



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:57 AM UTC

PDB ID : 1E69 / pdb_00001e69
Title : SMC head domain from *Thermotoga maritima*
Authors : Lowe, J.; Cordell, S.C.; van den Ent, F.
Deposited on : 2000-08-09
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

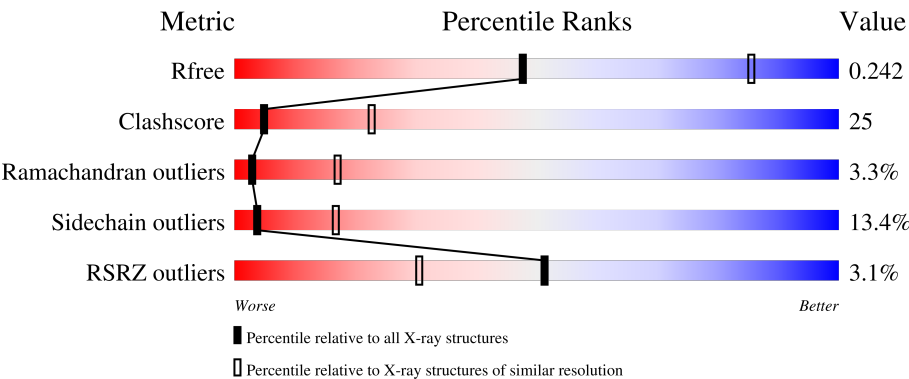
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	322	2% 48% 28% 6% • 18%
1	B	322	3% 42% 32% 7% • 18%
1	C	322	2% 44% 29% 7% • 18%
1	D	322	• 43% 31% 6% • 18%
1	E	322	3% 43% 31% 7% • 18%

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Mol	Chain	Length	Quality of chain
1	F	322	4% 44% 30% 6% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12396 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.

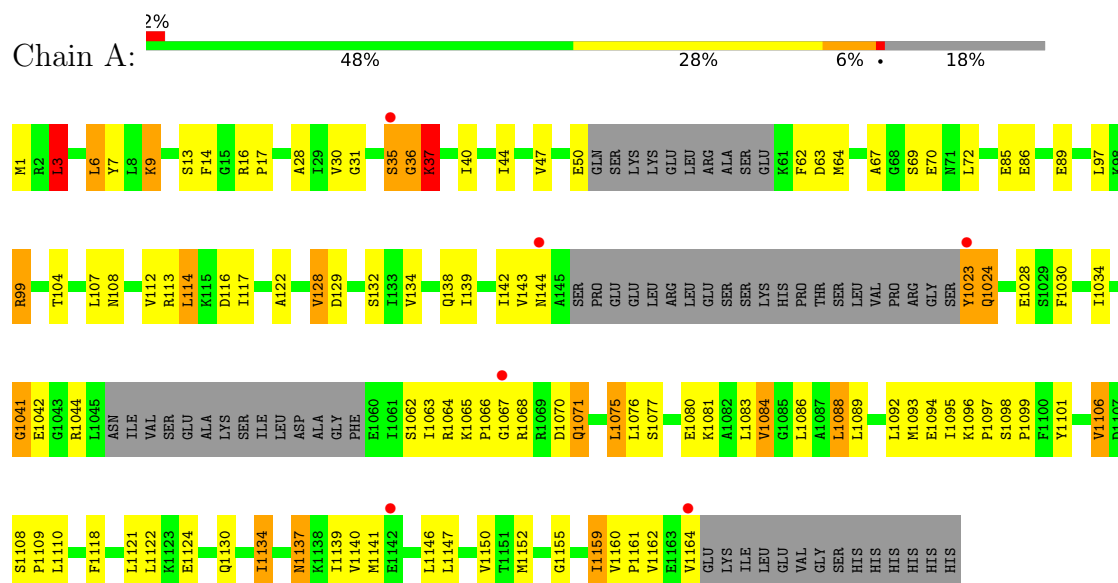
- Molecule 1 is a protein called CHROMOSOME SEGREGATION SMC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2066	1326	356	379	5			
1	B	263	Total	C	N	O	S	0	0	0
			2066	1326	356	379	5			
1	C	263	Total	C	N	O	S	0	0	0
			2066	1326	356	379	5			
1	D	263	Total	C	N	O	S	0	0	0
			2066	1326	356	379	5			
1	E	263	Total	C	N	O	S	0	0	0
			2066	1326	356	379	5			
1	F	263	Total	C	N	O	S	0	0	0
			2066	1326	356	379	5			

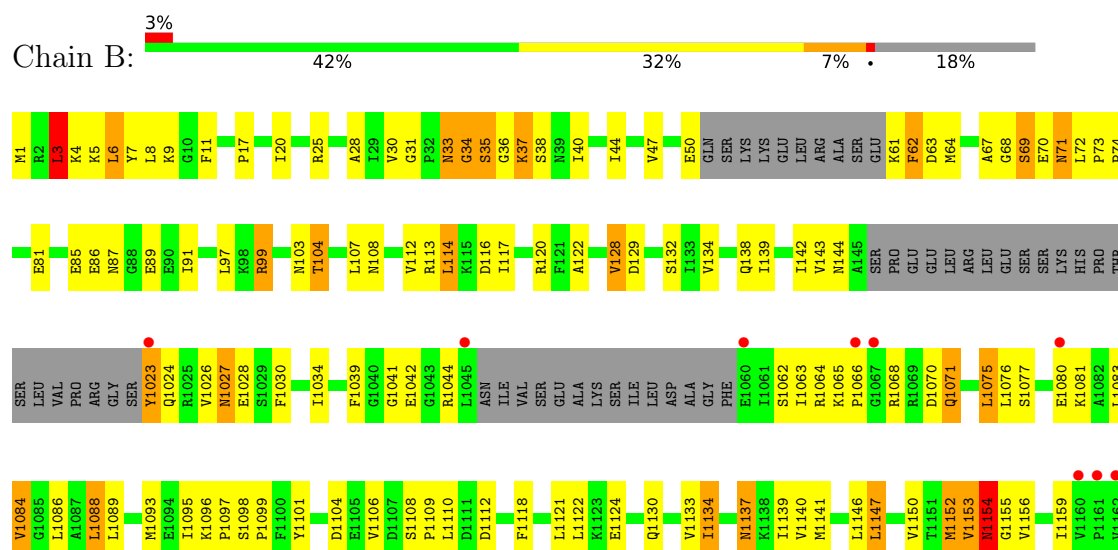
3 Residue-property plots

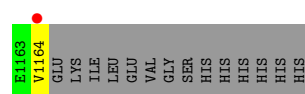
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

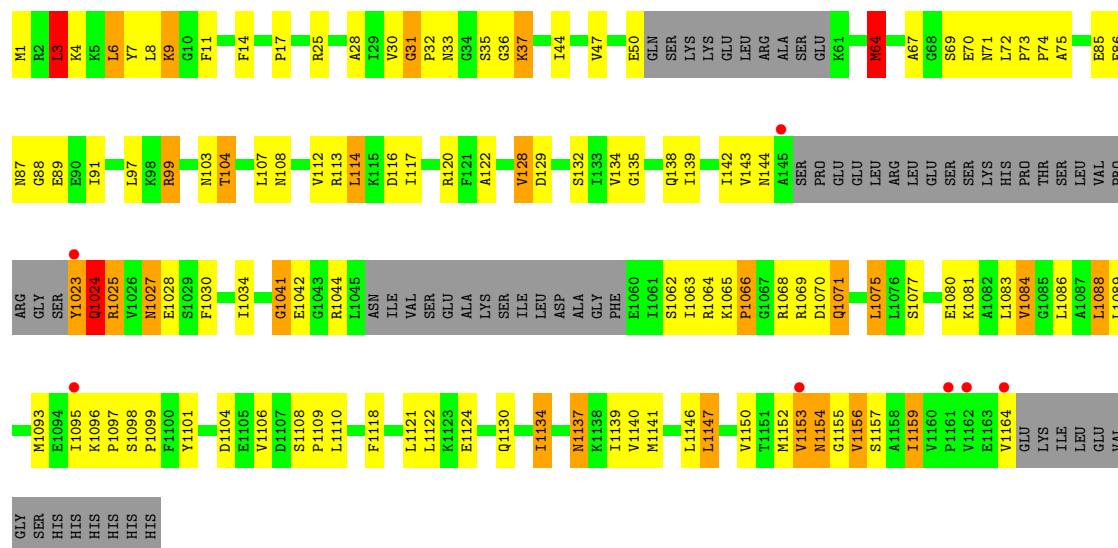
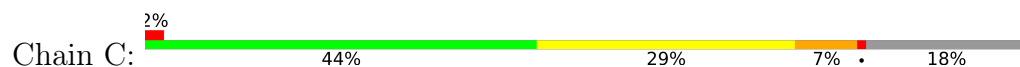


• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

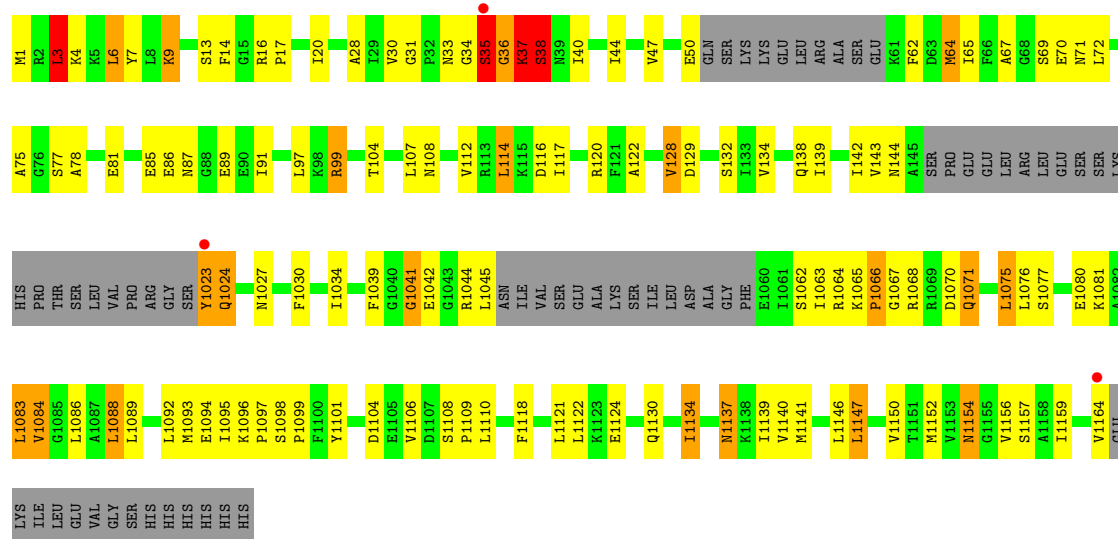
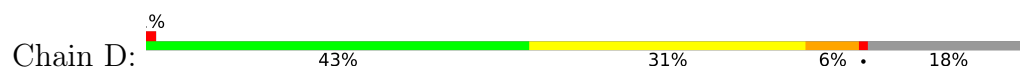




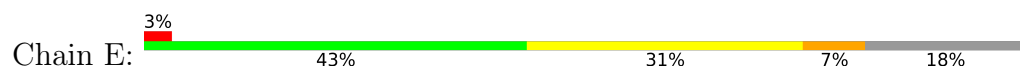
• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

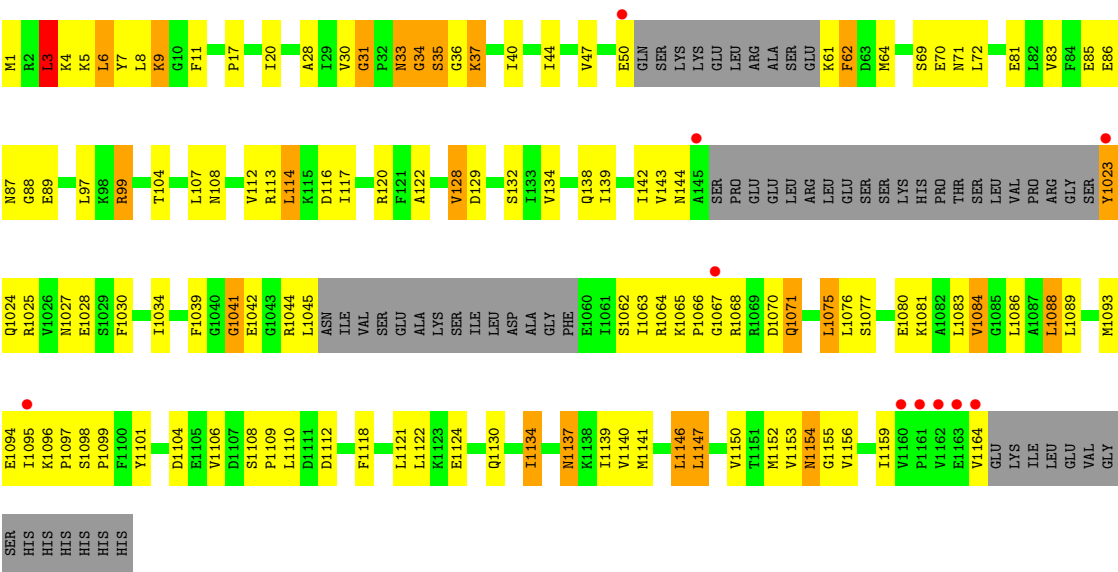


• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

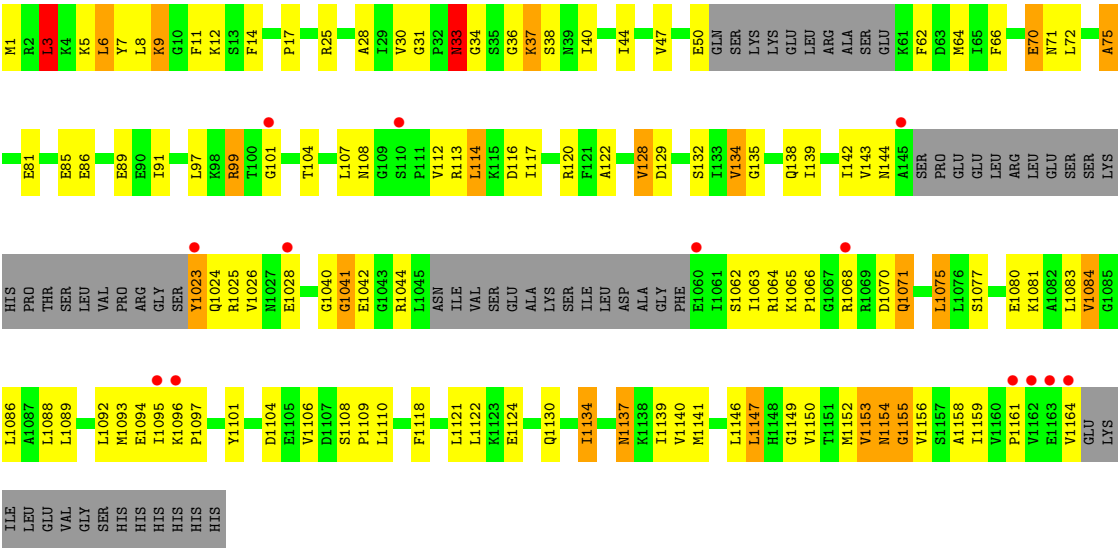


• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN





• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.00Å 49.19Å 233.88Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	100.00 – 3.10 100.00 – 3.14	Depositor EDS
% Data completeness (in resolution range)	97.3 (100.00-3.10) 94.9 (100.00-3.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 3.12Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.250 , 0.272 0.249 , 0.242	Depositor DCC
R_{free} test set	2619 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12396	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.49% 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	0.60	1/2102 (0.0%)	1.03	9/2826 (0.3%)
1	B	0.51	0/2102	1.00	10/2826 (0.4%)
1	C	0.53	0/2102	1.01	9/2826 (0.3%)
1	D	0.54	0/2102	1.03	9/2826 (0.3%)
1	E	0.53	0/2102	0.99	7/2826 (0.2%)
1	F	0.58	0/2102	1.01	8/2826 (0.3%)
All	All	0.55	1/12612 (0.0%)	1.01	52/16956 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	LYS	N-CA	5.69	1.53	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	GLY	N-CA-C	-9.78	90.01	113.18
1	D	36	GLY	N-CA-C	-8.12	93.95	113.18
1	D	67	ALA	N-CA-C	6.89	120.91	112.23
1	D	38	SER	N-CA-C	6.85	125.38	110.80
1	E	64	MET	N-CA-C	-6.80	105.14	113.50
1	D	64	MET	N-CA-C	-6.47	105.31	113.72
1	F	75	ALA	N-CA-C	6.43	119.57	110.50
1	B	64	MET	N-CA-C	-6.18	105.22	112.89
1	B	68	GLY	N-CA-C	6.15	118.27	110.96
1	F	33	ASN	N-CA-C	6.09	121.36	111.37
1	C	64	MET	N-CA-C	-6.04	104.98	112.90
1	D	1068	ARG	N-CA-C	6.03	119.49	109.96
1	A	37	LYS	N-CA-C	6.03	123.65	110.80
1	A	16	ARG	CA-C-N	5.83	127.12	119.84
1	A	16	ARG	C-N-CA	5.83	127.12	119.84
1	A	31	GLY	CA-C-N	5.75	126.55	120.11
1	A	31	GLY	C-N-CA	5.75	126.55	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1068	ARG	N-CA-C	5.71	118.97	109.96
1	E	31	GLY	CA-C-N	5.64	126.89	119.84
1	E	31	GLY	C-N-CA	5.64	126.89	119.84
1	B	1068	ARG	N-CA-C	5.62	118.84	109.96
1	D	35	SER	N-CA-C	-5.61	106.79	113.97
1	C	67	ALA	N-CA-C	5.54	118.50	111.69
1	F	1155	GLY	N-CA-C	-5.53	100.07	113.18
1	C	1068	ARG	N-CA-C	5.51	118.66	109.96
1	B	31	GLY	CA-C-N	5.45	126.65	119.84
1	B	31	GLY	C-N-CA	5.45	126.65	119.84
1	A	3	LEU	N-CA-C	-5.37	101.22	109.76
1	A	67	ALA	N-CA-C	5.35	119.52	112.89
1	B	25	ARG	CB-CA-C	-5.30	108.80	116.54
1	C	3	LEU	N-CA-C	-5.25	101.41	109.76
1	C	88	GLY	N-CA-C	-5.23	107.77	115.30
1	E	1068	ARG	N-CA-C	5.21	118.19	109.96
1	B	73	PRO	CA-C-N	-5.17	114.43	119.76
1	B	73	PRO	C-N-CA	-5.17	114.43	119.76
1	D	37	LYS	CA-C-N	5.17	131.41	121.54
1	D	37	LYS	C-N-CA	5.17	131.41	121.54
1	C	31	GLY	CA-C-N	5.16	126.29	119.84
1	C	31	GLY	C-N-CA	5.16	126.29	119.84
1	D	3	LEU	N-CA-C	-5.14	100.93	109.46
1	E	3	LEU	N-CA-C	-5.13	101.61	109.76
1	C	25	ARG	CB-CA-C	-5.12	109.07	116.54
1	B	3	LEU	N-CA-C	-5.12	100.97	109.46
1	F	3	LEU	N-CA-C	-5.11	100.97	109.46
1	C	1025	ARG	N-CA-C	-5.10	107.19	113.41
1	E	1112	ASP	N-CA-C	5.10	116.84	111.28
1	E	88	GLY	N-CA-C	-5.09	107.97	115.30
1	A	1068	ARG	N-CA-C	5.09	118.00	109.96
1	F	134	VAL	N-CA-C	5.09	115.23	108.11
1	B	1112	ASP	N-CA-C	5.06	116.79	111.28
1	F	1040	GLY	N-CA-C	5.03	125.11	113.18
1	F	25	ARG	CB-CA-C	-5.02	109.21	116.54

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	2066	0	2099	96	0
1	B	2066	0	2099	110	0
1	C	2066	0	2099	111	0
1	D	2066	0	2099	116	0
1	E	2066	0	2099	122	0
1	F	2066	0	2099	105	0
All	All	12396	0	12594	633	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 25.

All (633) 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:E:3:LEU:H	1:E:1130:GLN:HE22	1.04	1.04
1:B:3:LEU:H	1:B:1130:GLN:HE22	1.06	1.00
1:A:3:LEU:H	1:A:1130:GLN:HE22	1.02	0.99
1:D:3:LEU:H	1:D:1130:GLN:HE22	1.04	0.94
1:A:3:LEU:H	1:A:1130:GLN:NE2	1.65	0.94
1:C:37:LYS:HE3	1:C:37:LYS:H	1.31	0.93
1:F:3:LEU:H	1:F:1130:GLN:HE22	1.01	0.93
1:C:3:LEU:H	1:C:1130:GLN:HE22	1.00	0.93
1:C:3:LEU:H	1:C:1130:GLN:NE2	1.66	0.91
1:E:35:SER:HA	1:E:1152:MET:HB2	1.51	0.91
1:D:1150:VAL:HG12	1:D:1159:ILE:HG12	1.49	0.91
1:E:128:VAL:HG23	1:E:129:ASP:H	1.35	0.90
1:E:1150:VAL:HG12	1:E:1159:ILE:HG12	1.54	0.90
1:F:3:LEU:H	1:F:1130:GLN:NE2	1.68	0.90
1:E:3:LEU:H	1:E:1130:GLN:NE2	1.69	0.90
1:A:128:VAL:HG23	1:A:129:ASP:H	1.38	0.88
1:B:3:LEU:H	1:B:1130:GLN:NE2	1.71	0.88
1:D:128:VAL:HG23	1:D:129:ASP:H	1.38	0.88
1:D:3:LEU:H	1:D:1130:GLN:NE2	1.71	0.87
1:A:35:SER:O	1:A:36:GLY:C	2.16	0.87
1:D:1027:ASN:OD1	1:D:1045:LEU:HB2	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HD11	1:D:1159:ILE:HD13	1.57	0.86
1:C:128:VAL:HG23	1:C:129:ASP:H	1.38	0.86
1:F:128:VAL:HG23	1:F:129:ASP:H	1.40	0.86
1:B:128:VAL:HG23	1:B:129:ASP:H	1.39	0.86
1:A:14:PHE:CE2	1:A:1159:ILE:HD11	2.11	0.86
1:C:3:LEU:N	1:C:1130:GLN:HE22	1.74	0.84
1:A:3:LEU:N	1:A:1130:GLN:HE22	1.75	0.84
1:A:1150:VAL:HG12	1:A:1159:ILE:HD13	1.57	0.84
1:A:30:VAL:HG21	1:A:1141:MET:HE3	1.59	0.84
1:D:9:LYS:HD3	1:D:17:PRO:HG3	1.61	0.83
1:F:3:LEU:N	1:F:1130:GLN:HE22	1.76	0.83
1:D:1075:LEU:HD13	1:D:1075:LEU:H	1.45	0.82
1:D:1077:SER:HB3	1:D:1080:GLU:HB2	1.60	0.82
1:A:37:LYS:HG2	1:A:1150:VAL:CG2	2.10	0.82
1:C:37:LYS:HE3	1:C:37:LYS:N	1.94	0.82
1:D:30:VAL:HG21	1:D:1141:MET:HE3	1.61	0.82
1:F:30:VAL:HG21	1:F:1141:MET:HE3	1.61	0.81
1:E:1077:SER:HB3	1:E:1080:GLU:HB2	1.61	0.81
1:A:1075:LEU:HD13	1:A:1075:LEU:H	1.45	0.81
1:C:30:VAL:HG21	1:C:1141:MET:HE3	1.60	0.81
1:A:1077:SER:HB3	1:A:1080:GLU:HB2	1.61	0.80
1:D:3:LEU:N	1:D:1130:GLN:HE22	1.79	0.80
1:E:3:LEU:N	1:E:1130:GLN:HE22	1.78	0.80
1:B:1077:SER:HB3	1:B:1080:GLU:HB2	1.65	0.79
1:B:3:LEU:N	1:B:1130:GLN:HE22	1.80	0.79
1:B:1075:LEU:HD13	1:B:1075:LEU:H	1.45	0.79
1:A:35:SER:O	1:A:36:GLY:O	2.01	0.79
1:C:1077:SER:HB3	1:C:1080:GLU:HB2	1.63	0.79
1:E:30:VAL:HG21	1:E:1141:MET:HE3	1.65	0.79
1:E:1075:LEU:HD13	1:E:1075:LEU:H	1.46	0.78
1:F:9:LYS:HD3	1:F:17:PRO:HG3	1.63	0.78
1:F:33:ASN:O	1:F:37:LYS:HE2	1.83	0.78
1:F:1077:SER:HB3	1:F:1080:GLU:HB2	1.66	0.77
1:E:37:LYS:H	1:E:37:LYS:HE3	1.50	0.76
1:C:1069:ARG:NH2	1:D:17:PRO:O	2.18	0.76
1:A:37:LYS:HG2	1:A:1150:VAL:HG21	1.65	0.76
1:B:9:LYS:HD3	1:B:17:PRO:HG3	1.66	0.76
1:A:134:VAL:HG11	1:A:1089:LEU:HD11	1.68	0.76
1:C:9:LYS:HD3	1:C:17:PRO:HG3	1.66	0.76
1:F:75:ALA:O	1:F:99:ARG:NH1	2.20	0.75
1:E:9:LYS:HD3	1:E:17:PRO:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1150:VAL:HG12	1:B:1159:ILE:HG12	1.69	0.75
1:B:30:VAL:HG21	1:B:1141:MET:HE3	1.68	0.75
1:D:13:SER:HB2	1:D:1152:MET:HE2	1.69	0.75
1:D:1067:GLY:CA	1:E:83:VAL:HG21	2.17	0.75
1:E:37:LYS:HE3	1:E:37:LYS:N	2.01	0.74
1:F:14:PHE:HE2	1:F:1159:ILE:HD11	1.52	0.74
1:F:1075:LEU:HD13	1:F:1075:LEU:H	1.52	0.74
1:C:37:LYS:H	1:C:37:LYS:CE	2.00	0.73
1:C:1075:LEU:HD13	1:C:1075:LEU:H	1.53	0.73
1:A:9:LYS:HD3	1:A:17:PRO:HG3	1.68	0.73
1:F:1023:TYR:CD1	1:F:1023:TYR:C	2.67	0.73
1:D:134:VAL:HG11	1:D:1089:LEU:HD11	1.71	0.73
1:F:134:VAL:HG11	1:F:1089:LEU:HD11	1.71	0.72
1:C:75:ALA:O	1:C:99:ARG:NH1	2.23	0.71
1:B:134:VAL:HG11	1:B:1089:LEU:HD11	1.72	0.71
1:A:37:LYS:HB3	1:A:1150:VAL:HG21	1.71	0.70
1:B:1071:GLN:HG2	1:B:1075:LEU:HD21	1.73	0.70
1:E:34:GLY:O	1:E:36:GLY:N	2.23	0.70
1:C:1152:MET:HE2	1:C:1155:GLY:O	1.91	0.70
1:E:134:VAL:HG11	1:E:1089:LEU:HD11	1.73	0.70
1:C:1023:TYR:CD1	1:C:1023:TYR:C	2.70	0.69
1:D:35:SER:O	1:D:36:GLY:C	2.35	0.69
1:F:1152:MET:HG3	1:F:1156:VAL:O	1.93	0.69
1:C:36:GLY:H	1:C:37:LYS:HE3	1.58	0.68
1:E:1025:ARG:NH1	1:E:1094:GLU:HG3	2.08	0.68
1:A:1071:GLN:HG2	1:A:1075:LEU:HD21	1.76	0.68
1:A:28:ALA:HB3	1:A:1147:LEU:HD12	1.76	0.68
1:C:1023:TYR:C	1:C:1025:ARG:H	2.02	0.68
1:D:20:ILE:HD11	1:D:1159:ILE:CD1	2.24	0.68
1:C:36:GLY:N	1:C:37:LYS:HE3	2.08	0.67
1:C:134:VAL:HG11	1:C:1089:LEU:HD11	1.75	0.67
1:F:1150:VAL:HG12	1:F:1159:ILE:HG13	1.77	0.67
1:D:1071:GLN:HG2	1:D:1075:LEU:HD21	1.76	0.67
1:E:1152:MET:HG3	1:E:1156:VAL:O	1.94	0.67
1:A:40:ILE:HD11	1:A:1159:ILE:HD12	1.76	0.67
1:D:65:ILE:HD13	1:D:77:SER:HA	1.76	0.67
1:B:1023:TYR:CD1	1:B:1023:TYR:C	2.73	0.67
1:A:1023:TYR:CD1	1:A:1023:TYR:C	2.74	0.66
1:C:1071:GLN:HG2	1:C:1075:LEU:HD21	1.76	0.66
1:F:36:GLY:H	1:F:37:LYS:HE3	1.59	0.66
1:D:1067:GLY:O	1:E:5:LYS:CD	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:SER:OG	1:E:72:LEU:HB2	1.95	0.66
1:A:14:PHE:HE2	1:A:1159:ILE:HD11	1.57	0.66
1:E:1137:ASN:ND2	1:E:1139:ILE:H	1.93	0.66
1:D:69:SER:HB3	1:D:72:LEU:HB2	1.78	0.66
1:D:1067:GLY:HA2	1:E:83:VAL:HG21	1.77	0.66
1:C:1024:GLN:O	1:C:1028:GLU:HB2	1.96	0.65
1:F:70:GLU:OE1	1:F:71:ASN:N	2.30	0.65
1:D:28:ALA:HB3	1:D:1147:LEU:HD12	1.78	0.65
1:D:1077:SER:O	1:D:1081:LYS:HG3	1.96	0.65
1:B:1137:ASN:ND2	1:B:1139:ILE:H	1.94	0.65
1:D:1023:TYR:CD1	1:D:1023:TYR:C	2.74	0.65
1:C:72:LEU:HD12	1:C:1156:VAL:CG1	2.27	0.65
1:E:20:ILE:HD11	1:E:1159:ILE:CD1	2.26	0.64
1:E:1071:GLN:HG2	1:E:1075:LEU:HD21	1.78	0.64
1:E:85:GLU:HA	1:E:89:GLU:O	1.97	0.64
1:A:37:LYS:CG	1:A:1150:VAL:HG21	2.28	0.64
1:D:1066:PRO:O	1:E:81:GLU:OE2	2.15	0.64
1:C:36:GLY:CA	1:C:37:LYS:HE3	2.28	0.64
1:D:1067:GLY:O	1:E:5:LYS:HD2	1.97	0.64
1:E:28:ALA:HB3	1:E:1147:LEU:HD12	1.81	0.63
1:B:1027:ASN:C	1:B:1027:ASN:HD22	2.07	0.63
1:C:85:GLU:HA	1:C:89:GLU:O	1.99	0.63
1:F:85:GLU:HA	1:F:89:GLU:O	1.98	0.63
1:D:65:ILE:HG12	1:D:78:ALA:HB2	1.78	0.63
1:D:1137:ASN:ND2	1:D:1139:ILE:H	1.97	0.63
1:B:1152:MET:HE2	1:B:1155:GLY:O	1.97	0.63
1:E:128:VAL:HG23	1:E:129:ASP:N	2.11	0.63
1:C:72:LEU:HD12	1:C:1156:VAL:HG11	1.79	0.63
1:F:12:LYS:O	1:F:66:PHE:HD1	1.82	0.63
1:F:37:LYS:HE3	1:F:37:LYS:N	2.14	0.63
1:F:28:ALA:HB3	1:F:1147:LEU:HD12	1.81	0.63
1:F:1137:ASN:ND2	1:F:1139:ILE:H	1.97	0.63
1:F:37:LYS:HE3	1:F:37:LYS:H	1.64	0.62
1:F:134:VAL:HG11	1:F:1089:LEU:CD1	2.30	0.62
1:C:28:ALA:HB3	1:C:1147:LEU:HD12	1.82	0.62
1:E:37:LYS:H	1:E:37:LYS:CE	2.11	0.62
1:B:72:LEU:HD12	1:B:1156:VAL:HG11	1.80	0.62
1:F:1071:GLN:HG2	1:F:1075:LEU:HD21	1.82	0.62
1:A:134:VAL:HG11	1:A:1089:LEU:CD1	2.29	0.61
1:B:85:GLU:HA	1:B:89:GLU:O	1.99	0.61
1:C:70:GLU:HG2	1:C:71:ASN:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:HD2	1:B:38:SER:H	1.64	0.61
1:F:1023:TYR:C	1:F:1023:TYR:HD1	2.07	0.61
1:B:28:ALA:HB3	1:B:1147:LEU:HD12	1.81	0.61
1:F:1023:TYR:HD1	1:F:1024:GLN:N	1.98	0.61
1:A:85:GLU:HA	1:A:89:GLU:O	2.01	0.61
1:F:1154:ASN:HB3	1:F:1156:VAL:HG22	1.81	0.61
1:D:134:VAL:HG11	1:D:1089:LEU:CD1	2.31	0.61
1:E:6:LEU:HD23	1:E:7:TYR:N	2.16	0.61
1:C:1077:SER:O	1:C:1081:LYS:HG3	2.00	0.61
1:D:1095:ILE:C	1:D:1097:PRO:HD3	2.26	0.61
1:E:1095:ILE:C	1:E:1097:PRO:HD3	2.26	0.60
1:F:1077:SER:O	1:F:1081:LYS:HG3	2.01	0.60
1:D:1039:PHE:HA	1:E:108:ASN:O	2.01	0.60
1:F:36:GLY:N	1:F:37:LYS:HE3	2.16	0.60
1:B:128:VAL:HG23	1:B:129:ASP:N	2.15	0.60
1:E:1077:SER:O	1:E:1081:LYS:HG3	2.01	0.60
1:F:1095:ILE:C	1:F:1097:PRO:HD3	2.27	0.60
1:A:37:LYS:CB	1:A:1150:VAL:HG21	2.31	0.60
1:B:6:LEU:HD23	1:B:7:TYR:N	2.15	0.60
1:A:1108:SER:HB2	1:A:1109:PRO:CD	2.30	0.60
1:B:69:SER:HB3	1:B:72:LEU:HB2	1.82	0.60
1:A:1134:ILE:O	1:A:1134:ILE:HG12	2.02	0.60
1:C:6:LEU:HD23	1:C:7:TYR:N	2.16	0.60
1:A:69:SER:HB3	1:A:72:LEU:HB2	1.83	0.60
1:A:14:PHE:CZ	1:A:1159:ILE:HD11	2.37	0.59
1:A:1064:ARG:NH2	1:B:81:GLU:OE2	2.34	0.59
1:A:1095:ILE:C	1:A:1097:PRO:HD3	2.27	0.59
1:C:70:GLU:HB3	1:C:1154:ASN:ND2	2.17	0.59
1:A:1077:SER:O	1:A:1081:LYS:HG3	2.01	0.59
1:E:20:ILE:HD11	1:E:1159:ILE:HD13	1.84	0.59
1:E:1024:GLN:O	1:E:1028:GLU:HB2	2.02	0.59
1:D:85:GLU:HA	1:D:89:GLU:O	2.02	0.59
1:A:1137:ASN:ND2	1:A:1139:ILE:H	2.01	0.59
1:A:1108:SER:HB2	1:A:1109:PRO:HD3	1.84	0.59
1:C:1095:ILE:C	1:C:1097:PRO:HD3	2.27	0.59
1:A:62:PHE:C	1:A:64:MET:H	2.11	0.58
1:E:134:VAL:HG11	1:E:1089:LEU:CD1	2.34	0.58
1:E:1023:TYR:CD1	1:E:1023:TYR:C	2.81	0.58
1:D:1108:SER:HB2	1:D:1109:PRO:CD	2.34	0.58
1:B:134:VAL:HG11	1:B:1089:LEU:CD1	2.33	0.58
1:B:1095:ILE:C	1:B:1097:PRO:HD3	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1064:ARG:NH2	1:E:81:GLU:OE2	2.37	0.57
1:C:1023:TYR:HD1	1:C:1024:GLN:N	2.02	0.57
1:D:128:VAL:HG23	1:D:129:ASP:N	2.15	0.57
1:D:1134:ILE:HG12	1:D:1134:ILE:O	2.04	0.57
1:A:139:ILE:CD1	1:A:1089:LEU:HD12	2.34	0.57
1:C:1137:ASN:ND2	1:C:1139:ILE:H	2.03	0.57
1:B:1024:GLN:O	1:B:1028:GLU:HB2	2.05	0.57
1:E:72:LEU:HD12	1:E:1156:VAL:HG11	1.87	0.57
1:E:1108:SER:HB2	1:E:1109:PRO:HD3	1.87	0.57
1:C:1023:TYR:C	1:C:1023:TYR:HD1	2.11	0.57
1:E:1108:SER:HB2	1:E:1109:PRO:CD	2.34	0.57
1:B:1108:SER:HB2	1:B:1109:PRO:HD3	1.87	0.56
1:C:1150:VAL:HG12	1:C:1159:ILE:HG13	1.86	0.56
1:F:72:LEU:HD12	1:F:1156:VAL:HG11	1.87	0.56
1:C:33:ASN:O	1:C:37:LYS:HE2	2.04	0.56
1:A:1024:GLN:H	1:A:1024:GLN:NE2	2.03	0.56
1:D:1067:GLY:O	1:E:5:LYS:HD3	2.06	0.56
1:E:70:GLU:CD	1:E:71:ASN:H	2.13	0.56
1:A:13:SER:HB2	1:A:1152:MET:HE3	1.88	0.56
1:B:34:GLY:O	1:B:36:GLY:N	2.38	0.56
1:B:1077:SER:O	1:B:1081:LYS:HG3	2.04	0.56
1:C:134:VAL:HG11	1:C:1089:LEU:CD1	2.35	0.56
1:B:139:ILE:CD1	1:B:1089:LEU:HD12	2.35	0.56
1:F:99:ARG:HH11	1:F:99:ARG:HG3	1.71	0.56
1:F:6:LEU:HD23	1:F:7:TYR:N	2.21	0.55
1:F:11:PHE:CE1	1:F:64:MET:HG3	2.41	0.55
1:B:1108:SER:HB2	1:B:1109:PRO:CD	2.36	0.55
1:D:1150:VAL:CG1	1:D:1159:ILE:HG12	2.29	0.55
1:A:1096:LYS:N	1:A:1097:PRO:HD3	2.22	0.55
1:C:99:ARG:HG3	1:C:99:ARG:HH11	1.72	0.55
1:E:99:ARG:HG3	1:E:99:ARG:HH11	1.71	0.55
1:C:36:GLY:H	1:C:37:LYS:CE	2.20	0.55
1:F:1086:LEU:HD21	1:F:1106:VAL:HG11	1.89	0.55
1:D:1152:MET:HA	1:D:1157:SER:HA	1.89	0.55
1:A:128:VAL:HG23	1:A:129:ASP:N	2.15	0.55
1:D:1108:SER:HB2	1:D:1109:PRO:HD3	1.88	0.55
1:D:1137:ASN:HD21	1:D:1139:ILE:HB	1.72	0.54
1:F:37:LYS:HD2	1:F:38:SER:H	1.72	0.54
1:C:139:ILE:CD1	1:C:1089:LEU:HD12	2.37	0.54
1:E:1137:ASN:HD21	1:E:1139:ILE:HB	1.72	0.54
1:F:62:PHE:CZ	1:F:101:GLY:HA2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1023:TYR:C	1:B:1023:TYR:HD1	2.15	0.54
1:C:128:VAL:HG23	1:C:129:ASP:N	2.16	0.54
1:C:1108:SER:HB2	1:C:1109:PRO:CD	2.38	0.54
1:D:139:ILE:CD1	1:D:1089:LEU:HD12	2.38	0.54
1:D:1023:TYR:C	1:D:1023:TYR:HD1	2.15	0.54
1:F:14:PHE:CE2	1:F:1159:ILE:HD11	2.38	0.54
1:E:1064:ARG:NH2	1:F:81:GLU:OE2	2.40	0.54
1:F:1108:SER:HB2	1:F:1109:PRO:CD	2.38	0.54
1:C:1096:LYS:N	1:C:1097:PRO:HD3	2.23	0.54
1:D:40:ILE:HD11	1:D:1159:ILE:CD1	2.38	0.54
1:F:139:ILE:CD1	1:F:1089:LEU:HD12	2.38	0.54
1:A:139:ILE:HD13	1:A:1089:LEU:HD12	1.90	0.54
1:B:34:GLY:O	1:B:37:LYS:HE3	2.08	0.54
1:D:33:ASN:O	1:D:36:GLY:N	2.41	0.54
1:D:1096:LYS:N	1:D:1097:PRO:HD3	2.23	0.54
1:F:1089:LEU:O	1:F:1089:LEU:HD23	2.08	0.54
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.73	0.54
1:A:1137:ASN:HD21	1:A:1139:ILE:HB	1.71	0.54
1:C:1137:ASN:HD21	1:C:1139:ILE:HB	1.73	0.54
1:B:1137:ASN:HD21	1:B:1139:ILE:HB	1.73	0.54
1:F:1089:LEU:HD23	1:F:1089:LEU:C	2.33	0.54
1:C:37:LYS:H	1:C:37:LYS:CD	2.20	0.53
1:D:6:LEU:HD23	1:D:7:TYR:N	2.23	0.53
1:D:114:LEU:O	1:D:114:LEU:HD23	2.07	0.53
1:A:1024:GLN:O	1:A:1028:GLU:HB2	2.09	0.53
1:B:1023:TYR:HD1	1:B:1024:GLN:N	2.05	0.53
1:B:1153:VAL:HG12	1:B:1154:ASN:N	2.24	0.53
1:D:70:GLU:HB3	1:D:1154:ASN:ND2	2.24	0.53
1:E:1096:LYS:N	1:E:1097:PRO:HD3	2.24	0.53
1:F:1137:ASN:HD21	1:F:1139:ILE:HB	1.73	0.53
1:A:1023:TYR:C	1:A:1023:TYR:HD1	2.15	0.53
1:C:1152:MET:HA	1:C:1157:SER:HA	1.88	0.53
1:B:1039:PHE:HD1	1:C:108:ASN:HB3	1.73	0.53
1:B:1086:LEU:HD21	1:B:1106:VAL:HG11	1.91	0.53
1:D:40:ILE:HD11	1:D:1159:ILE:HD11	1.91	0.53
1:D:62:PHE:CZ	1:D:99:ARG:O	2.62	0.53
1:D:70:GLU:OE1	1:D:1154:ASN:HB2	2.09	0.53
1:D:99:ARG:HG3	1:D:99:ARG:HH11	1.74	0.53
1:F:1096:LYS:N	1:F:1097:PRO:HD3	2.23	0.52
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.73	0.52
1:C:139:ILE:HD13	1:C:1089:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1071:GLN:HG2	1:D:1075:LEU:CD2	2.39	0.52
1:F:1041:GLY:HA3	1:F:1064:ARG:O	2.09	0.52
1:F:1093:MET:HG2	1:F:1101:TYR:CZ	2.44	0.52
1:F:33:ASN:CG	1:F:34:GLY:N	2.66	0.52
1:F:1108:SER:HB2	1:F:1109:PRO:HD3	1.91	0.52
1:B:1063:ILE:HD11	1:B:1084:VAL:HB	1.92	0.52
1:C:1066:PRO:O	1:D:81:GLU:OE2	2.28	0.52
1:E:114:LEU:HD23	1:E:114:LEU:O	2.10	0.52
1:F:1134:ILE:O	1:F:1134:ILE:HG12	2.08	0.52
1:E:139:ILE:CD1	1:E:1089:LEU:HD12	2.40	0.52
1:E:1086:LEU:HD13	1:E:1118:PHE:CD1	2.45	0.52
1:B:1071:GLN:HG2	1:B:1075:LEU:CD2	2.40	0.52
1:C:1152:MET:HG3	1:C:1156:VAL:O	2.10	0.52
1:E:1063:ILE:HD11	1:E:1084:VAL:HB	1.91	0.52
1:F:1150:VAL:HA	1:F:1158:ALA:O	2.10	0.52
1:A:1137:ASN:HD22	1:A:1140:VAL:H	1.56	0.52
1:C:1041:GLY:HA3	1:C:1064:ARG:O	2.09	0.52
1:B:1096:LYS:N	1:B:1097:PRO:HD3	2.25	0.51
1:B:69:SER:OG	1:B:1154:ASN:ND2	2.43	0.51
1:F:14:PHE:HE2	1:F:1159:ILE:CD1	2.22	0.51
1:B:35:SER:HA	1:B:1152:MET:HB2	1.92	0.51
1:B:62:PHE:CE2	1:B:99:ARG:O	2.63	0.51
1:F:114:LEU:O	1:F:114:LEU:HD23	2.10	0.51
1:A:1086:LEU:HD21	1:A:1106:VAL:HG11	1.92	0.51
1:B:1104:ASP:HA	1:B:1134:ILE:HG23	1.93	0.51
1:E:33:ASN:O	1:E:37:LYS:HE2	2.11	0.51
1:F:128:VAL:HG23	1:F:129:ASP:N	2.16	0.51
1:E:70:GLU:CG	1:E:71:ASN:N	2.72	0.51
1:E:1154:ASN:ND2	1:E:1155:GLY:H	2.07	0.51
1:C:128:VAL:HG23	1:C:129:ASP:OD1	2.10	0.51
1:C:1108:SER:HB2	1:C:1109:PRO:HD3	1.92	0.51
1:B:1147:LEU:HD22	1:B:1164:VAL:HG22	1.93	0.51
1:C:114:LEU:HD23	1:C:114:LEU:O	2.10	0.51
1:E:69:SER:HB2	1:E:1154:ASN:HD22	1.76	0.51
1:B:139:ILE:HD13	1:B:1089:LEU:HD12	1.92	0.51
1:B:1086:LEU:HD13	1:B:1118:PHE:CD1	2.46	0.51
1:C:64:MET:N	1:C:64:MET:HE2	2.26	0.51
1:C:1086:LEU:HD21	1:C:1106:VAL:HG11	1.92	0.51
1:C:1089:LEU:C	1:C:1089:LEU:HD23	2.36	0.51
1:E:1134:ILE:HG12	1:E:1134:ILE:O	2.11	0.51
1:A:128:VAL:HG23	1:A:129:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1080:GLU:O	1:D:1084:VAL:HG12	2.11	0.50
1:F:36:GLY:H	1:F:37:LYS:CE	2.24	0.50
1:A:1063:ILE:HD11	1:A:1084:VAL:HB	1.93	0.50
1:C:1147:LEU:HD22	1:C:1164:VAL:HG22	1.93	0.50
1:E:1147:LEU:HD22	1:E:1164:VAL:HG22	1.93	0.50
1:B:1089:LEU:HD23	1:B:1089:LEU:C	2.37	0.50
1:C:1023:TYR:C	1:C:1025:ARG:N	2.65	0.50
1:A:44:ILE:O	1:A:47:VAL:HG12	2.11	0.50
1:A:1067:GLY:O	1:B:5:LYS:CD	2.60	0.49
1:D:139:ILE:HD13	1:D:1089:LEU:HD12	1.94	0.49
1:E:1089:LEU:HD23	1:E:1089:LEU:O	2.12	0.49
1:F:139:ILE:HD13	1:F:1089:LEU:HD12	1.94	0.49
1:A:1089:LEU:O	1:A:1089:LEU:HD23	2.12	0.49
1:C:1137:ASN:HD22	1:C:1140:VAL:H	1.59	0.49
1:E:1147:LEU:HD22	1:E:1164:VAL:CG2	2.42	0.49
1:A:1071:GLN:HG2	1:A:1075:LEU:CD2	2.42	0.49
1:C:73:PRO:O	1:C:74:PRO:C	2.56	0.49
1:C:112:VAL:HG22	1:C:116:ASP:HB2	1.94	0.49
1:C:1063:ILE:HD11	1:C:1084:VAL:HB	1.93	0.49
1:B:112:VAL:HG22	1:B:116:ASP:HB2	1.95	0.49
1:C:70:GLU:CG	1:C:71:ASN:N	2.75	0.49
1:C:1071:GLN:HG2	1:C:1075:LEU:CD2	2.40	0.49
1:D:1086:LEU:HD21	1:D:1106:VAL:HG11	1.93	0.49
1:D:1064:ARG:HH22	1:E:81:GLU:CD	2.21	0.49
1:A:138:GLN:O	1:A:142:ILE:HG12	2.12	0.49
1:D:128:VAL:HG23	1:D:129:ASP:OD1	2.13	0.49
1:F:1147:LEU:HD22	1:F:1164:VAL:CG2	2.43	0.49
1:A:1152:MET:HE2	1:A:1155:GLY:HA2	1.94	0.49
1:B:1080:GLU:O	1:B:1084:VAL:HG12	2.13	0.49
1:D:1063:ILE:HD11	1:D:1084:VAL:HB	1.93	0.49
1:E:1071:GLN:HG2	1:E:1075:LEU:CD2	2.42	0.49
1:E:1093:MET:HG2	1:E:1101:TYR:CZ	2.48	0.49
1:A:1080:GLU:O	1:A:1084:VAL:HG12	2.13	0.49
1:B:1089:LEU:HD23	1:B:1089:LEU:O	2.12	0.49
1:C:1093:MET:HG2	1:C:1101:TYR:CZ	2.47	0.49
1:B:1134:ILE:HG12	1:B:1134:ILE:O	2.13	0.48
1:D:1137:ASN:HD22	1:D:1140:VAL:H	1.61	0.48
1:E:1089:LEU:HD23	1:E:1089:LEU:C	2.38	0.48
1:D:138:GLN:O	1:D:142:ILE:HG12	2.13	0.48
1:E:139:ILE:HD13	1:E:1089:LEU:HD12	1.93	0.48
1:A:1041:GLY:HA3	1:A:1064:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:VAL:HG12	1:B:1106:VAL:O	2.14	0.48
1:D:1041:GLY:HA3	1:D:1064:ARG:O	2.13	0.48
1:C:1147:LEU:HD22	1:C:1164:VAL:CG2	2.43	0.48
1:D:1039:PHE:CD1	1:E:108:ASN:HB3	2.48	0.48
1:F:1063:ILE:HD11	1:F:1084:VAL:HB	1.95	0.48
1:A:40:ILE:HD11	1:A:1159:ILE:CD1	2.42	0.48
1:B:69:SER:HB2	1:B:1156:VAL:HG13	1.96	0.48
1:B:138:GLN:O	1:B:142:ILE:HG12	2.12	0.48
1:D:1064:ARG:NH2	1:E:81:GLU:CD	2.71	0.48
1:D:1076:LEU:O	1:D:1081:LYS:HE3	2.13	0.48
1:F:44:ILE:O	1:F:47:VAL:HG12	2.14	0.48
1:F:62:PHE:HZ	1:F:101:GLY:HA2	1.79	0.48
1:B:1093:MET:HG2	1:B:1101:TYR:CZ	2.48	0.48
1:A:1042:GLU:OE2	1:A:1064:ARG:NH1	2.47	0.48
1:B:44:ILE:O	1:B:47:VAL:HG12	2.14	0.48
1:C:1134:ILE:HG12	1:C:1134:ILE:O	2.12	0.48
1:A:1150:VAL:CG1	1:A:1159:ILE:HD13	2.37	0.48
1:B:1147:LEU:HD22	1:B:1164:VAL:CG2	2.44	0.48
1:E:35:SER:HA	1:E:1152:MET:CB	2.35	0.48
1:D:31:GLY:O	1:D:37:LYS:HE3	2.14	0.47
1:E:1086:LEU:HD21	1:E:1106:VAL:HG11	1.95	0.47
1:F:1149:GLY:O	1:F:1159:ILE:HA	2.14	0.47
1:C:1153:VAL:HG12	1:C:1154:ASN:N	2.29	0.47
1:D:1089:LEU:C	1:D:1089:LEU:HD23	2.39	0.47
1:F:1147:LEU:HD22	1:F:1164:VAL:HG22	1.95	0.47
1:A:1089:LEU:HD23	1:A:1089:LEU:C	2.39	0.47
1:D:1147:LEU:HD22	1:D:1164:VAL:HG22	1.97	0.47
1:A:1147:LEU:O	1:A:1161:PRO:HA	2.15	0.47
1:C:1027:ASN:HD22	1:C:1027:ASN:C	2.23	0.47
1:C:1089:LEU:HD23	1:C:1089:LEU:O	2.14	0.47
1:E:1044:ARG:HB2	1:E:1062:SER:HB2	1.97	0.47
1:D:1093:MET:HG2	1:D:1101:TYR:CZ	2.50	0.47
1:F:1023:TYR:C	1:F:1025:ARG:N	2.69	0.47
1:E:112:VAL:HG22	1:E:116:ASP:HB2	1.97	0.47
1:E:128:VAL:HG23	1:E:129:ASP:OD1	2.14	0.47
1:F:112:VAL:HG22	1:F:116:ASP:HB2	1.96	0.47
1:E:69:SER:HB2	1:E:1154:ASN:ND2	2.29	0.47
1:B:1152:MET:HE2	1:B:1155:GLY:C	2.40	0.47
1:D:4:LYS:HD3	1:D:4:LYS:HA	1.71	0.47
1:F:1023:TYR:CD1	1:F:1024:GLN:N	2.80	0.47
1:F:1154:ASN:CG	1:F:1155:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD23	1:B:114:LEU:O	2.14	0.47
1:C:4:LYS:HA	1:C:4:LYS:HD3	1.69	0.47
1:D:69:SER:C	1:D:71:ASN:N	2.73	0.46
1:A:114:LEU:HD23	1:A:114:LEU:O	2.15	0.46
1:A:1086:LEU:HD13	1:A:1118:PHE:CD1	2.50	0.46
1:D:1039:PHE:O	1:E:108:ASN:HA	2.16	0.46
1:E:112:VAL:HG22	1:E:113:ARG:N	2.29	0.46
1:A:6:LEU:HD23	1:A:7:TYR:N	2.29	0.46
1:B:1153:VAL:C	1:B:1155:GLY:H	2.23	0.46
1:D:1086:LEU:HD13	1:D:1118:PHE:CD1	2.50	0.46
1:E:1137:ASN:ND2	1:E:1139:ILE:N	2.61	0.46
1:A:1093:MET:HG2	1:A:1101:TYR:CZ	2.50	0.46
1:D:91:ILE:HD12	1:D:120:ARG:HH12	1.81	0.46
1:F:143:VAL:C	1:F:144:ASN:HD22	2.23	0.46
1:D:107:LEU:HD23	1:D:108:ASN:OD1	2.15	0.46
1:E:1098:SER:OG	1:E:1099:PRO:HD2	2.15	0.46
1:E:40:ILE:HD11	1:E:1159:ILE:HD11	1.97	0.46
1:F:1086:LEU:HD21	1:F:1106:VAL:CG1	2.45	0.46
1:D:1067:GLY:N	1:E:83:VAL:HG21	2.31	0.46
1:E:1023:TYR:C	1:E:1023:TYR:HD1	2.23	0.46
1:E:1104:ASP:HA	1:E:1134:ILE:HG23	1.96	0.46
1:F:112:VAL:HG22	1:F:113:ARG:N	2.31	0.46
1:B:128:VAL:HG23	1:B:129:ASP:OD1	2.16	0.46
1:C:138:GLN:O	1:C:142:ILE:HG12	2.15	0.46
1:D:1089:LEU:HD23	1:D:1089:LEU:O	2.15	0.46
1:B:1042:GLU:HG3	1:B:1064:ARG:NH1	2.31	0.45
1:D:1030:PHE:O	1:D:1034:ILE:HG12	2.16	0.45
1:D:1106:VAL:HG12	1:D:1106:VAL:O	2.15	0.45
1:B:1137:ASN:C	1:B:1137:ASN:HD22	2.24	0.45
1:C:14:PHE:HE2	1:C:1159:ILE:HD12	1.81	0.45
1:D:30:VAL:HG12	1:D:31:GLY:N	2.31	0.45
1:C:1024:GLN:HE21	1:C:1024:GLN:HB2	1.62	0.45
1:D:36:GLY:O	1:D:38:SER:N	2.50	0.45
1:F:91:ILE:HD12	1:F:120:ARG:HH12	1.81	0.45
1:B:1044:ARG:HB2	1:B:1062:SER:HB2	1.99	0.45
1:B:1086:LEU:HD13	1:B:1118:PHE:CE1	2.52	0.45
1:E:61:LYS:HG2	1:E:62:PHE:N	2.30	0.45
1:F:1071:GLN:HG2	1:F:1075:LEU:CD2	2.45	0.45
1:D:28:ALA:HB3	1:D:1147:LEU:CD1	2.45	0.45
1:E:1042:GLU:HG3	1:E:1064:ARG:NH1	2.32	0.45
1:F:1106:VAL:HG12	1:F:1106:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1153:VAL:HG12	1:B:1154:ASN:H	1.82	0.45
1:E:1080:GLU:O	1:E:1084:VAL:HG12	2.17	0.45
1:E:1106:VAL:HG12	1:E:1106:VAL:O	2.17	0.45
1:F:128:VAL:HG23	1:F:129:ASP:OD1	2.16	0.45
1:C:1080:GLU:O	1:C:1084:VAL:HG12	2.17	0.45
1:D:1147:LEU:HD22	1:D:1164:VAL:CG2	2.47	0.45
1:C:44:ILE:O	1:C:47:VAL:HG12	2.17	0.45
1:E:1:MET:HB2	1:E:86:GLU:OE1	2.17	0.45
1:E:44:ILE:O	1:E:47:VAL:HG12	2.16	0.45
1:B:20:ILE:HD11	1:B:1159:ILE:CD1	2.46	0.45
1:C:1104:ASP:HA	1:C:1134:ILE:HG23	1.98	0.45
1:F:1104:ASP:HA	1:F:1134:ILE:HG23	1.99	0.45
1:A:62:PHE:C	1:A:64:MET:N	2.75	0.44
1:A:1030:PHE:O	1:A:1034:ILE:HG12	2.16	0.44
1:B:107:LEU:HD23	1:B:108:ASN:OD1	2.17	0.44
1:C:1137:ASN:ND2	1:C:1140:VAL:H	2.15	0.44
1:E:143:VAL:C	1:E:144:ASN:HD22	2.25	0.44
1:E:1067:GLY:O	1:F:5:LYS:CD	2.65	0.44
1:A:1106:VAL:HG12	1:A:1106:VAL:O	2.17	0.44
1:C:8:LEU:HD22	1:C:11:PHE:HB3	1.97	0.44
1:C:1086:LEU:HD13	1:C:1118:PHE:CD1	2.52	0.44
1:E:8:LEU:HD22	1:E:11:PHE:HB3	1.99	0.44
1:A:1075:LEU:H	1:A:1075:LEU:CD1	2.25	0.44
1:A:1076:LEU:O	1:A:1081:LYS:HE3	2.17	0.44
1:D:14:PHE:HE2	1:D:1159:ILE:HG13	1.83	0.44
1:E:107:LEU:HB2	1:E:112:VAL:HG11	2.00	0.44
1:E:138:GLN:O	1:E:142:ILE:HG12	2.17	0.44
1:B:1:MET:HB2	1:B:86:GLU:OE1	2.18	0.44
1:B:8:LEU:HD22	1:B:11:PHE:HB3	2.00	0.44
1:B:1086:LEU:HD21	1:B:1106:VAL:CG1	2.48	0.44
1:E:1042:GLU:OE2	1:E:1064:ARG:NH1	2.50	0.44
1:F:1023:TYR:O	1:F:1026:VAL:N	2.50	0.44
1:E:1041:GLY:HA3	1:E:1064:ARG:O	2.18	0.44
1:E:1086:LEU:HD13	1:E:1118:PHE:CE1	2.51	0.44
1:A:62:PHE:CE2	1:A:99:ARG:O	2.70	0.44
1:A:1137:ASN:ND2	1:A:1140:VAL:H	2.16	0.44
1:C:35:SER:HA	1:C:1152:MET:HB2	2.00	0.44
1:C:107:LEU:HD23	1:C:108:ASN:OD1	2.18	0.44
1:D:1137:ASN:ND2	1:D:1139:ILE:N	2.63	0.44
1:A:1064:ARG:HH22	1:B:81:GLU:CD	2.26	0.44
1:C:70:GLU:HB3	1:C:1154:ASN:CG	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:VAL:C	1:C:144:ASN:HD22	2.25	0.44
1:F:1042:GLU:HG3	1:F:1064:ARG:NH1	2.33	0.44
1:C:37:LYS:N	1:C:37:LYS:CD	2.81	0.44
1:C:1069:ARG:CZ	1:D:17:PRO:O	2.66	0.44
1:F:1137:ASN:HD22	1:F:1140:VAL:H	1.64	0.44
1:B:67:ALA:O	1:B:74:PRO:HB3	2.17	0.43
1:D:1075:LEU:H	1:D:1075:LEU:CD1	2.24	0.43
1:E:99:ARG:HH11	1:E:99:ARG:CG	2.31	0.43
1:E:1137:ASN:HD22	1:E:1137:ASN:C	2.26	0.43
1:F:30:VAL:HG12	1:F:31:GLY:N	2.33	0.43
1:B:4:LYS:HA	1:B:4:LYS:HD3	1.71	0.43
1:B:1030:PHE:O	1:B:1034:ILE:HG12	2.18	0.43
1:C:1030:PHE:O	1:C:1034:ILE:HG12	2.19	0.43
1:D:1023:TYR:HD1	1:D:1024:GLN:N	2.17	0.43
1:F:70:GLU:CD	1:F:71:ASN:HB3	2.43	0.43
1:A:112:VAL:HG22	1:A:113:ARG:N	2.34	0.43
1:B:112:VAL:HG22	1:B:113:ARG:N	2.31	0.43
1:A:6:LEU:CD1	1:A:40:ILE:HG23	2.48	0.43
1:B:71:ASN:OD1	1:B:71:ASN:N	2.50	0.43
1:B:143:VAL:C	1:B:144:ASN:HD22	2.25	0.43
1:C:1044:ARG:HB2	1:C:1062:SER:HB2	2.00	0.43
1:D:14:PHE:CE2	1:D:1159:ILE:HD11	2.53	0.43
1:D:1027:ASN:OD1	1:D:1045:LEU:CB	2.55	0.43
1:E:1075:LEU:H	1:E:1075:LEU:CD1	2.25	0.43
1:F:1153:VAL:HG12	1:F:1154:ASN:N	2.33	0.43
1:A:1044:ARG:HB2	1:A:1062:SER:HB2	2.01	0.43
1:C:142:ILE:HG22	1:C:1088:LEU:HD13	2.00	0.43
1:C:1042:GLU:HG3	1:C:1064:ARG:NH1	2.33	0.43
1:B:87:ASN:C	1:B:89:GLU:H	2.26	0.43
1:C:1106:VAL:HG12	1:C:1106:VAL:O	2.19	0.43
1:D:70:GLU:CD	1:D:1154:ASN:HB2	2.43	0.43
1:E:1137:ASN:HD22	1:E:1140:VAL:H	1.65	0.43
1:A:112:VAL:HG22	1:A:116:ASP:HB2	2.01	0.43
1:D:142:ILE:HG22	1:D:1088:LEU:HD13	2.01	0.43
1:D:1039:PHE:C	1:E:108:ASN:C	2.86	0.43
1:E:1030:PHE:O	1:E:1034:ILE:HG12	2.19	0.43
1:F:1:MET:HB2	1:F:86:GLU:OE1	2.18	0.43
1:C:30:VAL:HG12	1:C:31:GLY:N	2.34	0.43
1:F:138:GLN:O	1:F:142:ILE:HG12	2.18	0.43
1:A:1086:LEU:HD21	1:A:1106:VAL:CG1	2.48	0.43
1:A:1092:LEU:C	1:A:1094:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ALA:HB3	1:B:1147:LEU:CD1	2.49	0.43
1:E:1086:LEU:HD21	1:E:1106:VAL:CG1	2.49	0.43
1:F:1152:MET:HA	1:F:1156:VAL:O	2.18	0.43
1:B:91:ILE:HD12	1:B:120:ARG:HH12	1.84	0.42
1:B:1075:LEU:H	1:B:1075:LEU:CD1	2.24	0.42
1:B:1137:ASN:ND2	1:B:1137:ASN:C	2.77	0.42
1:B:1137:ASN:ND2	1:B:1139:ILE:N	2.62	0.42
1:C:8:LEU:O	1:C:9:LYS:HB2	2.19	0.42
1:D:1086:LEU:HD13	1:D:1118:PHE:CE1	2.54	0.42
1:F:1023:TYR:O	1:F:1024:GLN:C	2.62	0.42
1:F:1024:GLN:O	1:F:1028:GLU:HB2	2.19	0.42
1:B:143:VAL:O	1:B:143:VAL:HG12	2.18	0.42
1:D:44:ILE:O	1:D:47:VAL:HG12	2.18	0.42
1:E:87:ASN:C	1:E:89:GLU:H	2.28	0.42
1:E:89:GLU:HA	1:E:89:GLU:OE1	2.18	0.42
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.19	0.42
1:C:1146:LEU:HD23	1:C:1147:LEU:N	2.34	0.42
1:A:1024:GLN:H	1:A:1024:GLN:CD	2.27	0.42
1:B:1098:SER:OG	1:B:1099:PRO:HD2	2.19	0.42
1:F:1044:ARG:HB2	1:F:1062:SER:HB2	2.01	0.42
1:B:87:ASN:C	1:B:89:GLU:N	2.76	0.42
1:E:142:ILE:HG22	1:E:1088:LEU:HD13	2.02	0.42
1:F:143:VAL:O	1:F:143:VAL:HG12	2.19	0.42
1:B:107:LEU:HB2	1:B:112:VAL:HG11	2.02	0.42
1:F:107:LEU:HB2	1:F:112:VAL:HG11	2.01	0.42
1:A:142:ILE:HG22	1:A:1088:LEU:HD13	2.01	0.42
1:C:1086:LEU:HD21	1:C:1106:VAL:CG1	2.49	0.42
1:D:1:MET:HB2	1:D:86:GLU:OE1	2.20	0.42
1:D:6:LEU:CD1	1:D:40:ILE:HG23	2.50	0.42
1:F:135:GLY:H	1:F:138:GLN:NE2	2.18	0.42
1:B:1023:TYR:O	1:B:1026:VAL:N	2.53	0.42
1:C:1064:ARG:HH22	1:D:81:GLU:CD	2.28	0.42
1:D:1042:GLU:OE2	1:D:1064:ARG:NH1	2.53	0.42
1:E:72:LEU:HD12	1:E:1156:VAL:CG1	2.50	0.42
1:E:1154:ASN:CG	1:E:1155:GLY:H	2.27	0.42
1:B:1076:LEU:O	1:B:1081:LYS:HE3	2.20	0.42
1:E:1027:ASN:HA	1:E:1045:LEU:HD12	2.01	0.42
1:A:1024:GLN:NE2	1:A:1024:GLN:N	2.68	0.41
1:C:36:GLY:C	1:C:37:LYS:HE3	2.45	0.41
1:F:1086:LEU:HD13	1:F:1118:PHE:CD1	2.55	0.41
1:A:28:ALA:HB3	1:A:1147:LEU:CD1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HD23	1:B:7:TYR:H	1.83	0.41
1:B:61:LYS:C	1:B:63:ASP:H	2.27	0.41
1:D:75:ALA:O	1:D:99:ARG:NH1	2.53	0.41
1:D:1044:ARG:HB2	1:D:1062:SER:HB2	2.02	0.41
1:D:1086:LEU:HD21	1:D:1106:VAL:CG1	2.49	0.41
1:D:1098:SER:OG	1:D:1099:PRO:HD2	2.20	0.41
1:E:70:GLU:CD	1:E:71:ASN:N	2.76	0.41
1:E:1039:PHE:HD1	1:F:108:ASN:O	2.03	0.41
1:E:1076:LEU:O	1:E:1081:LYS:HE3	2.20	0.41
1:F:6:LEU:CD1	1:F:40:ILE:HG23	2.50	0.41
1:A:35:SER:C	1:A:37:LYS:N	2.67	0.41
1:A:143:VAL:C	1:A:144:ASN:HD22	2.28	0.41
1:C:91:ILE:HD12	1:C:120:ARG:HH12	1.84	0.41
1:D:1083:LEU:HD12	1:D:1083:LEU:HA	1.89	0.41
1:F:99:ARG:HH11	1:F:99:ARG:CG	2.32	0.41
1:A:1:MET:HB2	1:A:86:GLU:OE1	2.21	0.41
1:D:1104:ASP:HA	1:D:1134:ILE:HG23	2.03	0.41
1:A:1042:GLU:HG3	1:A:1064:ARG:NH1	2.36	0.41
1:A:1098:SER:OG	1:A:1099:PRO:HD2	2.20	0.41
1:C:1023:TYR:CD1	1:C:1024:GLN:N	2.86	0.41
1:E:70:GLU:HG2	1:E:71:ASN:N	2.34	0.41
1:B:28:ALA:HA	1:B:1133:VAL:O	2.21	0.41
1:C:87:ASN:C	1:C:89:GLU:N	2.78	0.41
1:E:87:ASN:C	1:E:89:GLU:N	2.76	0.41
1:B:33:ASN:O	1:B:37:LYS:HE2	2.21	0.41
1:B:70:GLU:OE1	1:B:71:ASN:ND2	2.54	0.41
1:B:89:GLU:OE1	1:B:89:GLU:HA	2.19	0.41
1:B:99:ARG:HH11	1:B:99:ARG:CG	2.34	0.41
1:D:87:ASN:C	1:D:89:GLU:N	2.78	0.41
1:D:143:VAL:C	1:D:144:ASN:HD22	2.29	0.41
1:E:30:VAL:HG12	1:E:31:GLY:N	2.36	0.41
1:E:1137:ASN:ND2	1:E:1140:VAL:H	2.19	0.41
1:E:1137:ASN:HD22	1:E:1139:ILE:N	2.17	0.41
1:F:1137:ASN:ND2	1:F:1139:ILE:N	2.66	0.41
1:B:6:LEU:CD1	1:B:40:ILE:HG23	2.51	0.41
1:B:103:ASN:C	1:B:104:THR:HG22	2.44	0.41
1:C:103:ASN:C	1:C:104:THR:HG22	2.45	0.41
1:C:1023:TYR:O	1:C:1025:ARG:N	2.54	0.41
1:C:1042:GLU:OE2	1:C:1064:ARG:NH1	2.54	0.41
1:D:112:VAL:HG22	1:D:116:ASP:HB2	2.02	0.41
1:E:40:ILE:HD11	1:E:1159:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:HD23	1:E:108:ASN:OD1	2.20	0.41
1:F:1080:GLU:O	1:F:1084:VAL:HG12	2.21	0.41
1:B:1137:ASN:HD22	1:B:1140:VAL:H	1.67	0.41
1:C:112:VAL:HG22	1:C:113:ARG:N	2.35	0.41
1:C:1098:SER:OG	1:C:1099:PRO:HD2	2.21	0.41
1:D:1092:LEU:C	1:D:1094:GLU:H	2.28	0.41
1:F:36:GLY:CA	1:F:37:LYS:HE3	2.51	0.41
1:A:1147:LEU:HD22	1:A:1164:VAL:HG22	2.03	0.40
1:B:33:ASN:O	1:B:37:LYS:CE	2.70	0.40
1:B:1039:PHE:CD1	1:C:108:ASN:HB3	2.55	0.40
1:C:1:MET:HB2	1:C:86:GLU:OE1	2.21	0.40
1:E:1137:ASN:ND2	1:E:1137:ASN:C	2.78	0.40
1:A:1067:GLY:O	1:B:5:LYS:HD2	2.21	0.40
1:A:1086:LEU:HD13	1:A:1118:PHE:CE1	2.56	0.40
1:B:69:SER:C	1:B:71:ASN:N	2.79	0.40
1:E:120:ARG:HA	1:E:120:ARG:HD2	1.87	0.40
1:F:28:ALA:HB3	1:F:1147:LEU:CD1	2.51	0.40
1:F:1042:GLU:OE2	1:F:1064:ARG:NH1	2.55	0.40
1:A:107:LEU:HD23	1:A:108:ASN:OD1	2.22	0.40
1:A:143:VAL:O	1:A:143:VAL:HG12	2.21	0.40
1:A:1160:VAL:O	1:A:1162:VAL:HG13	2.21	0.40
1:B:142:ILE:HG22	1:B:1088:LEU:HD13	2.02	0.40
1:C:69:SER:HB2	1:C:72:LEU:HB2	2.03	0.40
1:C:72:LEU:CD1	1:C:1156:VAL:HG11	2.49	0.40
1:E:69:SER:O	1:E:70:GLU:C	2.64	0.40
1:F:1089:LEU:C	1:F:1089:LEU:CD2	2.95	0.40
1:B:120:ARG:HD2	1:B:120:ARG:HA	1.85	0.40
1:C:135:GLY:H	1:C:138:GLN:NE2	2.19	0.40
1:D:16:ARG:HA	1:D:17:PRO:HD3	1.93	0.40
1:D:89:GLU:OE1	1:D:89:GLU:HA	2.21	0.40
1:D:91:ILE:HD12	1:D:120:ARG:NH1	2.36	0.40
1:E:4:LYS:HA	1:E:4:LYS:HD3	1.70	0.40
1:D:1137:ASN:ND2	1:D:1140:VAL:H	2.19	0.40
1:E:1146:LEU:HD23	1:E:1147:LEU:N	2.37	0.40
1:F:8:LEU:HD22	1:F:11:PHE:HB3	2.02	0.40
1:F:1024:GLN:HE21	1:F:1024:GLN:HB2	1.74	0.40
1:F:1092:LEU:C	1:F:1094:GLU:H	2.29	0.40
1:F:1137:ASN:ND2	1:F:1140:VAL:H	2.19	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	255/322 (79%)	223 (88%)	26 (10%)	6 (2%)	4	22
1	B	255/322 (79%)	219 (86%)	27 (11%)	9 (4%)	3	16
1	C	255/322 (79%)	221 (87%)	25 (10%)	9 (4%)	3	16
1	D	255/322 (79%)	221 (87%)	25 (10%)	9 (4%)	3	16
1	E	255/322 (79%)	215 (84%)	30 (12%)	10 (4%)	2	14
1	F	255/322 (79%)	222 (87%)	25 (10%)	8 (3%)	3	18
All	All	1530/1932 (79%)	1321 (86%)	158 (10%)	51 (3%)	3	17

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	B	35	SER
1	C	1153	VAL
1	D	37	LYS
1	D	38	SER
1	D	1066	PRO
1	E	35	SER
1	E	1153	VAL
1	E	1154	ASN
1	F	1153	VAL
1	F	1154	ASN
1	A	1041	GLY
1	A	1066	PRO
1	B	34	GLY
1	B	1041	GLY
1	B	1066	PRO
1	B	1153	VAL
1	C	9	LYS
1	C	1066	PRO
1	C	1154	ASN

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Mol	Chain	Res	Type
1	D	1041	GLY
1	E	34	GLY
1	E	1041	GLY
1	E	1066	PRO
1	F	1066	PRO
1	A	122	ALA
1	A	128	VAL
1	B	122	ALA
1	B	128	VAL
1	B	1154	ASN
1	C	1041	GLY
1	D	34	GLY
1	D	122	ALA
1	E	122	ALA
1	F	9	LYS
1	F	122	ALA
1	F	1161	PRO
1	C	122	ALA
1	C	128	VAL
1	D	9	LYS
1	D	128	VAL
1	D	1154	ASN
1	E	128	VAL
1	F	128	VAL
1	A	9	LYS
1	B	62	PHE
1	E	9	LYS
1	E	62	PHE
1	F	1041	GLY
1	C	1024	GLN
1	C	32	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/275 (81%)	191 (86%)	31 (14%)	3	15
1	B	222/275 (81%)	190 (86%)	32 (14%)	3	14
1	C	222/275 (81%)	192 (86%)	30 (14%)	4	16
1	D	222/275 (81%)	192 (86%)	30 (14%)	4	16
1	E	222/275 (81%)	195 (88%)	27 (12%)	5	20
1	F	222/275 (81%)	194 (87%)	28 (13%)	4	19
All	All	1332/1650 (81%)	1154 (87%)	178 (13%)	4	17

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	LEU
1	A	35	SER
1	A	37	LYS
1	A	50	GLU
1	A	63	ASP
1	A	70	GLU
1	A	97	LEU
1	A	99	ARG
1	A	104	THR
1	A	114	LEU
1	A	117	ILE
1	A	132	SER
1	A	1023	TYR
1	A	1024	GLN
1	A	1065	LYS
1	A	1070	ASP
1	A	1071	GLN
1	A	1075	LEU
1	A	1083	LEU
1	A	1084	VAL
1	A	1088	LEU
1	A	1106	VAL
1	A	1110	LEU
1	A	1121	LEU
1	A	1122	LEU
1	A	1124	GLU

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Mol	Chain	Res	Type
1	A	1134	ILE
1	A	1137	ASN
1	A	1146	LEU
1	A	1159	ILE
1	B	3	LEU
1	B	6	LEU
1	B	33	ASN
1	B	37	LYS
1	B	50	GLU
1	B	69	SER
1	B	71	ASN
1	B	97	LEU
1	B	99	ARG
1	B	104	THR
1	B	114	LEU
1	B	117	ILE
1	B	132	SER
1	B	1023	TYR
1	B	1027	ASN
1	B	1065	LYS
1	B	1070	ASP
1	B	1071	GLN
1	B	1075	LEU
1	B	1083	LEU
1	B	1084	VAL
1	B	1088	LEU
1	B	1110	LEU
1	B	1121	LEU
1	B	1122	LEU
1	B	1124	GLU
1	B	1134	ILE
1	B	1137	ASN
1	B	1146	LEU
1	B	1147	LEU
1	B	1152	MET
1	B	1154	ASN
1	C	3	LEU
1	C	6	LEU
1	C	37	LYS
1	C	50	GLU
1	C	64	MET
1	C	97	LEU

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Mol	Chain	Res	Type
1	C	99	ARG
1	C	104	THR
1	C	114	LEU
1	C	117	ILE
1	C	132	SER
1	C	1023	TYR
1	C	1024	GLN
1	C	1027	ASN
1	C	1065	LYS
1	C	1070	ASP
1	C	1071	GLN
1	C	1075	LEU
1	C	1083	LEU
1	C	1084	VAL
1	C	1088	LEU
1	C	1110	LEU
1	C	1121	LEU
1	C	1122	LEU
1	C	1124	GLU
1	C	1134	ILE
1	C	1137	ASN
1	C	1147	LEU
1	C	1156	VAL
1	C	1159	ILE
1	D	3	LEU
1	D	6	LEU
1	D	35	SER
1	D	37	LYS
1	D	50	GLU
1	D	64	MET
1	D	97	LEU
1	D	99	ARG
1	D	104	THR
1	D	114	LEU
1	D	117	ILE
1	D	132	SER
1	D	1023	TYR
1	D	1024	GLN
1	D	1065	LYS
1	D	1070	ASP
1	D	1071	GLN
1	D	1075	LEU

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Mol	Chain	Res	Type
1	D	1083	LEU
1	D	1084	VAL
1	D	1088	LEU
1	D	1110	LEU
1	D	1121	LEU
1	D	1122	LEU
1	D	1124	GLU
1	D	1134	ILE
1	D	1137	ASN
1	D	1146	LEU
1	D	1147	LEU
1	D	1156	VAL
1	E	3	LEU
1	E	6	LEU
1	E	33	ASN
1	E	37	LYS
1	E	50	GLU
1	E	97	LEU
1	E	99	ARG
1	E	104	THR
1	E	114	LEU
1	E	117	ILE
1	E	132	SER
1	E	1023	TYR
1	E	1065	LYS
1	E	1070	ASP
1	E	1071	GLN
1	E	1075	LEU
1	E	1083	LEU
1	E	1084	VAL
1	E	1088	LEU
1	E	1110	LEU
1	E	1121	LEU
1	E	1122	LEU
1	E	1124	GLU
1	E	1134	ILE
1	E	1137	ASN
1	E	1146	LEU
1	E	1147	LEU
1	F	3	LEU
1	F	6	LEU
1	F	33	ASN

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Mol	Chain	Res	Type
1	F	37	LYS
1	F	50	GLU
1	F	70	GLU
1	F	97	LEU
1	F	99	ARG
1	F	104	THR
1	F	114	LEU
1	F	117	ILE
1	F	132	SER
1	F	1023	TYR
1	F	1065	LYS
1	F	1070	ASP
1	F	1071	GLN
1	F	1075	LEU
1	F	1083	LEU
1	F	1084	VAL
1	F	1088	LEU
1	F	1110	LEU
1	F	1121	LEU
1	F	1122	LEU
1	F	1124	GLU
1	F	1134	ILE
1	F	1137	ASN
1	F	1146	LEU
1	F	1147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	1024	GLN
1	A	1071	GLN
1	A	1114	ASN
1	A	1128	HIS
1	A	1130	GLN
1	A	1137	ASN
1	B	33	ASN
1	B	144	ASN
1	B	1024	GLN
1	B	1027	ASN
1	B	1071	GLN
1	B	1114	ASN

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Mol	Chain	Res	Type
1	B	1128	HIS
1	B	1130	GLN
1	B	1137	ASN
1	B	1154	ASN
1	C	71	ASN
1	C	144	ASN
1	C	1024	GLN
1	C	1071	GLN
1	C	1114	ASN
1	C	1130	GLN
1	C	1137	ASN
1	D	144	ASN
1	D	1071	GLN
1	D	1114	ASN
1	D	1128	HIS
1	D	1130	GLN
1	D	1137	ASN
1	E	71	ASN
1	E	144	ASN
1	E	1027	ASN
1	E	1071	GLN
1	E	1114	ASN
1	E	1128	HIS
1	E	1130	GLN
1	E	1137	ASN
1	E	1154	ASN
1	F	144	ASN
1	F	1024	GLN
1	F	1071	GLN
1	F	1114	ASN
1	F	1128	HIS
1	F	1130	GLN
1	F	1137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/322 (81%)	0.24	6 (2%) 61 39	34, 66, 91, 119	0
1	B	263/322 (81%)	0.23	10 (3%) 44 25	47, 76, 99, 125	0
1	C	263/322 (81%)	0.29	7 (2%) 56 35	49, 74, 102, 126	0
1	D	263/322 (81%)	0.15	3 (1%) 78 59	51, 73, 97, 121	0
1	E	263/322 (81%)	0.29	10 (3%) 44 25	46, 76, 99, 125	0
1	F	263/322 (81%)	0.44	13 (4%) 35 18	47, 70, 94, 125	0
All	All	1578/1932 (81%)	0.27	49 (3%) 51 30	34, 73, 99, 126	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1164	VAL	6.1
1	C	1164	VAL	5.6
1	F	1023	TYR	4.3
1	F	1162	VAL	3.8
1	E	1162	VAL	3.7
1	C	1023	TYR	3.5
1	A	1023	TYR	3.4
1	B	1023	TYR	3.4
1	E	1164	VAL	3.3
1	C	1095	ILE	3.1
1	E	1023	TYR	3.0
1	C	1162	VAL	3.0
1	F	1060	GLU	3.0
1	E	145	ALA	2.7
1	D	1164	VAL	2.7
1	A	1067	GLY	2.7
1	A	1164	VAL	2.7
1	F	1095	ILE	2.7
1	A	1142	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1066	PRO	2.7
1	B	1162	VAL	2.7
1	D	1023	TYR	2.6
1	F	110	SER	2.6
1	B	1067	GLY	2.6
1	B	1160	VAL	2.6
1	C	1153	VAL	2.5
1	F	101	GLY	2.5
1	E	1067	GLY	2.5
1	F	1068	ARG	2.5
1	E	1161	PRO	2.5
1	F	145	ALA	2.4
1	B	1164	VAL	2.4
1	E	50	GLU	2.4
1	B	1161	PRO	2.4
1	E	1163	GLU	2.4
1	F	1028	GLU	2.3
1	A	144	ASN	2.3
1	E	1160	VAL	2.3
1	C	1161	PRO	2.3
1	F	1161	PRO	2.2
1	B	1080	GLU	2.1
1	D	35	SER	2.1
1	A	35	SER	2.1
1	F	1096	LYS	2.1
1	B	1045	LEU	2.1
1	F	1163	GLU	2.1
1	C	145	ALA	2.0
1	E	1095	ILE	2.0
1	B	1060	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 ⓘ

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.