14 (5%)	23	48
1	D	302/318 (95%)	288 (95%)	14 (5%)	24	49
1	E	270/318 (85%)	253 (94%)	17 (6%)	16	41
1	F	287/318 (90%)	270 (94%)	17 (6%)	18	43
2	H	322/408 (79%)	300 (93%)	22 (7%)	14	39
2	I	308/408 (76%)	292 (95%)	16 (5%)	21	47
2	J	317/408 (78%)	310 (98%)	7 (2%)	45	63
2	K	305/408 (75%)	297 (97%)	8 (3%)	40	60
All	All	2967/3540 (84%)	2811 (95%)	156 (5%)	20	46

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	85	ILE
1	A	95	ARG
1	A	141	SER
1	A	143	TYR
1	A	152	VAL
1	A	159	VAL
1	A	160	THR
1	A	192	ILE
1	A	202	THR
1	A	209	VAL
1	A	256	ARG
1	A	263	GLN
1	A	303	THR
1	A	317	ILE
1	A	322	PRO
1	A	327	ILE
1	A	349	LEU
1	A	354	GLN
1	A	368	SER
1	B	14	SER
1	B	37	ARG
1	B	75	ILE
1	B	76	VAL

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Mol	Chain	Res	Type
1	B	85	ILE
1	B	99	GLU
1	B	107	GLU
1	B	118	LYS
1	B	134	VAL
1	B	145	SER
1	B	151	ILE
1	B	165	ILE
1	B	176	LEU
1	B	185	LEU
1	B	212	ILE
1	B	213	LYS
1	B	219	VAL
1	B	227	MET
1	B	270	GLU
1	B	341	ILE
1	B	361	GLU
1	C	27	PRO
1	C	32	PRO
1	C	34	ILE
1	C	35	VAL
1	C	105	LEU
1	C	153	MET
1	C	211	ASP
1	C	214	GLU
1	C	248	ILE
1	C	298	VAL
1	C	327	ILE
1	C	334	GLU
1	C	337	TYR
1	C	341	ILE
1	D	25	ASP
1	D	34	ILE
1	D	51	ASP
1	D	56	ASP
1	D	71	ILE
1	D	87	HIS
1	D	120	THR
1	D	208	ILE
1	D	229	THR
1	D	234	SER
1	D	250	ILE

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Mol	Chain	Res	Type
1	D	258	PRO
1	D	298	VAL
1	D	334	GLU
1	E	59	GLN
1	E	66	THR
1	E	99	GLU
1	E	104	LEU
1	E	129	THR
1	E	149	THR
1	E	165	ILE
1	E	169	TYR
1	E	175	ILE
1	E	226	GLU
1	E	247	VAL
1	E	249	THR
1	E	267	LEU
1	E	276	GLU
1	E	325	MET
1	E	330	ILE
1	E	334	GLU
1	F	30	VAL
1	F	56	ASP
1	F	57	GLU
1	F	104	LEU
1	F	208	ILE
1	F	219	VAL
1	F	221	LEU
1	F	309	ILE
1	F	318	THR
1	F	322	PRO
1	F	324	THR
1	F	327	ILE
1	F	334	GLU
1	F	350	SER
1	F	351	THR
1	F	359	LYS
1	F	370	VAL
2	H	37	LEU
2	H	59	GLU
2	H	160	THR
2	H	161	HIS
2	H	162	GLU

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Mol	Chain	Res	Type
2	H	167	THR
2	H	175	ILE
2	H	182	ASN
2	H	185	VAL
2	H	192	GLN
2	H	200	ASP
2	H	209	THR
2	H	213	ASN
2	H	216	ILE
2	H	220	ASN
2	H	221	SER
2	H	226	ASP
2	H	233	ASP
2	H	257	VAL
2	H	279	LYS
2	H	322	ILE
2	H	360	HIS
2	I	28	ILE
2	I	45	LEU
2	I	96	GLU
2	I	133	VAL
2	I	175	ILE
2	I	176	LEU
2	I	179	VAL
2	I	180	MET
2	I	181	LEU
2	I	197	PRO
2	I	211	SER
2	I	220	ASN
2	I	230	PRO
2	I	315	THR
2	I	331	ASN
2	I	337	ASP
2	J	43	ILE
2	J	116	ASN
2	J	167	THR
2	J	170	GLU
2	J	216	ILE
2	J	248	SER
2	J	279	LYS
2	K	49	TYR
2	K	110	LYS

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Mol	Chain	Res	Type
2	K	170	GLU
2	K	197	PRO
2	K	224	PHE
2	K	292	ILE
2	K	320	GLN
2	K	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	78	ASN
1	A	87	HIS
1	A	128	ASN
1	A	161	HIS
1	A	225	GLN
1	A	296	ASN
1	A	354	GLN
1	B	88	HIS
1	B	101	HIS
1	B	121	GLN
1	B	128	ASN
1	B	225	GLN
1	B	252	ASN
1	B	360	GLN
1	C	128	ASN
1	D	12	ASN
1	D	92	ASN
1	D	115	ASN
1	D	128	ASN
1	D	252	ASN
1	D	275	HIS
1	D	296	ASN
1	E	59	GLN
1	E	87	HIS
1	E	111	ASN
1	E	275	HIS
1	E	371	HIS
1	F	225	GLN
1	F	252	ASN
2	H	151	ASN
2	H	278	HIS

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Mol	Chain	Res	Type
2	H	346	GLN
2	H	368	ASN
2	I	116	ASN
2	I	129	HIS
2	I	182	ASN
2	I	278	HIS
2	I	320	GLN
2	I	331	ASN
2	I	346	GLN
2	I	355	GLN
2	I	360	HIS
2	I	363	GLN
2	J	129	HIS
2	J	278	HIS
2	J	355	GLN
2	K	74	GLN
2	K	151	ASN
2	K	184	ASN
2	K	305	HIS
2	K	320	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	322/375 (85%)	1.90	134 (41%) 0 1	30, 96, 106, 116	0
1	B	343/375 (91%)	1.65	111 (32%) 1 1	40, 84, 100, 161	0
1	C	342/375 (91%)	0.74	28 (8%) 17 15	30, 43, 57, 75	0
1	D	354/375 (94%)	0.76	30 (8%) 16 14	30, 46, 58, 78	0
1	E	318/375 (84%)	0.91	35 (11%) 10 11	32, 49, 63, 77	0
1	F	338/375 (90%)	0.91	25 (7%) 20 17	38, 52, 62, 92	0
2	H	348/441 (78%)	0.79	30 (8%) 16 14	30, 47, 65, 88	0
2	I	335/441 (75%)	0.91	37 (11%) 10 11	33, 46, 61, 77	0
2	J	343/441 (77%)	0.80	30 (8%) 16 14	27, 43, 59, 75	0
2	K	331/441 (75%)	1.12	53 (16%) 5 6	36, 52, 72, 515	0
All	All	3374/4014 (84%)	1.04	513 (15%) 5 7	27, 50, 98, 515	0

All (513) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	220	ASN	10.3
2	K	275	ILE	9.3
1	F	63	GLY	6.9
2	I	184	ASN	6.1
1	B	83	GLU	6.1
2	K	217	MET	6.0
2	I	186	GLU	5.7
2	I	169	ASP	5.4
2	I	363	GLN	5.4
2	J	309	GLU	5.3
1	B	217	CYS	5.2
1	B	357	ILE	5.2
1	A	83	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	271	SER	5.2
1	A	35	VAL	5.1
1	A	309	ILE	5.0
1	B	141	SER	5.0
2	J	214	PRO	5.0
1	D	36	GLY	5.0
1	A	348	SER	5.0
2	I	177	SER	5.0
2	I	180	MET	4.9
1	B	358	SER	4.8
1	B	353	GLN	4.8
1	A	375	PHE	4.8
2	J	256	PHE	4.8
1	A	272	CYS	4.7
1	C	355	MET	4.4
1	A	294	TYR	4.3
1	B	359	LYS	4.3
1	A	34	ILE	4.3
1	C	250	ILE	4.3
2	K	276	GLU	4.3
2	K	274	TYR	4.3
2	I	206	LEU	4.1
1	E	212	ILE	4.1
2	K	138	SER	4.1
2	K	248	SER	4.1
1	A	80	ASP	4.0
1	C	133	TYR	4.0
1	B	293	LEU	4.0
1	A	32	PRO	4.0
1	B	24	ASP	4.0
1	B	63	GLY	3.9
1	B	211	ASP	3.9
1	E	169	TYR	3.9
1	A	231	ALA	3.9
1	A	159	VAL	3.9
1	B	32	PRO	3.9
1	B	195	GLU	3.8
1	B	355	MET	3.8
2	H	362	LEU	3.8
1	C	242	LEU	3.8
1	B	188	TYR	3.7
1	B	275	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	367	PRO	3.7
1	D	66	THR	3.7
2	K	159	VAL	3.7
1	E	272	CYS	3.7
2	I	220	ASN	3.7
1	B	108	ALA	3.6
1	F	169	TYR	3.6
2	K	209	THR	3.6
1	B	294	TYR	3.6
2	H	80	ILE	3.6
2	K	206	LEU	3.6
2	H	20	SER	3.6
2	K	200	ASP	3.6
1	A	26	ALA	3.6
2	K	219	PRO	3.6
1	B	240	TYR	3.6
1	B	346	LEU	3.5
1	B	297	THR	3.5
2	J	219	PRO	3.5
1	B	242	LEU	3.5
1	A	250	ILE	3.5
1	B	279	PHE	3.5
1	A	328	LYS	3.5
1	A	79	TRP	3.5
1	A	143	TYR	3.5
1	C	134	VAL	3.5
1	D	65	LEU	3.5
1	A	341	ILE	3.5
1	B	198	TYR	3.4
1	B	92	ASN	3.4
1	B	366	GLY	3.4
2	I	176	LEU	3.4
1	B	212	ILE	3.4
1	E	327	ILE	3.4
2	H	157	TYR	3.4
2	K	150	TYR	3.4
1	B	180	LEU	3.4
2	H	203	ARG	3.4
1	A	374	CYS	3.4
1	A	21	PHE	3.4
1	A	127	PHE	3.4
1	A	103	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	158	ALA	3.4
2	K	212	ALA	3.4
1	A	98	PRO	3.4
1	D	354	GLN	3.4
2	K	111	SER	3.3
1	A	95	ARG	3.3
1	B	374	CYS	3.3
1	D	56	ASP	3.3
2	I	140	LEU	3.3
1	A	344	SER	3.3
1	A	369	ILE	3.3
2	H	163	THR	3.3
1	B	127	PHE	3.3
1	B	339	VAL	3.3
1	A	33	SER	3.3
1	A	9	VAL	3.3
1	B	60	SER	3.2
1	A	370	VAL	3.2
2	J	258	ALA	3.2
1	D	20	GLY	3.2
1	A	330	ILE	3.2
1	B	95	ARG	3.2
1	A	31	PHE	3.2
1	F	34	ILE	3.2
1	A	22	ALA	3.2
1	A	84	LYS	3.2
2	I	222	PRO	3.2
1	A	109	PRO	3.1
1	A	322	PRO	3.1
2	H	329	LYS	3.1
2	H	357	ALA	3.1
2	K	350	PHE	3.1
1	A	275	HIS	3.1
2	K	215	GLY	3.1
2	K	366	PHE	3.1
1	B	34	ILE	3.1
1	F	64	ILE	3.1
1	C	58	ALA	3.1
1	B	33	SER	3.1
1	F	157	ASP	3.1
2	H	38	ASP	3.1
2	K	160	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	39	ARG	3.1
2	I	61	SER	3.1
1	B	299	LEU	3.0
2	K	213	ASN	3.0
1	A	249	THR	3.0
1	D	241	GLU	3.0
2	K	238	ALA	3.0
1	B	256	ARG	3.0
1	B	282	ILE	3.0
1	D	355	MET	3.0
2	K	168	LEU	3.0
1	B	119	MET	3.0
1	B	133	TYR	3.0
1	C	56	ASP	3.0
2	I	88	LYS	3.0
1	B	132	MET	3.0
2	K	359	HIS	3.0
1	A	255	PHE	3.0
1	A	221	LEU	2.9
1	E	216	LEU	2.9
1	B	79	TRP	2.9
1	B	291	LYS	2.9
1	A	329	ILE	2.9
1	A	125	GLU	2.9
1	B	224	GLU	2.9
1	A	86	TRP	2.9
1	A	247	VAL	2.9
1	F	127	PHE	2.9
1	F	221	LEU	2.9
1	A	204	ALA	2.9
2	H	257	VAL	2.9
1	F	95	ARG	2.9
1	B	59	GLN	2.8
2	I	200	ASP	2.8
2	K	273	ASP	2.8
2	K	272	THR	2.8
1	E	84	LYS	2.8
1	A	132	MET	2.8
1	A	327	ILE	2.8
1	C	240	TYR	2.8
1	A	203	THR	2.8
2	J	38	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	187	LEU	2.8
1	A	8	LEU	2.8
1	A	347	ALA	2.8
1	A	372	ARG	2.8
1	B	247	VAL	2.8
1	E	60	SER	2.8
2	I	225	THR	2.8
1	A	154	ASP	2.8
2	I	183	ASP	2.8
1	F	153	MET	2.8
1	A	27	PRO	2.8
1	C	159	VAL	2.8
2	K	142	VAL	2.8
1	B	8	LEU	2.8
1	A	93	GLU	2.8
1	A	274	ILE	2.8
1	B	248	ILE	2.8
1	B	375	PHE	2.7
1	A	287	VAL	2.7
1	E	226	GLU	2.7
1	F	14	SER	2.7
1	E	15	GLY	2.7
1	B	62	ARG	2.7
2	J	195	ARG	2.7
1	A	188	TYR	2.7
1	B	328	LYS	2.7
2	I	179	VAL	2.7
1	D	327	ILE	2.7
1	A	355	MET	2.7
1	B	148	THR	2.7
1	D	25	ASP	2.7
1	A	161	HIS	2.7
2	H	208	ASN	2.7
2	I	257	VAL	2.7
1	A	67	LEU	2.7
1	A	353	GLN	2.7
1	A	248	ILE	2.7
1	B	123	MET	2.7
2	J	217	MET	2.7
1	F	365	SER	2.7
1	F	69	TYR	2.7
1	A	289	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	2.7
2	K	328	ILE	2.7
1	D	359	LYS	2.7
1	E	23	GLY	2.7
2	H	117	GLU	2.7
1	A	323	SER	2.7
1	E	155	SER	2.7
1	A	337	TYR	2.7
1	C	128	ASN	2.7
2	K	237	ILE	2.6
2	K	62	GLY	2.6
1	A	257	CYS	2.6
1	B	178	LEU	2.6
2	I	308	SER	2.6
1	A	81	ASP	2.6
2	J	45	LEU	2.6
1	B	326	LYS	2.6
1	A	200	PHE	2.6
2	K	271	LEU	2.6
1	A	198	TYR	2.6
1	E	344	SER	2.6
1	F	12	ASN	2.6
2	K	229	VAL	2.6
1	B	16	MET	2.6
1	A	150	GLY	2.6
1	A	94	LEU	2.6
1	A	104	LEU	2.6
1	E	159	VAL	2.6
1	E	66	THR	2.6
1	C	208	ILE	2.5
1	B	223	PHE	2.5
2	K	49	TYR	2.5
1	A	308	GLY	2.5
1	A	252	ASN	2.5
1	A	253	GLU	2.5
1	B	213	LYS	2.5
2	H	88	LYS	2.5
2	H	287	LYS	2.5
1	B	86	TRP	2.5
2	J	160	THR	2.5
1	C	257	CYS	2.5
1	B	12	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	26	ALA	2.5
2	J	327	ASN	2.5
2	K	223	ASN	2.5
1	A	165	ILE	2.5
1	A	277	THR	2.5
1	A	113	LYS	2.5
1	D	336	LYS	2.5
1	E	94	LEU	2.5
2	I	341	GLU	2.5
1	A	340	TRP	2.5
1	A	306	TYR	2.5
2	K	222	PRO	2.5
2	I	185	VAL	2.5
1	D	33	SER	2.5
2	I	46	SER	2.5
2	K	279	LYS	2.5
2	J	130	LEU	2.5
1	A	218	TYR	2.5
1	B	166	TYR	2.5
2	K	199	LYS	2.4
1	B	152	VAL	2.4
1	E	175	ILE	2.4
1	A	16	MET	2.4
1	A	82	MET	2.4
1	E	153	MET	2.4
2	H	213	ASN	2.4
1	A	112	PRO	2.4
1	A	209	VAL	2.4
1	C	192	ILE	2.4
1	F	122	ILE	2.4
1	B	255	PHE	2.4
2	J	68	GLU	2.4
2	K	224	PHE	2.4
1	E	221	LEU	2.4
1	A	288	ASP	2.4
1	A	91	TYR	2.4
1	A	371	HIS	2.4
1	C	204	ALA	2.4
1	A	313	MET	2.4
1	A	256	ARG	2.4
1	B	37	ARG	2.4
1	D	242	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	35	VAL	2.4
1	B	15	GLY	2.4
2	H	207	GLY	2.4
2	K	148	ASP	2.4
1	D	135	ALA	2.4
2	J	64	PHE	2.4
1	A	105	LEU	2.4
1	A	349	LEU	2.4
1	B	185	LEU	2.4
2	H	156	GLU	2.4
2	I	91	GLU	2.4
1	E	14	SER	2.4
1	A	76	VAL	2.4
1	B	367	PRO	2.4
2	J	159	VAL	2.4
2	H	280	THR	2.3
1	A	92	ASN	2.3
1	A	111	ASN	2.3
1	A	220	ALA	2.3
2	K	265	TYR	2.3
1	C	354	GLN	2.3
2	I	256	PHE	2.3
1	B	72	GLU	2.3
2	I	141	SER	2.3
1	B	373	LYS	2.3
1	D	34	ILE	2.3
1	B	179	ASP	2.3
1	A	110	LEU	2.3
1	B	104	LEU	2.3
1	B	266	PHE	2.3
1	E	225	GLN	2.3
2	J	205	GLU	2.3
1	A	118	LYS	2.3
1	B	245	GLY	2.3
1	A	229	THR	2.3
1	A	351	THR	2.3
1	D	16	MET	2.3
1	E	16	MET	2.3
1	B	252	ASN	2.3
1	C	236	LEU	2.3
2	J	173	GLN	2.3
2	H	162	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	328	ILE	2.3
2	K	230	PRO	2.3
1	C	158	GLY	2.3
1	A	297	THR	2.3
1	B	186	THR	2.3
2	H	32	LEU	2.3
2	H	184	ASN	2.3
1	C	225	GLN	2.3
1	B	238	LYS	2.3
1	B	241	GLU	2.3
1	B	130	PRO	2.3
1	E	182	GLY	2.3
2	I	244	ALA	2.3
1	B	356	TRP	2.3
1	A	299	LEU	2.3
1	E	133	TYR	2.3
1	A	363	ASP	2.3
1	E	57	GLU	2.2
1	B	330	ILE	2.2
1	A	268	GLY	2.2
2	J	335	LEU	2.2
1	E	31	PHE	2.2
1	E	337	TYR	2.2
1	A	134	VAL	2.2
1	A	219	VAL	2.2
1	C	247	VAL	2.2
1	B	329	ILE	2.2
1	B	153	MET	2.2
1	F	106	THR	2.2
2	J	135	LYS	2.2
2	K	339	HIS	2.2
2	K	363	GLN	2.2
1	A	117	GLU	2.2
1	F	5	ILE	2.2
1	C	343	GLY	2.2
1	F	18	LYS	2.2
1	B	160	THR	2.2
1	E	186	THR	2.2
2	J	161	HIS	2.2
1	E	152	VAL	2.2
1	D	300	SER	2.2
1	A	193	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	140	LEU	2.2
2	H	137	GLU	2.2
2	I	32	LEU	2.2
2	I	130	LEU	2.2
2	I	131	GLU	2.2
2	J	54	LEU	2.2
1	B	36	GLY	2.2
1	D	181	ALA	2.2
1	E	38	PRO	2.2
2	H	214	PRO	2.2
1	A	315	LYS	2.2
1	B	286	ASP	2.2
1	C	223	PHE	2.2
1	D	129	THR	2.2
1	E	351	THR	2.2
2	K	332	TYR	2.2
1	F	52	SER	2.2
1	F	137	GLN	2.2
1	D	346	LEU	2.2
1	B	138	ALA	2.2
1	E	259	GLU	2.2
1	A	157	ASP	2.2
1	A	179	ASP	2.2
1	F	318	THR	2.1
2	K	269	VAL	2.1
2	I	49	TYR	2.1
1	B	327	ILE	2.1
1	D	282	ILE	2.1
1	B	320	LEU	2.1
1	F	354	GLN	2.1
2	I	94	LEU	2.1
2	I	181	LEU	2.1
1	C	235	SER	2.1
2	H	367	LYS	2.1
2	K	46	SER	2.1
2	K	48	LYS	2.1
1	F	6	ALA	2.1
1	B	13	GLY	2.1
1	B	109	PRO	2.1
1	B	332	PRO	2.1
1	F	36	GLY	2.1
1	C	272	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	88	HIS	2.1
2	I	359	HIS	2.1
1	D	303	THR	2.1
1	E	10	ILE	2.1
2	J	49	TYR	2.1
2	K	45	LEU	2.1
1	A	354	GLN	2.1
1	B	254	ARG	2.1
2	H	27	SER	2.1
1	A	223	PHE	2.1
1	B	159	VAL	2.1
1	D	159	VAL	2.1
2	H	161	HIS	2.1
1	C	297	THR	2.1
1	A	69	TYR	2.1
1	B	143	TYR	2.1
1	D	166	TYR	2.1
1	D	169	TYR	2.1
2	H	125	LEU	2.1
1	B	82	MET	2.1
1	A	114	ALA	2.1
1	B	144	ALA	2.1
2	J	290	GLN	2.1
1	B	21	PHE	2.1
1	B	338	SER	2.1
2	J	199	LYS	2.1
1	A	346	LEU	2.1
2	K	125	LEU	2.1
2	K	352	LEU	2.1
1	A	77	THR	2.1
1	A	169	TYR	2.1
1	B	77	THR	2.1
2	K	157	TYR	2.1
2	H	171	ALA	2.1
1	B	168	GLY	2.1
1	A	226	GLU	2.1
1	D	243	PRO	2.1
1	D	334	GLU	2.1
1	E	83	GLU	2.1
2	H	256	PHE	2.1
2	K	61	SER	2.1
2	H	223	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	182	ASN	2.1
1	A	192	ILE	2.1
1	C	327	ILE	2.1
1	E	86	TRP	2.1
1	B	351	THR	2.1
2	J	358	MET	2.1
1	B	260	ALA	2.1
1	A	266	PHE	2.1
1	B	253	GLU	2.1
1	B	352	PHE	2.1
1	B	134	VAL	2.0
2	I	231	VAL	2.0
2	K	287	LYS	2.0
1	A	300	SER	2.0
2	I	306	SER	2.0
1	A	85	ILE	2.0
1	A	122	ILE	2.0
1	B	157	ASP	2.0
2	I	219	PRO	2.0
2	I	51	GLU	2.0
1	A	152	VAL	2.0
1	A	293	LEU	2.0
2	J	140	LEU	2.0
1	A	75	ILE	2.0
1	A	208	ILE	2.0
1	E	323	SER	2.0
1	F	10	ILE	2.0
1	A	325	MET	2.0
1	A	166	TYR	2.0
1	B	126	THR	2.0
1	B	135	ALA	2.0
1	C	303	THR	2.0
1	F	24	ASP	2.0
1	A	90	PHE	2.0
1	B	257	CYS	2.0
2	J	222	PRO	2.0
1	A	259	GLU	2.0
1	A	276	GLU	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.