



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:26 PM UTC

PDB ID : 3K4W / pdb_00003k4w
Title : CRYSTAL STRUCTURE OF Uncharacterized Tim-Barrel Protein Bb4693
From Bordetella Bronchiseptica
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New
York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-10-06
Resolution : 1.92 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:

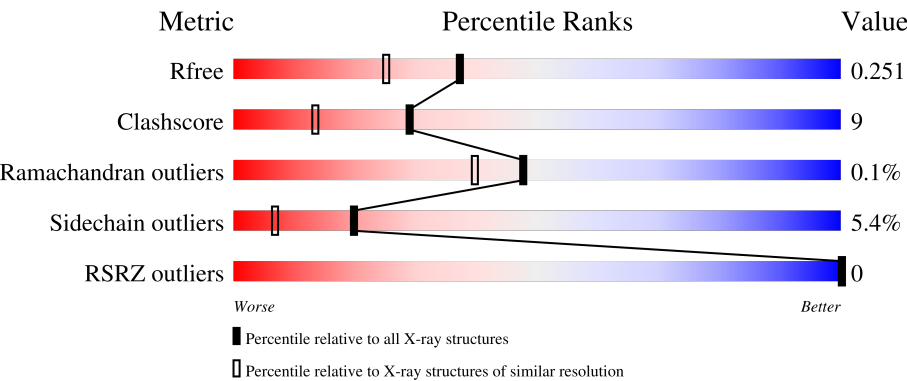
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	291	77%18% . .
1	B	291	73%20% . .
1	C	291	78%16% . .
1	D	291	69%23% . . .
1	E	291	74%21% . .

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Mol	Chain	Length	Quality of chain
1	F	291	76%19%
1	G	291	69%24%
1	H	291	73%20%
1	I	291	76%18%
1	J	291	78%18%
1	K	291	80%15%
1	L	291	69%24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28586 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 uncharacterized protein Bb4693.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	1	0
			2215	1417	381	402	15			
1	B	281	Total	C	N	O	S	0	6	0
			2236	1430	382	408	16			
1	C	281	Total	C	N	O	S	0	2	0
			2220	1420	382	403	15			
1	D	281	Total	C	N	O	S	0	2	0
			2220	1421	381	402	16			
1	E	281	Total	C	N	O	S	0	5	0
			2231	1427	382	406	16			
1	F	281	Total	C	N	O	S	0	3	0
			2230	1428	384	401	17			
1	G	281	Total	C	N	O	S	0	2	0
			2223	1423	381	403	16			
1	H	281	Total	C	N	O	S	0	4	0
			2226	1424	382	404	16			
1	I	281	Total	C	N	O	S	0	2	0
			2224	1423	384	402	15			
1	J	281	Total	C	N	O	S	0	2	0
			2220	1420	382	403	15			
1	K	281	Total	C	N	O	S	0	3	0
			2223	1422	381	404	16			
1	L	281	Total	C	N	O	S	0	1	0
			2215	1417	381	402	15			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	insertion	UNP Q7WEE2
A	1	LEU	-	insertion	UNP Q7WEE2
A	282	GLU	-	insertion	UNP Q7WEE2
A	283	GLY	-	insertion	UNP Q7WEE2
A	284	HIS	-	insertion	UNP Q7WEE2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	285	HIS	-	insertion	UNP Q7WEE2
A	286	HIS	-	insertion	UNP Q7WEE2
A	287	HIS	-	insertion	UNP Q7WEE2
A	288	HIS	-	insertion	UNP Q7WEE2
A	289	HIS	-	insertion	UNP Q7WEE2
B	0	SER	-	insertion	UNP Q7WEE2
B	1	LEU	-	insertion	UNP Q7WEE2
B	282	GLU	-	insertion	UNP Q7WEE2
B	283	GLY	-	insertion	UNP Q7WEE2
B	284	HIS	-	insertion	UNP Q7WEE2
B	285	HIS	-	insertion	UNP Q7WEE2
B	286	HIS	-	insertion	UNP Q7WEE2
B	287	HIS	-	insertion	UNP Q7WEE2
B	288	HIS	-	insertion	UNP Q7WEE2
B	289	HIS	-	insertion	UNP Q7WEE2
C	0	SER	-	insertion	UNP Q7WEE2
C	1	LEU	-	insertion	UNP Q7WEE2
C	282	GLU	-	insertion	UNP Q7WEE2
C	283	GLY	-	insertion	UNP Q7WEE2
C	284	HIS	-	insertion	UNP Q7WEE2
C	285	HIS	-	insertion	UNP Q7WEE2
C	286	HIS	-	insertion	UNP Q7WEE2
C	287	HIS	-	insertion	UNP Q7WEE2
C	288	HIS	-	insertion	UNP Q7WEE2
C	289	HIS	-	insertion	UNP Q7WEE2
D	0	SER	-	insertion	UNP Q7WEE2
D	1	LEU	-	insertion	UNP Q7WEE2
D	282	GLU	-	insertion	UNP Q7WEE2
D	283	GLY	-	insertion	UNP Q7WEE2
D	284	HIS	-	insertion	UNP Q7WEE2
D	285	HIS	-	insertion	UNP Q7WEE2
D	286	HIS	-	insertion	UNP Q7WEE2
D	287	HIS	-	insertion	UNP Q7WEE2
D	288	HIS	-	insertion	UNP Q7WEE2
D	289	HIS	-	insertion	UNP Q7WEE2
E	0	SER	-	insertion	UNP Q7WEE2
E	1	LEU	-	insertion	UNP Q7WEE2
E	282	GLU	-	insertion	UNP Q7WEE2
E	283	GLY	-	insertion	UNP Q7WEE2
E	284	HIS	-	insertion	UNP Q7WEE2
E	285	HIS	-	insertion	UNP Q7WEE2
E	286	HIS	-	insertion	UNP Q7WEE2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	287	HIS	-	insertion	UNP Q7WEE2
E	288	HIS	-	insertion	UNP Q7WEE2
E	289	HIS	-	insertion	UNP Q7WEE2
F	0	SER	-	insertion	UNP Q7WEE2
F	1	LEU	-	insertion	UNP Q7WEE2
F	282	GLU	-	insertion	UNP Q7WEE2
F	283	GLY	-	insertion	UNP Q7WEE2
F	284	HIS	-	insertion	UNP Q7WEE2
F	285	HIS	-	insertion	UNP Q7WEE2
F	286	HIS	-	insertion	UNP Q7WEE2
F	287	HIS	-	insertion	UNP Q7WEE2
F	288	HIS	-	insertion	UNP Q7WEE2
F	289	HIS	-	insertion	UNP Q7WEE2
G	0	SER	-	insertion	UNP Q7WEE2
G	1	LEU	-	insertion	UNP Q7WEE2
G	282	GLU	-	insertion	UNP Q7WEE2
G	283	GLY	-	insertion	UNP Q7WEE2
G	284	HIS	-	insertion	UNP Q7WEE2
G	285	HIS	-	insertion	UNP Q7WEE2
G	286	HIS	-	insertion	UNP Q7WEE2
G	287	HIS	-	insertion	UNP Q7WEE2
G	288	HIS	-	insertion	UNP Q7WEE2
G	289	HIS	-	insertion	UNP Q7WEE2
H	0	SER	-	insertion	UNP Q7WEE2
H	1	LEU	-	insertion	UNP Q7WEE2
H	282	GLU	-	insertion	UNP Q7WEE2
H	283	GLY	-	insertion	UNP Q7WEE2
H	284	HIS	-	insertion	UNP Q7WEE2
H	285	HIS	-	insertion	UNP Q7WEE2
H	286	HIS	-	insertion	UNP Q7WEE2
H	287	HIS	-	insertion	UNP Q7WEE2
H	288	HIS	-	insertion	UNP Q7WEE2
H	289	HIS	-	insertion	UNP Q7WEE2
I	0	SER	-	insertion	UNP Q7WEE2
I	1	LEU	-	insertion	UNP Q7WEE2
I	282	GLU	-	insertion	UNP Q7WEE2
I	283	GLY	-	insertion	UNP Q7WEE2
I	284	HIS	-	insertion	UNP Q7WEE2
I	285	HIS	-	insertion	UNP Q7WEE2
I	286	HIS	-	insertion	UNP Q7WEE2
I	287	HIS	-	insertion	UNP Q7WEE2
I	288	HIS	-	insertion	UNP Q7WEE2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	289	HIS	-	insertion	UNP Q7WEE2
J	0	SER	-	insertion	UNP Q7WEE2
J	1	LEU	-	insertion	UNP Q7WEE2
J	282	GLU	-	insertion	UNP Q7WEE2
J	283	GLY	-	insertion	UNP Q7WEE2
J	284	HIS	-	insertion	UNP Q7WEE2
J	285	HIS	-	insertion	UNP Q7WEE2
J	286	HIS	-	insertion	UNP Q7WEE2
J	287	HIS	-	insertion	UNP Q7WEE2
J	288	HIS	-	insertion	UNP Q7WEE2
J	289	HIS	-	insertion	UNP Q7WEE2
K	0	SER	-	insertion	UNP Q7WEE2
K	1	LEU	-	insertion	UNP Q7WEE2
K	282	GLU	-	insertion	UNP Q7WEE2
K	283	GLY	-	insertion	UNP Q7WEE2
K	284	HIS	-	insertion	UNP Q7WEE2
K	285	HIS	-	insertion	UNP Q7WEE2
K	286	HIS	-	insertion	UNP Q7WEE2
K	287	HIS	-	insertion	UNP Q7WEE2
K	288	HIS	-	insertion	UNP Q7WEE2
K	289	HIS	-	insertion	UNP Q7WEE2
L	0	SER	-	insertion	UNP Q7WEE2
L	1	LEU	-	insertion	UNP Q7WEE2
L	282	GLU	-	insertion	UNP Q7WEE2
L	283	GLY	-	insertion	UNP Q7WEE2
L	284	HIS	-	insertion	UNP Q7WEE2
L	285	HIS	-	insertion	UNP Q7WEE2
L	286	HIS	-	insertion	UNP Q7WEE2
L	287	HIS	-	insertion	UNP Q7WEE2
L	288	HIS	-	insertion	UNP Q7WEE2
L	289	HIS	-	insertion	UNP Q7WEE2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	159	Total O 159 159	0	0
2	B	147	Total O 147 147	0	0
2	C	195	Total O 195 195	0	0
2	D	142	Total O 142 142	0	0

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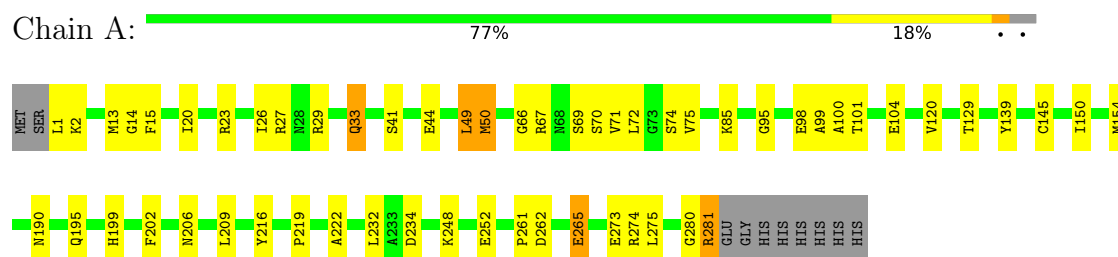
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	168	Total 168	O 168	0	0
2	F	171	Total 171	O 171	0	0
2	G	114	Total 114	O 114	0	0
2	H	155	Total 155	O 155	0	0
2	I	159	Total 159	O 159	0	0
2	J	161	Total 161	O 161	0	0
2	K	175	Total 175	O 175	0	0
2	L	157	Total 157	O 157	0	0

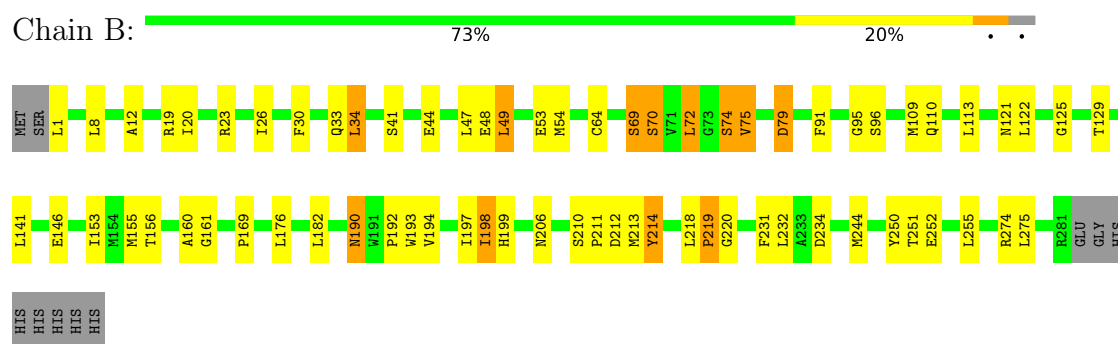
3 Residue-property plots

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.

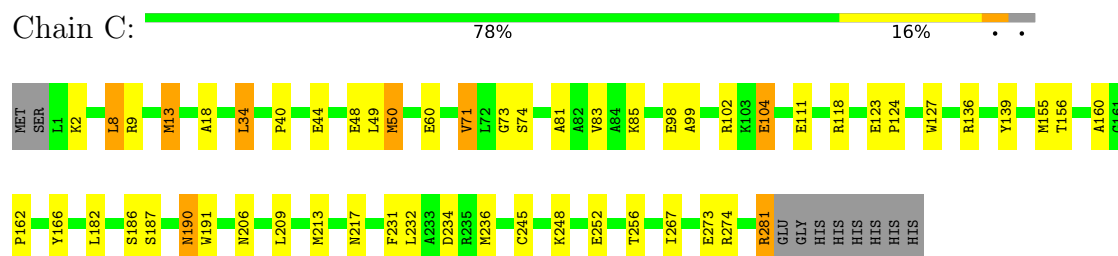
• Molecule 1: uncharacterized protein Bb4693



• Molecule 1: uncharacterized protein Bb4693

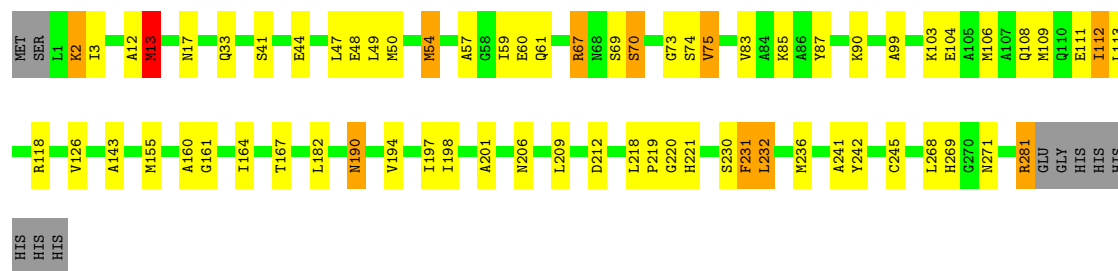


• Molecule 1: uncharacterized protein Bb4693



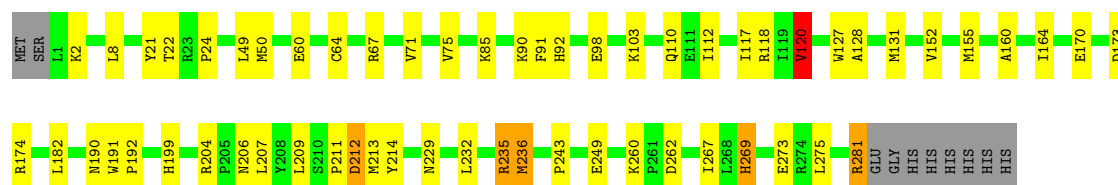
• Molecule 1: uncharacterized protein Bb4693





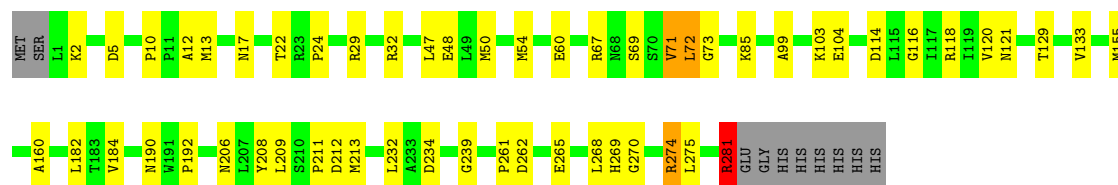
- Molecule 1: uncharacterized protein Bb4693

Chain I: 76% 18% ..



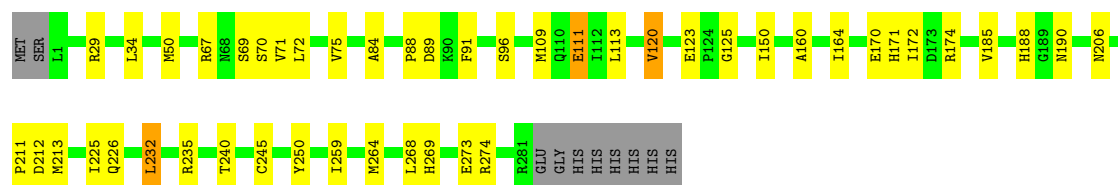
- Molecule 1: uncharacterized protein Bb4693

Chain J: 78% 18% ..



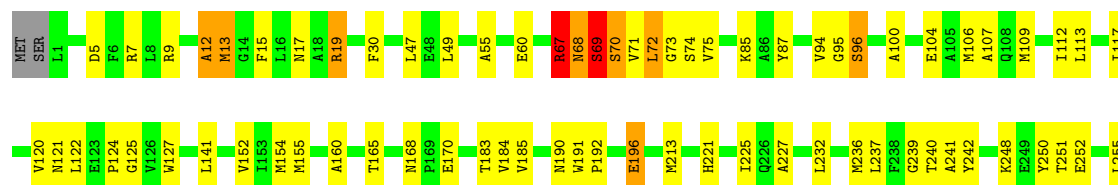
- Molecule 1: uncharacterized protein Bb4693

Chain K: 80% 15% ..



- Molecule 1: uncharacterized protein Bb4693

Chain L: 69% 24% ..



I259	I260	P261	I267	L275	A279	G280	R281	GLU	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.92Å 248.77Å 90.62Å 90.00° 104.92° 90.00°	Depositor
Resolution (Å)	25.97 – 1.92 25.97 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.5 (25.97-1.92) 95.5 (25.97-1.92)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.251 0.192 , 0.251	Depositor DCC
R_{free} test set	13295 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28586	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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	1.36	6/2277 (0.3%)	1.27	5/3097 (0.2%)
1	B	1.34	9/2313 (0.4%)	1.25	11/3146 (0.3%)
1	C	1.35	4/2285 (0.2%)	1.24	8/3108 (0.3%)
1	D	1.43	12/2285 (0.5%)	1.33	16/3107 (0.5%)
1	E	1.33	5/2305 (0.2%)	1.21	1/3135 (0.0%)
1	F	1.36	5/2298 (0.2%)	1.22	7/3123 (0.2%)
1	G	1.34	12/2288 (0.5%)	1.32	10/3111 (0.3%)
1	H	1.33	9/2297 (0.4%)	1.23	11/3124 (0.4%)
1	I	1.32	3/2290 (0.1%)	1.21	6/3115 (0.2%)
1	J	1.38	12/2285 (0.5%)	1.31	5/3108 (0.2%)
1	K	1.31	8/2291 (0.3%)	1.21	6/3116 (0.2%)
1	L	1.36	8/2277 (0.4%)	1.29	13/3097 (0.4%)
All	All	1.35	93/27491 (0.3%)	1.26	99/37387 (0.3%)

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	212	ASP	C-O	-8.54	1.16	1.24
1	G	193	TRP	C-O	-8.29	1.13	1.24
1	E	94	VAL	C-N	-8.10	1.29	1.33
1	D	71	VAL	CA-CB	-7.86	1.47	1.55
1	L	68	ASN	CA-C	-7.74	1.46	1.53
1	G	68	ASN	C-O	-7.51	1.15	1.24
1	L	13	MET	C-O	-7.49	1.17	1.24
1	I	120	VAL	CA-CB	7.43	1.64	1.54
1	A	145	CYS	C-O	-7.41	1.15	1.24
1	D	207	LEU	C-O	-7.24	1.15	1.24
1	K	212	ASP	C-O	-7.15	1.17	1.24
1	J	212	ASP	C-O	-7.02	1.18	1.24
1	J	133	VAL	CA-CB	6.96	1.64	1.54
1	A	222	ALA	CA-CB	6.91	1.64	1.53
1	G	213	MET	C-O	-6.75	1.16	1.24
1	L	55	ALA	CA-CB	6.73	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	32	ARG	C-O	-6.65	1.16	1.24
1	B	212	ASP	C-O	-6.63	1.15	1.24
1	F	198	ILE	CA-CB	6.63	1.62	1.54
1	A	150	ILE	CA-C	6.57	1.58	1.53
1	B	153	ILE	C-O	-6.53	1.17	1.24
1	D	257	LEU	C-O	-6.50	1.15	1.23
1	D	71	VAL	CA-C	-6.48	1.44	1.52
1	K	150	ILE	CA-CB	6.27	1.60	1.53
1	A	280	GLY	C-O	-6.25	1.16	1.24
1	D	205	PRO	C-O	-6.22	1.16	1.24
1	K	185	VAL	CA-CB	6.18	1.61	1.54
1	H	143	ALA	CA-CB	6.17	1.63	1.53
1	J	211	PRO	C-O	-6.15	1.16	1.24
1	I	211	PRO	C-O	-6.15	1.16	1.24
1	A	195	GLN	N-CA	6.06	1.53	1.46
1	B	198	ILE	CA-CB	-6.05	1.47	1.54
1	F	80	VAL	CA-CB	6.02	1.61	1.54
1	D	225	ILE	CA-CB	6.01	1.61	1.54
1	J	10	PRO	CA-C	5.95	1.57	1.52
1	D	197	ILE	CA-CB	5.94	1.61	1.54
1	G	36	PHE	N-CA	5.93	1.52	1.45
1	E	13	MET	C-O	-5.89	1.18	1.24
1	K	111	GLU	C-O	-5.86	1.17	1.24
1	G	210	SER	C-O	-5.84	1.17	1.24
1	G	211	PRO	C-O	-5.83	1.17	1.24
1	L	259	ILE	CA-CB	5.79	1.61	1.54
1	C	102	ARG	C-O	-5.79	1.17	1.24
1	F	137	ARG	C-O	-5.74	1.16	1.24
1	I	212	ASP	C-O	-5.73	1.16	1.24
1	L	15	PHE	C-O	-5.66	1.17	1.24
1	K	123	GLU	C-O	-5.64	1.17	1.24
1	F	267	ILE	CA-CB	-5.63	1.47	1.54
1	L	165	THR	CA-CB	5.61	1.63	1.53
1	G	133	VAL	CA-CB	5.60	1.62	1.54
1	J	274	ARG	CD-NE	-5.60	1.38	1.46
1	D	256	THR	C-O	-5.60	1.16	1.24
1	K	172	ILE	CA-CB	5.59	1.62	1.54
1	B	146	GLU	N-CA	-5.58	1.39	1.46
1	B	210	SER	C-O	-5.58	1.17	1.24
1	E	267	ILE	N-CA	-5.58	1.39	1.46
1	H	112	ILE	C-O	-5.57	1.17	1.24
1	H	111	GLU	C-O	-5.56	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	245	CYS	CA-C	-5.54	1.47	1.52
1	H	126	VAL	CA-CB	5.52	1.61	1.54
1	D	206	ASN	C-O	-5.50	1.16	1.24
1	E	59	ILE	CA-C	5.49	1.59	1.53
1	L	68	ASN	C-O	-5.46	1.19	1.24
1	J	268	LEU	C-O	-5.45	1.17	1.24
1	C	186	SER	C-O	5.44	1.30	1.23
1	G	212	ASP	C-O	-5.43	1.17	1.24
1	H	75	VAL	CA-CB	5.40	1.61	1.54
1	A	15	PHE	C-O	-5.40	1.17	1.24
1	B	211	PRO	C-O	-5.40	1.17	1.24
1	L	227	ALA	CA-CB	5.40	1.61	1.53
1	J	121	ASN	CA-C	-5.39	1.46	1.52
1	J	213	MET	SD-CE	-5.36	1.66	1.79
1	H	268	LEU	C-O	-5.34	1.17	1.24
1	G	71	VAL	CA-CB	-5.31	1.48	1.54
1	J	184	VAL	C-O	-5.28	1.18	1.24
1	D	195	GLN	N-CA	5.28	1.52	1.46
1	D	146	GLU	N-CA	-5.28	1.40	1.46
1	J	270	GLY	C-O	-5.22	1.17	1.23
1	G	55	ALA	CA-CB	5.22	1.61	1.53
1	G	67	ARG	CA-C	-5.20	1.47	1.52
1	D	279	ALA	CA-C	5.18	1.59	1.52
1	J	208	TYR	C-O	5.18	1.30	1.24
1	C	13	MET	C-O	-5.18	1.19	1.24
1	G	195	GLN	C-O	-5.15	1.18	1.24
1	B	176	LEU	CA-CB	5.09	1.61	1.53
1	K	226	GLN	CA-C	5.09	1.59	1.52
1	H	271	ASN	C-O	-5.09	1.18	1.24
1	K	211	PRO	C-O	-5.09	1.17	1.24
1	B	125	GLY	C-O	-5.06	1.18	1.24
1	C	81	ALA	CA-CB	-5.06	1.45	1.53
1	F	191	TRP	C-O	-5.03	1.17	1.24
1	J	281	ARG	CB-CG	-5.02	1.37	1.52
1	B	250	TYR	C-O	-5.00	1.18	1.24

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68	ASN	N-CA-C	19.12	132.20	111.36
1	J	71	VAL	N-CA-C	18.47	127.89	110.53
1	G	71	VAL	N-CA-C	12.82	126.12	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	68	ASN	N-CA-C	10.62	126.03	108.08
1	B	69	SER	N-CA-C	9.76	121.92	111.28
1	D	69	SER	N-CA-C	9.54	124.28	108.73
1	G	194	VAL	N-CA-C	9.46	120.27	110.62
1	L	196	GLU	N-CA-C	9.16	120.87	111.07
1	F	129	THR	CB-CA-C	-8.85	102.47	110.44
1	A	74	SER	N-CA-C	8.30	122.79	108.76
1	B	74	SER	N-CA-C	8.29	122.25	110.23
1	H	75	VAL	CB-CA-C	8.26	120.56	110.73
1	D	161	GLY	CA-C-N	8.06	127.73	119.19
1	D	161	GLY	C-N-CA	8.06	127.73	119.19
1	J	274	ARG	NE-CZ-NH2	-7.75	112.22	119.20
1	G	68	ASN	N-CA-C	7.42	121.11	107.99
1	L	68	ASN	CB-CA-C	-7.33	108.13	116.63
1	K	69	SER	CA-C-N	-7.13	111.19	123.25
1	K	69	SER	C-N-CA	-7.13	111.19	123.25
1	G	203	ARG	N-CA-C	6.92	118.82	111.28
1	J	69	SER	N-CA-C	6.81	119.72	111.82
1	L	87	TYR	CA-C-N	6.78	126.73	119.28
1	L	87	TYR	C-N-CA	6.78	126.73	119.28
1	D	139	TYR	CA-C-N	-6.47	112.16	119.28
1	D	139	TYR	C-N-CA	-6.47	112.16	119.28
1	A	216	TYR	N-CA-C	6.46	118.97	108.63
1	G	145	CYS	N-CA-C	6.40	118.26	111.28
1	B	129	THR	CB-CA-C	-6.37	103.83	110.33
1	K	171	HIS	N-CA-C	6.33	117.97	111.14
1	H	87	TYR	CA-C-N	6.30	126.21	119.28
1	H	87	TYR	C-N-CA	6.30	126.21	119.28
1	L	69	SER	N-CA-C	6.15	119.62	110.52
1	L	165	THR	N-CA-C	-6.13	104.89	112.38
1	D	68	ASN	CA-C-N	-6.07	114.69	122.77
1	D	68	ASN	C-N-CA	-6.07	114.69	122.77
1	F	92	HIS	CA-C-N	-5.98	112.37	119.84
1	F	92	HIS	C-N-CA	-5.98	112.37	119.84
1	F	161	GLY	CA-C-N	5.96	125.58	119.56
1	F	161	GLY	C-N-CA	5.96	125.58	119.56
1	H	268	LEU	N-CA-C	5.95	117.84	111.36
1	D	72	LEU	N-CA-C	-5.89	101.32	110.10
1	B	214	TYR	N-CA-C	5.76	119.93	113.01
1	G	72	LEU	CA-C-N	-5.76	110.12	121.41
1	G	72	LEU	C-N-CA	-5.76	110.12	121.41
1	L	67	ARG	N-CA-C	-5.75	105.84	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	96	SER	CB-CA-C	5.75	119.89	109.37
1	H	161	GLY	CA-C-N	5.74	125.28	119.19
1	H	161	GLY	C-N-CA	5.74	125.28	119.19
1	F	71	VAL	CB-CA-C	5.70	117.20	110.93
1	L	12	ALA	N-CA-C	5.67	118.69	109.06
1	A	100	ALA	N-CA-C	-5.65	103.95	111.24
1	K	69	SER	N-CA-C	-5.62	103.23	110.19
1	B	75	VAL	CB-CA-C	5.60	117.40	110.73
1	C	245	CYS	CA-C-N	5.59	125.52	119.76
1	C	245	CYS	C-N-CA	5.59	125.52	119.76
1	B	79	ASP	N-CA-C	5.57	117.43	111.36
1	G	69	SER	N-CA-C	5.55	116.70	108.60
1	D	206	ASN	N-CA-C	5.55	120.05	113.28
1	I	92	HIS	CA-C-N	-5.50	114.31	120.14
1	I	92	HIS	C-N-CA	-5.50	114.31	120.14
1	D	267	ILE	N-CA-C	-5.49	104.61	112.35
1	J	71	VAL	CB-CA-C	-5.49	104.83	112.02
1	I	249	GLU	N-CA-C	5.47	117.05	111.14
1	A	129	THR	CA-C-N	5.42	125.35	119.76
1	A	129	THR	C-N-CA	5.42	125.35	119.76
1	I	235	ARG	N-CA-C	5.42	119.68	112.30
1	H	231	PHE	N-CA-C	5.40	118.67	111.75
1	D	79	ASP	N-CA-C	5.38	117.23	111.36
1	L	95	GLY	CA-C-N	-5.37	114.22	122.87
1	L	95	GLY	C-N-CA	-5.37	114.22	122.87
1	B	161	GLY	CA-C-N	5.35	125.01	119.56
1	B	161	GLY	C-N-CA	5.35	125.01	119.56
1	J	71	VAL	N-CA-CB	-5.34	103.73	110.57
1	K	96	SER	CB-CA-C	5.23	118.27	109.48
1	H	13	MET	N-CA-CB	5.22	119.31	110.49
1	C	104	GLU	N-CA-C	-5.21	105.50	111.07
1	G	281	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	F	274	ARG	CG-CD-NE	-5.19	100.58	112.00
1	K	120	VAL	N-CA-C	5.16	116.73	108.89
1	D	174	ARG	N-CA-C	5.14	116.57	111.07
1	H	106	MET	CB-CG-SD	5.13	128.09	112.70
1	I	204	ARG	CA-C-N	5.11	124.73	119.56
1	I	204	ARG	C-N-CA	5.11	124.73	119.56
1	D	23	ARG	CA-C-N	-5.11	113.66	119.28
1	D	23	ARG	C-N-CA	-5.11	113.66	119.28
1	B	26	ILE	CB-CA-C	-5.10	105.44	111.97
1	B	23	ARG	CA-C-N	-5.10	114.36	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ARG	C-N-CA	-5.10	114.36	119.56
1	L	107	ALA	N-CA-C	-5.06	105.84	111.36
1	E	106	MET	CB-CG-SD	5.04	127.82	112.70
1	C	104	GLU	CA-CB-CG	5.04	124.17	114.10
1	C	187	SER	N-CA-C	-5.04	102.24	110.20
1	C	217	ASN	CA-C-N	-5.03	116.72	123.96
1	C	217	ASN	C-N-CA	-5.03	116.72	123.96
1	D	99	ALA	N-CA-C	5.02	116.87	108.99
1	G	275	LEU	CB-CG-CD1	-5.02	95.65	110.70
1	H	209	LEU	CA-C-N	-5.01	116.99	123.16
1	H	209	LEU	C-N-CA	-5.01	116.99	123.16
1	C	71	VAL	CB-CA-C	-5.00	105.64	111.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2215	0	2186	41	0
1	B	2236	0	2210	40	0
1	C	2220	0	2192	36	0
1	D	2220	0	2195	47	0
1	E	2231	0	2206	46	0
1	F	2230	0	2212	30	0
1	G	2223	0	2196	58	0
1	H	2226	0	2202	32	0
1	I	2224	0	2194	35	0
1	J	2220	0	2192	27	0
1	K	2223	0	2195	17	0
1	L	2215	0	2186	70	0
2	A	159	0	0	5	0
2	B	147	0	0	1	0
2	C	195	0	0	5	0
2	D	142	0	0	3	0
2	E	168	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	171	0	0	5	0
2	G	114	0	0	3	0
2	H	155	0	0	1	0
2	I	159	0	0	3	0
2	J	161	0	0	4	0
2	K	175	0	0	1	0
2	L	157	0	0	3	0
All	All	28586	0	26366	460	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 9.

All (460) 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:G:281:ARG:HG2	2:G:1454:HOH:O	1.47	1.15
1:L:68:ASN:O	1:L:74:SER:HB2	1.53	1.06
1:G:67:ARG:HH21	1:G:67:ARG:HG3	1.16	1.05
1:C:136:ARG:HD2	2:E:292:HOH:O	1.60	1.00
1:D:71:VAL:HG12	1:D:72:LEU:O	1.62	0.99
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.27	0.97
2:C:594:HOH:O	1:J:13:MET:HE2	1.68	0.92
1:G:23:ARG:HG3	1:G:23:ARG:HH11	1.34	0.89
1:D:68:ASN:HD22	1:D:69:SER:N	1.71	0.89
1:D:34:LEU:HD11	1:D:213:MET:HE3	1.54	0.88
1:H:118:ARG:HD2	1:H:281:ARG:NH1	1.88	0.87
1:L:13:MET:HE2	2:L:2003:HOH:O	1.74	0.87
1:D:68:ASN:C	1:D:68:ASN:ND2	2.29	0.84
1:I:269[A]:HIS:CE1	1:I:273:GLU:CD	2.55	0.84
1:G:72:LEU:N	1:G:72:LEU:CD1	2.39	0.84
1:I:269[A]:HIS:CE1	1:I:273:GLU:OE1	2.31	0.84
1:J:155:MET:HE3	1:J:160:ALA:HA	1.57	0.84
1:C:13:MET:HE3	1:C:83:VAL:HG22	1.59	0.84
1:G:67:ARG:HG3	1:G:67:ARG:NH2	1.93	0.84
1:D:68:ASN:HD22	1:D:68:ASN:C	1.85	0.83
1:L:232:LEU:HD23	1:L:236:MET:CE	2.08	0.83
1:A:281:ARG:HH11	1:A:281:ARG:CG	1.92	0.81
1:L:155:MET:HE3	1:L:160:ALA:HA	1.63	0.80
1:A:66:GLY:HA3	2:A:1552:HOH:O	1.80	0.80
1:L:68:ASN:CG	1:L:69:SER:HG	1.90	0.80
1:H:2:LYS:HG3	1:H:60:GLU:OE2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:SER:HB3	2:C:1121:HOH:O	1.81	0.79
1:J:281:ARG:NH1	2:J:533:HOH:O	2.14	0.79
1:D:118:ARG:HD2	1:D:281:ARG:NH2	1.98	0.78
1:F:79:ASP:OD2	1:J:274:ARG:HD3	1.84	0.78
1:J:71:VAL:HG23	1:J:72:LEU:N	1.98	0.78
1:E:67:ARG:CG	1:E:67:ARG:HH21	1.95	0.78
1:D:71:VAL:CG1	1:D:72:LEU:O	2.32	0.77
1:L:71:VAL:HG22	1:L:72:LEU:N	1.98	0.77
1:D:71:VAL:CG1	1:D:72:LEU:N	2.47	0.77
1:G:67:ARG:HH21	1:G:67:ARG:CG	1.90	0.77
1:C:118:ARG:HD2	1:C:281:ARG:NH1	2.00	0.77
1:D:70:SER:O	1:D:71:VAL:HG23	1.85	0.76
1:G:265:GLU:HG3	1:G:266:LYS:N	2.00	0.76
1:A:281:ARG:HG3	1:A:281:ARG:NH1	1.88	0.76
1:E:29:ARG:HD2	2:E:516:HOH:O	1.85	0.76
1:E:32:ARG:NH2	1:E:37:GLU:OE2	2.19	0.75
1:E:188:HIS:CE1	1:E:213:MET:HE2	2.22	0.74
1:L:71:VAL:HG22	1:L:72:LEU:CD1	2.16	0.74
1:C:13:MET:HE3	1:C:83:VAL:CG2	2.17	0.74
1:G:22:THR:O	1:G:23:ARG:HD2	1.88	0.73
1:L:68:ASN:CG	1:L:69:SER:OG	2.30	0.73
1:I:118:ARG:HD2	1:I:281:ARG:NH2	2.05	0.72
1:G:262:ASP:O	1:G:265:GLU:HG2	1.91	0.70
1:I:110:GLN:NE2	2:I:877:HOH:O	2.24	0.69
1:B:155:MET:HE3	1:B:160:ALA:HA	1.75	0.69
1:G:72:LEU:N	1:G:72:LEU:HD13	2.05	0.69
1:L:71:VAL:HG22	1:L:72:LEU:HD12	1.73	0.69
1:I:209:LEU:HD12	1:I:232:LEU:HD21	1.75	0.69
1:I:50:MET:HE1	1:I:91:PHE:HZ	1.59	0.68
1:I:269[A]:HIS:NE2	1:I:273:GLU:OE1	2.26	0.68
1:E:30:PHE:HD1	2:E:923:HOH:O	1.77	0.68
1:G:99:ALA:HB1	1:G:104:GLU:HB3	1.76	0.68
1:F:50:MET:HE1	1:F:91:PHE:HZ	1.58	0.68
1:G:67:ARG:NH2	1:G:67:ARG:CG	2.51	0.67
1:J:71:VAL:HG23	1:J:72:LEU:H	1.59	0.67
1:E:118:ARG:HD2	1:E:281:ARG:NH2	2.09	0.67
1:G:109:MET:HE2	1:G:113:LEU:HG	1.77	0.67
1:I:155:MET:HE3	1:I:160:ALA:HA	1.76	0.66
1:J:99:ALA:HB1	1:J:104:GLU:HB3	1.78	0.66
1:L:279:ALA:HA	2:L:1359:HOH:O	1.95	0.66
1:A:66:GLY:CA	2:A:1552:HOH:O	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:MET:HE3	1:E:113:LEU:HG	1.78	0.65
1:L:168:ASN:OD1	1:L:170:GLU:HG2	1.96	0.65
1:L:17:ASN:O	1:L:73:GLY:HA2	1.96	0.65
1:L:71:VAL:HG22	1:L:72:LEU:H	1.58	0.65
1:G:191:TRP:CZ3	1:I:199:HIS:HB2	2.30	0.65
1:E:67:ARG:HH21	1:E:67:ARG:HG3	1.60	0.65
1:L:68:ASN:OD1	1:L:69:SER:N	2.29	0.65
1:L:30:PHE:CE1	1:L:213:MET:HE3	2.31	0.65
1:G:72:LEU:N	1:G:72:LEU:HD12	2.09	0.64
1:D:71:VAL:HG13	1:D:72:LEU:N	2.12	0.64
1:E:99:ALA:HB1	1:E:104:GLU:HB3	1.79	0.64
1:A:101:THR:HB	2:A:1591:HOH:O	1.98	0.64
1:L:68:ASN:HB2	1:L:96:SER:OG	1.98	0.64
1:A:29:ARG:O	1:A:33:GLN:HB2	1.98	0.64
1:D:71:VAL:HG12	1:D:72:LEU:C	2.22	0.64
1:J:262:ASP:O	1:J:265:GLU:HG3	1.98	0.64
1:C:248:LYS:O	1:C:252:GLU:HG3	1.98	0.63
1:D:97:ILE:HD12	1:D:120:VAL:HG21	1.81	0.63
1:G:69:SER:OG	1:G:70:SER:N	2.30	0.63
1:L:7:ARG:NH2	1:L:67:ARG:NH2	2.47	0.63
1:B:12:ALA:HB2	1:B:47:LEU:HD22	1.80	0.63
1:B:34:LEU:HD21	1:B:213:MET:HB2	1.81	0.63
1:D:68:ASN:ND2	1:D:69:SER:N	2.42	0.63
1:J:118:ARG:HG3	1:J:281:ARG:HD2	1.81	0.63
1:L:68:ASN:O	1:L:74:SER:CB	2.39	0.62
1:A:202:PHE:HE2	1:B:30:PHE:CE1	2.17	0.62
1:I:207:LEU:O	1:I:235:ARG:HD2	1.98	0.62
1:A:23:ARG:HH21	1:A:26:ILE:HD11	1.64	0.62
1:L:7:ARG:HH21	1:L:67:ARG:NH2	1.97	0.62
1:F:60:GLU:HG2	2:F:1334:HOH:O	2.00	0.62
1:E:155:MET:HE3	1:E:160:ALA:HA	1.80	0.62
1:G:23:ARG:HG3	1:G:23:ARG:NH1	2.10	0.62
1:D:248:LYS:O	1:D:252:GLU:HG3	2.00	0.62
1:L:71:VAL:CG2	1:L:72:LEU:N	2.63	0.61
1:C:209:LEU:HD12	1:C:232:LEU:HD21	1.82	0.61
1:B:109:MET:HE2	1:B:113:LEU:HG	1.83	0.61
1:L:232:LEU:HD23	1:L:236:MET:HE2	1.82	0.61
1:B:110:GLN:HA	1:B:110:GLN:NE2	2.16	0.61
1:D:22:THR:O	1:D:24:PRO:HD3	2.01	0.60
1:F:269:HIS:O	1:F:273:GLU:HG2	2.01	0.60
1:I:213:MET:HE2	1:I:214:TYR:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:ASN:OD1	1:L:68:ASN:C	2.41	0.60
1:A:75:VAL:HG13	1:A:75:VAL:O	2.02	0.60
1:E:67:ARG:CG	1:E:67:ARG:NH2	2.57	0.60
1:C:85:LYS:NZ	2:C:979:HOH:O	2.35	0.60
1:E:96:SER:HB3	1:E:121:ASN:HB3	1.83	0.60
1:B:41[B]:SER:HB2	1:B:49:LEU:HB3	1.83	0.60
1:G:265:GLU:HG3	1:G:266:LYS:H	1.66	0.60
1:L:280:GLY:O	1:L:281:ARG:HB2	2.01	0.59
1:D:234:ASP:O	1:D:274:ARG:NH2	2.36	0.59
1:H:155:MET:HE3	1:H:160:ALA:HA	1.84	0.59
1:L:9:ARG:N	1:L:9:ARG:HD3	2.17	0.59
1:G:155:MET:HE3	1:G:160:ALA:HA	1.83	0.59
1:L:71:VAL:CG2	1:L:72:LEU:HD12	2.33	0.59
1:H:118:ARG:HD2	1:H:281:ARG:HH11	1.65	0.59
1:E:109:MET:CE	1:E:113:LEU:HG	2.33	0.58
1:A:209:LEU:HD12	1:A:232:LEU:HD21	1.86	0.58
1:C:13:MET:HE2	2:C:1872:HOH:O	2.04	0.58
1:L:67:ARG:H	1:L:75:VAL:HG12	1.67	0.58
1:L:71:VAL:CG2	1:L:72:LEU:H	2.17	0.58
1:B:8:LEU:C	1:B:8:LEU:HD23	2.28	0.58
1:K:84:ALA:O	1:K:88:PRO:HA	2.04	0.57
1:C:231:PHE:CE1	1:C:232:LEU:HD13	2.40	0.57
1:L:68:ASN:CG	1:L:69:SER:N	2.55	0.57
1:A:67:ARG:NH1	1:A:72:LEU:CD1	2.68	0.57
1:L:71:VAL:HG22	1:L:72:LEU:HD13	1.86	0.57
1:B:122:LEU:HD11	1:B:141:LEU:HD23	1.87	0.56
1:E:67:ARG:NH2	1:E:67:ARG:HG2	2.21	0.56
1:F:79:ASP:OD2	1:J:274:ARG:CD	2.52	0.56
1:B:199:HIS:HB2	1:C:191:TRP:CH2	2.40	0.56
1:C:156:THR:O	1:C:190:ASN:HA	2.05	0.56
1:G:262:ASP:O	1:G:265:GLU:CG	2.53	0.56
1:G:72:LEU:CD1	1:G:72:LEU:H	2.19	0.56
1:A:33:GLN:HG2	1:C:231:PHE:HB2	1.88	0.56
1:K:71:VAL:CG1	1:K:72:LEU:N	2.69	0.56
1:J:118:ARG:HD3	1:J:281:ARG:HB3	1.88	0.56
1:A:67:ARG:NH1	1:A:72:LEU:HD12	2.21	0.55
1:H:218:LEU:HB3	1:H:219:PRO:HD2	1.87	0.55
1:L:154:MET:HE3	1:L:184:VAL:CG1	2.35	0.55
1:B:69:SER:O	1:B:70:SER:HB3	2.06	0.55
1:J:71:VAL:CG2	1:J:72:LEU:N	2.69	0.55
1:A:67:ARG:HH11	1:A:72:LEU:CD1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ARG:HE	1:G:126:VAL:CG2	2.19	0.55
1:G:134:ASP:OD2	1:G:174:ARG:HD2	2.07	0.55
1:A:104:GLU:HG2	2:A:1077:HOH:O	2.05	0.55
1:A:262:ASP:O	1:A:265:GLU:HG3	2.07	0.55
1:A:14:GLY:HA3	1:A:75:VAL:HG23	1.87	0.55
1:C:123:GLU:HB3	1:C:155:MET:HE2	1.89	0.55
1:B:64[A]:CYS:SG	1:B:91:PHE:HB3	2.47	0.55
1:E:46:SER:OG	1:E:49:LEU:HB2	2.07	0.55
1:G:218:LEU:HB3	1:G:219:PRO:HD2	1.89	0.54
1:L:122:LEU:HD21	1:L:141:LEU:HD21	1.89	0.54
1:L:236:MET:HB3	1:L:267:ILE:HG12	1.89	0.54
1:L:109:MET:CE	1:L:113:LEU:HD21	2.37	0.54
1:C:182:LEU:O	1:C:206[B]:ASN:HB2	2.07	0.54
1:I:236:MET:HB3	1:I:267:ILE:HG12	1.90	0.54
1:B:69:SER:OG	1:B:74:SER:HB3	2.08	0.54
1:H:99:ALA:HB1	1:H:104:GLU:HB3	1.90	0.54
1:G:72:LEU:HD12	1:G:72:LEU:H	1.73	0.54
1:G:191:TRP:CH2	1:I:199:HIS:HB2	2.42	0.54
1:B:72:LEU:HD12	1:B:72:LEU:H	1.73	0.54
1:C:162:PRO:HD2	1:C:166:TYR:CE2	2.43	0.54
1:L:154:MET:HE3	1:L:184:VAL:HG13	1.90	0.54
1:K:232:LEU:HD12	1:K:235:ARG:HB2	1.90	0.54
1:E:212:ASP:OD1	1:E:213:MET:HG2	2.09	0.53
1:F:83:VAL:HG23	2:F:1980:HOH:O	2.08	0.53
1:K:109:MET:HE3	1:K:113:LEU:HG	1.89	0.53
1:L:232:LEU:CD2	1:L:236:MET:HE2	2.39	0.53
1:F:92:HIS:ND1	2:F:1689:HOH:O	2.33	0.53
1:H:230[A]:SER:OG	1:H:231:PHE:N	2.41	0.53
1:L:241:ALA:O	1:L:242:TYR:C	2.51	0.53
1:C:99:ALA:HB1	1:C:104:GLU:HB3	1.90	0.53
1:F:252:GLU:O	1:F:256:THR:HG23	2.07	0.53
1:L:232:LEU:HD23	1:L:236:MET:HE3	1.86	0.53
1:B:213:MET:HE3	1:B:214:TYR:CZ	2.43	0.53
1:H:109:MET:HE3	1:H:113:LEU:HG	1.90	0.53
1:J:281:ARG:NE	2:J:1900:HOH:O	2.41	0.53
1:G:17:ASN:O	1:G:73:GLY:HA2	2.09	0.53
1:L:12:ALA:HB2	1:L:47:LEU:HD22	1.91	0.53
1:I:191:TRP:CG	1:I:192:PRO:HA	2.44	0.53
1:J:17:ASN:O	1:J:73:GLY:HA2	2.09	0.53
1:B:44:GLU:OE1	1:B:49:LEU:HD12	2.08	0.53
1:D:71:VAL:HG12	1:D:72:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:VAL:CG1	1:L:121:ASN:HB2	2.39	0.53
1:J:281:ARG:HG3	2:J:1900:HOH:O	2.08	0.52
1:H:69:SER:OG	1:H:74:SER:HB3	2.09	0.52
1:E:41[B]:SER:OG	1:E:50:MET:N	2.42	0.52
1:D:3:ILE:HB	1:D:59:ILE:HA	1.90	0.52
1:L:7:ARG:HH21	1:L:67:ARG:HH22	1.56	0.52
1:K:88:PRO:HD2	1:K:89:ASP:OD1	2.10	0.52
1:L:183:THR:HG21	1:L:275:LEU:CD2	2.40	0.52
1:F:70:SER:O	1:J:281:ARG:HA	2.10	0.52
1:F:102:ARG:HG3	1:F:103:LYS:N	2.24	0.52
1:I:262:ASP:HB2	2:I:1014:HOH:O	2.10	0.51
1:E:41[B]:SER:HB2	1:E:53:GLU:CD	2.34	0.51
1:L:248:LYS:O	1:L:252:GLU:HG3	2.10	0.51
1:G:2:LYS:NZ	2:G:844:HOH:O	2.43	0.51
1:L:30:PHE:CZ	1:L:213:MET:CE	2.94	0.51
1:E:120:VAL:CG2	1:E:121:ASN:N	2.74	0.51
1:G:169:PRO:HD3	1:G:193:TRP:CG	2.46	0.51
1:H:231:PHE:CE1	1:H:232:LEU:HD13	2.45	0.51
1:L:221:HIS:O	1:L:225:ILE:HG12	2.11	0.51
1:C:18:ALA:HA	1:C:73:GLY:HA3	1.93	0.51
1:F:118:ARG:HD2	1:F:281:ARG:NH1	2.25	0.51
1:F:168:ASN:OD1	1:F:170:GLU:HG2	2.10	0.51
1:G:281:ARG:CG	2:G:1454:HOH:O	2.24	0.51
1:D:92:HIS:ND1	2:D:759:HOH:O	2.33	0.50
1:H:182:LEU:O	1:H:206[A]:ASN:HB2	2.10	0.50
1:C:118:ARG:CD	1:C:281:ARG:NH1	2.74	0.50
1:I:50:MET:HE1	1:I:91:PHE:CZ	2.43	0.50
1:C:234:ASP:O	1:C:274:ARG:NH2	2.45	0.50
1:B:199:HIS:HB2	1:C:191:TRP:CZ3	2.47	0.50
1:F:209:LEU:HD12	1:F:232:LEU:HD21	1.93	0.50
1:H:57:ALA:O	1:J:261:PRO:HG2	2.11	0.50
1:A:261:PRO:O	1:A:265:GLU:HG2	2.12	0.50
1:L:19:ARG:CG	1:L:19:ARG:HH21	2.25	0.50
1:J:182:LEU:O	1:J:206[A]:ASN:HB2	2.12	0.50
1:C:118:ARG:HD2	1:C:281:ARG:HH11	1.75	0.50
1:K:50:MET:HE1	1:K:91:PHE:HZ	1.76	0.49
1:C:236:MET:HB3	1:C:267:ILE:HG12	1.94	0.49
1:E:69:SER:HB2	1:E:71:VAL:HG12	1.94	0.49
1:G:22:THR:C	1:G:23:ARG:HD2	2.36	0.49
1:D:102:ARG:O	1:D:106[A]:MET:HG2	2.12	0.49
1:K:269:HIS:O	1:K:273:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ALA:HB2	1:E:75:VAL:CG2	2.42	0.49
1:G:202:PHE:CE1	1:H:33:GLN:HG2	2.48	0.49
1:H:48:GLU:CD	1:H:48:GLU:H	2.21	0.49
1:G:241:ALA:O	1:G:242:TYR:C	2.54	0.49
1:G:150:ILE:HA	1:G:281:ARG:NH1	2.28	0.49
1:I:213:MET:HE2	1:I:214:TYR:CE2	2.46	0.49
1:H:269:HIS:HE1	2:H:1348:HOH:O	1.95	0.49
1:A:71:VAL:HG12	1:A:72:LEU:HD23	1.95	0.48
1:I:174:ARG:HA	2:I:1603:HOH:O	2.11	0.48
1:H:13:MET:HE2	1:H:83:VAL:HA	1.96	0.48
1:F:40:PRO:O	1:F:44:GLU:HG3	2.14	0.48
1:G:34:LEU:HD11	1:G:213:MET:HE3	1.96	0.48
1:G:218:LEU:HB3	1:G:219:PRO:CD	2.43	0.48
1:E:67:ARG:HH21	1:E:67:ARG:HG2	1.78	0.48
1:B:79:ASP:OD2	2:B:1051:HOH:O	2.20	0.48
1:E:194:VAL:HG21	1:E:220:GLY:HA3	1.95	0.48
1:E:234:ASP:O	1:E:274:ARG:NH2	2.46	0.48
1:E:49:LEU:O	1:E:53:GLU:HG3	2.14	0.48
1:A:139:TYR:CZ	1:D:136:ARG:HD3	2.49	0.48
1:I:75:VAL:HG13	1:I:75:VAL:O	2.14	0.48
1:F:134:ASP:OD2	1:F:174:ARG:HD2	2.14	0.48
1:G:67:ARG:HE	1:G:126:VAL:HG23	1.77	0.48
1:I:212:ASP:OD1	1:I:213:MET:HG2	2.14	0.48
1:A:219:PRO:HD3	2:C:587:HOH:O	2.15	0.47
1:L:109:MET:HE3	1:L:113:LEU:CD2	2.44	0.47
1:B:234:ASP:O	1:B:274:ARG:NH2	2.48	0.47
1:L:122:LEU:HD21	1:L:141:LEU:CD2	2.44	0.47
1:F:187:SER:O	1:F:188:HIS:HB2	2.15	0.47
1:B:251:THR:O	1:B:255:LEU:HG	2.15	0.47
1:J:22:THR:C	1:J:24:PRO:HD3	2.39	0.47
1:L:125:GLY:HA3	1:L:160:ALA:O	2.15	0.47
1:B:95:GLY:O	1:B:121:ASN:N	2.43	0.47
1:E:41[B]:SER:HB3	1:E:242:TYR:HH	1.78	0.47
1:E:97:ILE:HD12	1:E:120:VAL:HG21	1.96	0.47
1:E:201:ALA:HB1	1:E:232:LEU:HD11	1.97	0.47
1:H:70:SER:O	1:H:70:SER:OG	2.30	0.47
1:H:108:GLN:O	1:H:112:ILE:HG13	2.14	0.47
1:H:167:THR:O	1:H:190:ASN:ND2	2.44	0.47
1:F:19:ARG:HA	1:F:22:THR:OG1	2.15	0.47
1:F:102:ARG:O	1:F:106[B]:MET:HG2	2.15	0.47
1:K:71:VAL:HG12	1:K:72:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:MET:HE3	1:F:160:ALA:HA	1.96	0.47
1:G:109:MET:HE3	1:G:112:ILE:HB	1.97	0.47
1:H:12:ALA:HB2	1:H:47:LEU:HD13	1.97	0.47
1:F:207:LEU:O	1:F:235:ARG:HD2	2.15	0.47
1:D:119:ILE:HG12	1:D:151:PRO:HG2	1.97	0.46
1:H:236:MET:HE3	1:H:236:MET:HB2	1.63	0.46
1:J:32:ARG:HD2	2:J:1316:HOH:O	2.15	0.46
1:L:94:VAL:HG11	1:L:121:ASN:HB2	1.96	0.46
1:I:127:TRP:CZ3	1:I:131:MET:HE3	2.51	0.46
1:A:206:ASN:HB3	2:A:1722:HOH:O	2.15	0.46
1:L:120:VAL:CG1	1:L:152:VAL:HG22	2.45	0.46
1:D:169:PRO:HD3	1:D:193:TRP:CG	2.51	0.46
1:H:67:ARG:O	1:H:74:SER:HB2	2.16	0.46
1:K:259:ILE:HB	1:K:264:MET:HE2	1.98	0.46
1:L:100:ALA:N	1:L:104:GLU:OE1	2.43	0.46
1:J:116:GLY:O	1:J:281:ARG:HD3	2.15	0.46
1:E:182:LEU:O	1:E:206[A]:ASN:HB2	2.15	0.46
1:B:30:PHE:CD2	1:B:244:MET:HE3	2.50	0.46
1:C:48:GLU:OE2	1:C:48:GLU:HA	2.16	0.46
1:C:73:GLY:HA2	1:J:85:LYS:HD2	1.97	0.46
1:H:41[B]:SER:HB2	1:H:49:LEU:HB3	1.98	0.46
1:L:109:MET:HE3	1:L:113:LEU:HG	1.97	0.46
1:A:99:ALA:HB1	1:A:104:GLU:HB3	1.98	0.46
1:B:194:VAL:O	1:B:198:ILE:HG12	2.16	0.45
1:D:33:GLN:HG2	1:F:231:PHE:HB2	1.98	0.45
1:D:241:ALA:O	1:D:242:TYR:C	2.59	0.45
1:G:12:ALA:HB2	1:G:47:LEU:HD13	1.96	0.45
1:G:15:PHE:HA	1:G:75:VAL:HG11	1.97	0.45
1:C:40:PRO:O	1:C:44:GLU:HG2	2.17	0.45
1:C:124:PRO:HA	1:C:127:TRP:CD2	2.51	0.45
1:E:240:THR:HG22	1:E:250:TYR:CD2	2.51	0.45
1:L:109:MET:HE3	1:L:113:LEU:HD21	1.99	0.45
1:D:70:SER:O	1:D:71:VAL:CG2	2.59	0.45
1:F:273:GLU:HG2	1:F:273:GLU:H	1.63	0.45
1:G:23:ARG:HB3	1:G:26:ILE:HD12	1.97	0.45
1:A:67:ARG:NH1	1:A:72:LEU:HD13	2.32	0.45
1:D:12:ALA:HB2	1:D:47:LEU:HD13	1.98	0.45
1:D:137:ARG:NH2	2:D:1062:HOH:O	2.38	0.45
1:C:34:LEU:HD11	1:C:213:MET:HB2	1.99	0.45
1:D:99:ALA:HB1	1:D:104:GLU:HB3	1.98	0.45
1:E:21:TYR:CZ	1:E:243:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ASP:OD1	1:E:213:MET:N	2.45	0.45
1:G:96:SER:HB3	1:G:121:ASN:HB3	1.99	0.45
1:E:230[A]:SER:OG	1:E:231:PHE:N	2.49	0.45
1:F:39:ALA:HB2	1:F:246:PRO:HA	1.98	0.45
1:C:139:TYR:CZ	1:E:136:ARG:HD3	2.52	0.45
1:E:212:ASP:HA	1:E:239:GLY:O	2.17	0.45
1:A:69:SER:HA	1:A:98:GLU:OE1	2.17	0.44
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.79	0.44
1:H:3:ILE:HB	1:H:59:ILE:HA	1.98	0.44
1:I:21:TYR:CZ	1:I:243:PRO:HG3	2.52	0.44
1:I:67:ARG:H	1:I:75:VAL:CG1	2.31	0.44
1:G:124:PRO:HA	1:G:127:TRP:CE2	2.53	0.44
1:I:232:LEU:HD23	1:I:236:MET:CE	2.48	0.44
1:D:67:ARG:NH2	1:D:155:MET:HE1	2.32	0.44
1:E:12:ALA:HB2	1:E:47:LEU:HD13	1.98	0.44
1:E:260:LYS:NZ	2:E:1373:HOH:O	2.33	0.44
1:L:106:MET:HG3	2:L:1925:HOH:O	2.17	0.44
1:G:123:GLU:HG2	1:G:155:MET:HB2	2.00	0.44
1:A:67:ARG:H	1:A:75:VAL:HG12	1.82	0.44
1:A:248:LYS:O	1:A:252:GLU:HG3	2.17	0.44
1:G:50:MET:HG3	1:G:242:TYR:CZ	2.52	0.44
1:J:71:VAL:CG2	1:J:72:LEU:H	2.28	0.44
1:B:194:VAL:HG21	1:B:220:GLY:HA3	1.99	0.44
1:K:268:LEU:HD23	1:K:268:LEU:HA	1.71	0.44
1:B:190:ASN:CB	1:B:197:ILE:HD13	2.48	0.44
1:C:155:MET:HE3	1:C:160:ALA:HA	1.99	0.44
1:I:120:VAL:HG12	1:I:152:VAL:HG22	2.00	0.44
1:D:22:THR:C	1:D:24:PRO:HD3	2.43	0.44
1:G:17:ASN:O	1:G:73:GLY:CA	2.66	0.44
1:G:164:ILE:HG22	1:I:170:GLU:HA	2.00	0.44
1:H:241:ALA:O	1:H:242:TYR:C	2.61	0.44
1:I:182:LEU:O	1:I:206[B]:ASN:HB2	2.18	0.44
1:J:209:LEU:HD12	1:J:232:LEU:HD21	2.00	0.44
1:A:67:ARG:HH11	1:A:72:LEU:HD12	1.81	0.43
1:C:8:LEU:HD21	1:C:50:MET:SD	2.58	0.43
1:K:125:GLY:HA3	1:K:160:ALA:O	2.17	0.43
1:B:194:VAL:HA	1:B:197:ILE:HG22	2.01	0.43
1:E:162:PRO:HD2	1:E:166:TYR:CE2	2.52	0.43
1:L:112:ILE:HG23	1:L:117:ILE:HB	2.00	0.43
1:F:55:ALA:O	2:F:593:HOH:O	2.21	0.43
1:H:201:ALA:HB1	1:H:232:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ASN:O	1:H:73:GLY:HA2	2.19	0.43
1:C:2:LYS:NZ	1:C:273:GLU:OE2	2.42	0.43
1:E:236:MET:HE2	1:E:236:MET:HB2	1.86	0.43
1:A:23:ARG:HE	1:A:26:ILE:HG13	1.83	0.43
1:D:155:MET:HE3	1:D:160:ALA:HA	1.99	0.43
1:E:98:GLU:HG3	1:E:127:TRP:CD1	2.53	0.43
1:E:41[B]:SER:OG	1:E:50:MET:HB2	2.19	0.43
1:E:202:PHE:HE2	1:F:30:PHE:CE1	2.36	0.43
1:K:206:ASN:HB2	2:K:1565:HOH:O	2.19	0.43
1:D:109:MET:CE	1:D:113:LEU:HD21	2.49	0.43
1:J:234:ASP:O	1:J:274:ARG:NH2	2.52	0.43
1:A:75:VAL:O	1:A:75:VAL:CG1	2.66	0.43
1:B:182:LEU:O	1:B:206[A]:ASN:HB2	2.19	0.43
1:E:120:VAL:HG22	1:E:121:ASN:N	2.34	0.43
1:I:8:LEU:O	1:I:64:CYS:HA	2.19	0.43
1:I:127:TRP:O	1:I:128:ALA:C	2.59	0.43
1:K:188:HIS:CE1	1:K:213:MET:CE	3.02	0.43
1:D:182:LEU:O	1:D:206:ASN:HB2	2.19	0.42
1:G:40:PRO:HD2	1:G:53:GLU:OE2	2.18	0.42
1:L:260:LYS:HA	1:L:261:PRO:HD3	1.96	0.42
1:B:169:PRO:HD3	1:B:193:TRP:CG	2.54	0.42
1:C:8:LEU:C	1:C:9:ARG:HD3	2.44	0.42
1:G:212:ASP:HA	1:G:239:GLY:O	2.19	0.42
1:I:2:LYS:HD3	1:I:269[A]:HIS:CE1	2.54	0.42
1:K:250:TYR:C	1:K:250:TYR:CD2	2.97	0.42
1:L:5:ASP:OD1	1:L:239:GLY:HA2	2.19	0.42
1:L:69:SER:HA	1:L:70:SER:HA	1.87	0.42
1:B:109:MET:HE2	1:B:113:LEU:CG	2.48	0.42
1:C:252:GLU:O	1:C:256:THR:HG23	2.20	0.42
1:D:125:GLY:HA3	1:D:160:ALA:O	2.18	0.42
1:F:12:ALA:O	1:F:13:MET:C	2.62	0.42
1:D:5:ASP:OD2	1:D:240:THR:HG23	2.20	0.42
1:L:30:PHE:CZ	1:L:213:MET:HE3	2.54	0.42
1:L:30:PHE:CD1	1:L:30:PHE:C	2.98	0.42
1:A:95:GLY:O	1:A:120:VAL:HA	2.20	0.42
1:B:12:ALA:CB	1:B:47:LEU:HD22	2.48	0.42
1:L:124:PRO:HA	1:L:127:TRP:CE2	2.54	0.42
1:G:21:TYR:O	1:G:45:LYS:CE	2.67	0.42
1:H:194:VAL:HA	1:H:197:ILE:HG22	2.01	0.42
1:D:50:MET:HG3	1:D:242:TYR:CZ	2.54	0.42
1:G:21:TYR:O	1:G:45:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:MET:HE3	1:H:54:MET:SD	2.60	0.42
1:B:49:LEU:O	1:B:53:GLU:HG3	2.19	0.42
1:B:110:GLN:NE2	1:B:110:GLN:CA	2.83	0.42
1:B:244:MET:HE3	1:B:244:MET:HB3	1.95	0.42
1:A:20:ILE:O	1:A:27:ARG:HD3	2.19	0.42
1:D:240:THR:HG21	1:D:247:LEU:HD23	2.02	0.42
1:I:112:ILE:HG23	1:I:117:ILE:HB	2.00	0.42
1:L:196:GLU:H	1:L:196:GLU:CD	2.28	0.42
1:D:122:LEU:HD11	1:D:141:LEU:HD23	2.02	0.42
1:B:96[A]:SER:HA	1:B:121:ASN:O	2.20	0.41
1:D:232:LEU:HD12	1:D:232:LEU:HA	1.87	0.41
1:F:34:LEU:HD23	1:F:34:LEU:HA	1.88	0.41
1:D:162:PRO:HD2	1:D:166:TYR:CD2	2.55	0.41
1:C:98:GLU:HG3	1:C:127:TRP:CD1	2.55	0.41
1:E:241:ALA:O	1:E:242:TYR:C	2.62	0.41
1:B:72:LEU:HD12	1:B:72:LEU:N	2.35	0.41
1:H:194:VAL:O	1:H:198:ILE:HG12	2.21	0.41
1:L:251:THR:O	1:L:255:LEU:HG	2.20	0.41
1:A:23:ARG:NH2	1:A:26:ILE:HD11	2.33	0.41
1:E:32:ARG:HH21	1:E:37:GLU:CD	2.25	0.41
1:G:118:ARG:HB3	1:G:279:ALA:HB1	2.03	0.41
1:I:98:GLU:HG3	1:I:127:TRP:CG	2.56	0.41
1:K:240:THR:O	1:K:245:CYS:HB2	2.21	0.41
1:A:154:MET:HE2	1:A:154:MET:HB3	1.93	0.41
1:L:68:ASN:OD1	1:L:69:SER:OG	2.30	0.41
1:A:234:ASP:O	1:A:274:ARG:NH2	2.54	0.41
1:C:13:MET:HE3	1:C:83:VAL:HG23	2.00	0.41
1:F:27:ARG:NH2	1:F:43:GLU:OE1	2.54	0.41
1:G:13:MET:HB3	1:G:14:GLY:H	1.60	0.41
1:A:50:MET:HE2	1:A:50:MET:HB3	1.83	0.41
1:B:109:MET:HE2	1:B:113:LEU:CD2	2.50	0.41
1:B:218:LEU:HB3	1:B:219:PRO:HD2	2.02	0.41
1:D:59:ILE:CD1	1:D:247:LEU:HD22	2.50	0.41
1:D:219:PRO:HD3	2:F:541:HOH:O	2.20	0.41
1:H:118:ARG:CD	1:H:281:ARG:NH1	2.73	0.41
1:H:220:GLY:O	1:H:221:HIS:C	2.62	0.41
1:I:22:THR:C	1:I:24:PRO:HD3	2.46	0.41
1:K:170:GLU:O	1:K:174:ARG:HG3	2.21	0.41
1:L:120:VAL:HG12	1:L:152:VAL:HG22	2.03	0.41
1:L:185:VAL:HG13	1:L:237:LEU:HD12	2.03	0.41
1:L:191:TRP:CG	1:L:192:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:240:THR:HG22	1:L:250:TYR:CD2	2.56	0.41
1:A:41:SER:HB3	1:A:49:LEU:HB3	2.03	0.41
1:B:156:THR:O	1:B:190:ASN:HA	2.21	0.41
1:B:231:PHE:CE1	1:B:232:LEU:HD13	2.55	0.41
1:G:19:ARG:HA	1:G:22:THR:OG1	2.21	0.41
1:A:199:HIS:HB3	1:B:192:PRO:HG3	2.03	0.40
1:D:194:VAL:HG21	1:D:220:GLY:HA3	2.03	0.40
1:G:229:ASN:O	1:G:260:LYS:HE2	2.21	0.40
1:J:12:ALA:HB2	1:J:47:LEU:HD22	2.02	0.40
1:L:67:ARG:H	1:L:75:VAL:CG1	2.34	0.40
1:D:156:THR:O	1:D:190:ASN:HA	2.21	0.40
1:F:118:ARG:O	1:F:281:ARG:NH2	2.49	0.40
1:F:131:MET:HE2	1:F:131:MET:HB3	1.91	0.40
1:G:118:ARG:HD2	1:G:281:ARG:NH2	2.37	0.40
1:J:5:ASP:OD1	1:J:239:GLY:HA2	2.21	0.40
1:A:2:LYS:NZ	1:A:273:GLU:OE2	2.43	0.40
1:D:235:ARG:NH1	2:D:766:HOH:O	2.54	0.40
1:G:164:ILE:N	1:I:173:ASP:OD2	2.54	0.40
1:I:229:ASN:O	1:I:260:LYS:NZ	2.54	0.40
1:D:44:GLU:HB2	1:D:46:SER:HB3	2.03	0.40
1:G:112:ILE:HG23	1:G:117:ILE:HB	2.04	0.40
1:L:152:VAL:O	1:L:184:VAL:HA	2.22	0.40
1:A:67:ARG:HH11	1:A:72:LEU:HD13	1.86	0.40
1:K:232:LEU:HD12	1:K:232:LEU:HA	1.73	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	280/291 (96%)	270 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	285/291 (98%)	278 (98%)	7 (2%)	0	100	100
1	C	281/291 (97%)	274 (98%)	7 (2%)	0	100	100
1	D	281/291 (97%)	270 (96%)	10 (4%)	1 (0%)	30	19
1	E	284/291 (98%)	274 (96%)	10 (4%)	0	100	100
1	F	282/291 (97%)	275 (98%)	7 (2%)	0	100	100
1	G	281/291 (97%)	270 (96%)	11 (4%)	0	100	100
1	H	283/291 (97%)	278 (98%)	5 (2%)	0	100	100
1	I	281/291 (97%)	272 (97%)	9 (3%)	0	100	100
1	J	281/291 (97%)	274 (98%)	6 (2%)	1 (0%)	30	19
1	K	282/291 (97%)	273 (97%)	9 (3%)	0	100	100
1	L	280/291 (96%)	272 (97%)	8 (3%)	0	100	100
All	All	3381/3492 (97%)	3280 (97%)	99 (3%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ARG
1	J	269	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/242 (97%)	222 (95%)	12 (5%)	21	8
1	B	239/242 (99%)	224 (94%)	15 (6%)	16	4
1	C	235/242 (97%)	226 (96%)	9 (4%)	29	14
1	D	235/242 (97%)	221 (94%)	14 (6%)	17	5
1	E	238/242 (98%)	230 (97%)	8 (3%)	32	16
1	F	236/242 (98%)	223 (94%)	13 (6%)	19	6
1	G	235/242 (97%)	220 (94%)	15 (6%)	16	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	237/242 (98%)	222 (94%)	15 (6%)	16	4
1	I	235/242 (97%)	221 (94%)	14 (6%)	17	5
1	J	235/242 (97%)	219 (93%)	16 (7%)	14	4
1	K	236/242 (98%)	224 (95%)	12 (5%)	21	8
1	L	234/242 (97%)	225 (96%)	9 (4%)	29	14
All	All	2829/2904 (97%)	2677 (95%)	152 (5%)	20	7

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	13	MET
1	A	33	GLN
1	A	44	GLU
1	A	49	LEU
1	A	50	MET
1	A	70	SER
1	A	85	LYS
1	A	190	ASN
1	A	265	GLU
1	A	275	LEU
1	A	281	ARG
1	B	1	LEU
1	B	19	ARG
1	B	20	ILE
1	B	33	GLN
1	B	34	LEU
1	B	48	GLU
1	B	49	LEU
1	B	54	MET
1	B	70	SER
1	B	72	LEU
1	B	75	VAL
1	B	190	ASN
1	B	219	PRO
1	B	252	GLU
1	B	275	LEU
1	C	8	LEU
1	C	34	LEU
1	C	49	LEU

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Mol	Chain	Res	Type
1	C	50	MET
1	C	60	GLU
1	C	71	VAL
1	C	111	GLU
1	C	190	ASN
1	C	281	ARG
1	D	1	LEU
1	D	33	GLN
1	D	46	SER
1	D	54	MET
1	D	67	ARG
1	D	68	ASN
1	D	69	SER
1	D	71	VAL
1	D	72	LEU
1	D	85	LYS
1	D	190	ASN
1	D	265	GLU
1	D	275	LEU
1	D	281	ARG
1	E	34	LEU
1	E	67	ARG
1	E	97	ILE
1	E	111	GLU
1	E	190	ASN
1	E	236	MET
1	E	275	LEU
1	E	281	ARG
1	F	1	LEU
1	F	2	LYS
1	F	49	LEU
1	F	60	GLU
1	F	71	VAL
1	F	85	LYS
1	F	89	ASP
1	F	129	THR
1	F	190	ASN
1	F	225	ILE
1	F	273	GLU
1	F	275	LEU
1	F	281	ARG
1	G	1	LEU

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Mol	Chain	Res	Type
1	G	13	MET
1	G	23	ARG
1	G	46	SER
1	G	49	LEU
1	G	54	MET
1	G	67	ARG
1	G	72	LEU
1	G	74	SER
1	G	75	VAL
1	G	85	LYS
1	G	90	LYS
1	G	190	ASN
1	G	275	LEU
1	G	281	ARG
1	H	2	LYS
1	H	13	MET
1	H	44	GLU
1	H	54	MET
1	H	61	GLN
1	H	67	ARG
1	H	70	SER
1	H	75	VAL
1	H	85	LYS
1	H	90	LYS
1	H	103	LYS
1	H	164	ILE
1	H	190	ASN
1	H	232	LEU
1	H	281	ARG
1	I	49	LEU
1	I	60	GLU
1	I	71	VAL
1	I	85	LYS
1	I	90	LYS
1	I	103	LYS
1	I	120	VAL
1	I	164	ILE
1	I	190	ASN
1	I	236	MET
1	I	269[A]	HIS
1	I	269[B]	HIS
1	I	275	LEU

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Mol	Chain	Res	Type
1	I	281	ARG
1	J	2	LYS
1	J	29	ARG
1	J	48	GLU
1	J	50	MET
1	J	54	MET
1	J	60	GLU
1	J	67	ARG
1	J	72	LEU
1	J	103	LYS
1	J	114	ASP
1	J	120	VAL
1	J	129	THR
1	J	190	ASN
1	J	192	PRO
1	J	275	LEU
1	J	281	ARG
1	K	29	ARG
1	K	34	LEU
1	K	67	ARG
1	K	70	SER
1	K	75	VAL
1	K	111	GLU
1	K	120	VAL
1	K	164	ILE
1	K	190	ASN
1	K	225	ILE
1	K	232	LEU
1	K	274	ARG
1	L	19	ARG
1	L	49	LEU
1	L	60	GLU
1	L	67	ARG
1	L	69	SER
1	L	70	SER
1	L	72	LEU
1	L	85	LYS
1	L	190	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	132	HIS
1	A	226	GLN
1	B	68	ASN
1	B	110	GLN
1	B	121	ASN
1	B	190	ASN
1	B	226	GLN
1	C	68	ASN
1	C	159	ASN
1	C	190	ASN
1	C	226	GLN
1	C	278	GLN
1	D	68	ASN
1	D	132	HIS
1	D	269	HIS
1	D	278	GLN
1	E	68	ASN
1	E	110	GLN
1	E	132	HIS
1	E	190	ASN
1	E	217	ASN
1	E	269	HIS
1	E	278	GLN
1	F	121	ASN
1	F	159	ASN
1	F	171	HIS
1	F	269	HIS
1	F	278	GLN
1	G	132	HIS
1	G	217	ASN
1	G	226	GLN
1	H	68	ASN
1	H	278	GLN
1	I	110	GLN
1	I	159	ASN
1	I	217	ASN
1	J	121	ASN
1	J	269	HIS
1	K	92	HIS
1	K	217	ASN
1	L	190	ASN
1	L	217	ASN

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Mol	Chain	Res	Type
1	L	269	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	281/291 (96%)	-1.53	0 100 100	6, 15, 34, 60	1 (0%)
1	B	281/291 (96%)	-1.54	0 100 100	4, 17, 30, 42	6 (2%)
1	C	281/291 (96%)	-1.58	0 100 100	4, 15, 25, 32	2 (0%)
1	D	281/291 (96%)	-1.49	0 100 100	6, 15, 36, 53	2 (0%)
1	E	281/291 (96%)	-1.54	0 100 100	5, 16, 29, 39	5 (1%)
1	F	281/291 (96%)	-1.58	0 100 100	4, 14, 26, 36	3 (1%)
1	G	281/291 (96%)	-1.50	0 100 100	6, 16, 31, 58	2 (0%)
1	H	281/291 (96%)	-1.53	0 100 100	3, 17, 27, 41	4 (1%)
1	I	281/291 (96%)	-1.55	0 100 100	5, 16, 29, 45	2 (0%)
1	J	281/291 (96%)	-1.58	0 100 100	5, 15, 28, 39	2 (0%)
1	K	281/291 (96%)	-1.56	0 100 100	5, 16, 28, 43	3 (1%)
1	L	281/291 (96%)	-1.54	0 100 100	7, 16, 30, 46	1 (0%)
All	All	3372/3492 (96%)	-1.54	0 100 100	3, 16, 30, 60	33 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.