



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:07 PM UTC

PDB ID : 3K4U / pdb_00003k4u
Title : CRYSTAL STRUCTURE OF putative binding component of ABC transporter from *Wolinella succinogenes* DSM 1740 complexed with lysine
Authors : Malashkevich, V.N.; Toro, R.; Morano, C.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-10-06
Resolution : 2.62 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

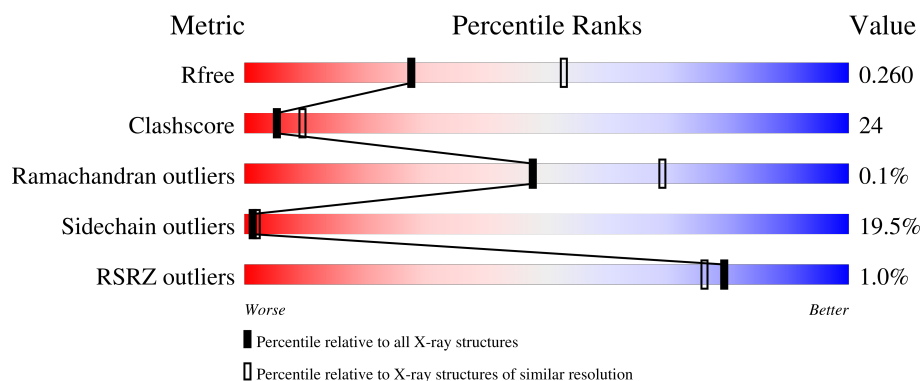
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	245	44% 37% 11% • 5%
1	B	245	56% 30% 8% • 5%
1	C	245	51% 31% 12% • 5%
1	D	245	53% 30% 11% • 5%
1	E	245	59% 27% 10% •

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Mol	Chain	Length	Quality of chain
1	F	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LYS	B	501	-	-	X	-
2	LYS	D	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11414 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 BINDING COMPONENT OF ABC TRANSPORTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	Se	0	0	0
			1872	1222	304	340	6			
1	B	233	Total	C	N	O	Se	0	0	0
			1872	1222	304	340	6			
1	C	233	Total	C	N	O	Se	0	0	0
			1872	1222	304	340	6			
1	D	233	Total	C	N	O	Se	0	0	0
			1872	1222	304	340	6			
1	E	234	Total	C	N	O	Se	0	0	0
			1878	1225	305	342	6			
1	F	233	Total	C	N	O	Se	0	0	0
			1872	1222	304	340	6			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q7MAG0
A	0	SER	-	expression tag	UNP Q7MAG0
A	1	LEU	-	expression tag	UNP Q7MAG0
A	236	GLU	-	expression tag	UNP Q7MAG0
A	237	GLY	-	expression tag	UNP Q7MAG0
A	238	HIS	-	expression tag	UNP Q7MAG0
A	239	HIS	-	expression tag	UNP Q7MAG0
A	240	HIS	-	expression tag	UNP Q7MAG0
A	241	HIS	-	expression tag	UNP Q7MAG0
A	242	HIS	-	expression tag	UNP Q7MAG0
A	243	HIS	-	expression tag	UNP Q7MAG0
B	-1	MSE	-	expression tag	UNP Q7MAG0
B	0	SER	-	expression tag	UNP Q7MAG0
B	1	LEU	-	expression tag	UNP Q7MAG0
B	236	GLU	-	expression tag	UNP Q7MAG0
B	237	GLY	-	expression tag	UNP Q7MAG0
B	238	HIS	-	expression tag	UNP Q7MAG0

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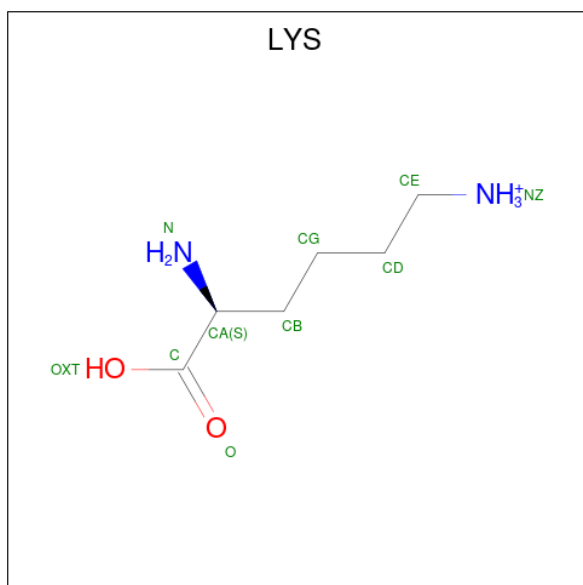
Chain	Residue	Modelled	Actual	Comment	Reference
B	239	HIS	-	expression tag	UNP Q7MAG0
B	240	HIS	-	expression tag	UNP Q7MAG0
B	241	HIS	-	expression tag	UNP Q7MAG0
B	242	HIS	-	expression tag	UNP Q7MAG0
B	243	HIS	-	expression tag	UNP Q7MAG0
C	-1	MSE	-	expression tag	UNP Q7MAG0
C	0	SER	-	expression tag	UNP Q7MAG0
C	1	LEU	-	expression tag	UNP Q7MAG0
C	236	GLU	-	expression tag	UNP Q7MAG0
C	237	GLY	-	expression tag	UNP Q7MAG0
C	238	HIS	-	expression tag	UNP Q7MAG0
C	239	HIS	-	expression tag	UNP Q7MAG0
C	240	HIS	-	expression tag	UNP Q7MAG0
C	241	HIS	-	expression tag	UNP Q7MAG0
C	242	HIS	-	expression tag	UNP Q7MAG0
C	243	HIS	-	expression tag	UNP Q7MAG0
D	-1	MSE	-	expression tag	UNP Q7MAG0
D	0	SER	-	expression tag	UNP Q7MAG0
D	1	LEU	-	expression tag	UNP Q7MAG0
D	236	GLU	-	expression tag	UNP Q7MAG0
D	237	GLY	-	expression tag	UNP Q7MAG0
D	238	HIS	-	expression tag	UNP Q7MAG0
D	239	HIS	-	expression tag	UNP Q7MAG0
D	240	HIS	-	expression tag	UNP Q7MAG0
D	241	HIS	-	expression tag	UNP Q7MAG0
D	242	HIS	-	expression tag	UNP Q7MAG0
D	243	HIS	-	expression tag	UNP Q7MAG0
E	-1	MSE	-	expression tag	UNP Q7MAG0
E	0	SER	-	expression tag	UNP Q7MAG0
E	1	LEU	-	expression tag	UNP Q7MAG0
E	236	GLU	-	expression tag	UNP Q7MAG0
E	237	GLY	-	expression tag	UNP Q7MAG0
E	238	HIS	-	expression tag	UNP Q7MAG0
E	239	HIS	-	expression tag	UNP Q7MAG0
E	240	HIS	-	expression tag	UNP Q7MAG0
E	241	HIS	-	expression tag	UNP Q7MAG0
E	242	HIS	-	expression tag	UNP Q7MAG0
E	243	HIS	-	expression tag	UNP Q7MAG0
F	-1	MSE	-	expression tag	UNP Q7MAG0
F	0	SER	-	expression tag	UNP Q7MAG0
F	1	LEU	-	expression tag	UNP Q7MAG0
F	236	GLU	-	expression tag	UNP Q7MAG0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	237	GLY	-	expression tag	UNP Q7MAG0
F	238	HIS	-	expression tag	UNP Q7MAG0
F	239	HIS	-	expression tag	UNP Q7MAG0
F	240	HIS	-	expression tag	UNP Q7MAG0
F	241	HIS	-	expression tag	UNP Q7MAG0
F	242	HIS	-	expression tag	UNP Q7MAG0
F	243	HIS	-	expression tag	UNP Q7MAG0

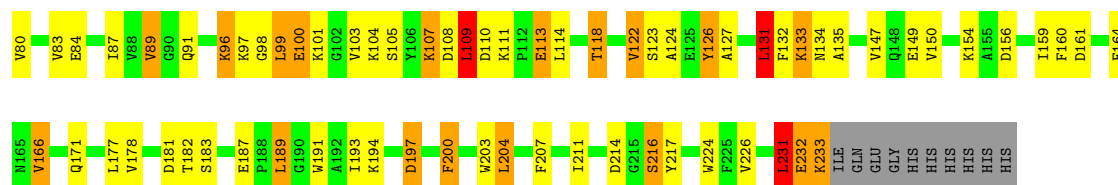
- Molecule 2 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



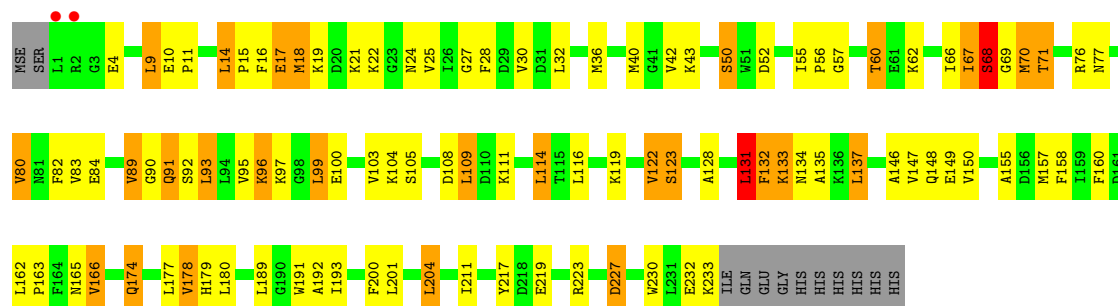
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		
2	E	1	Total	C	N	O	0	0
			10	6	2	2		
2	F	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is water.

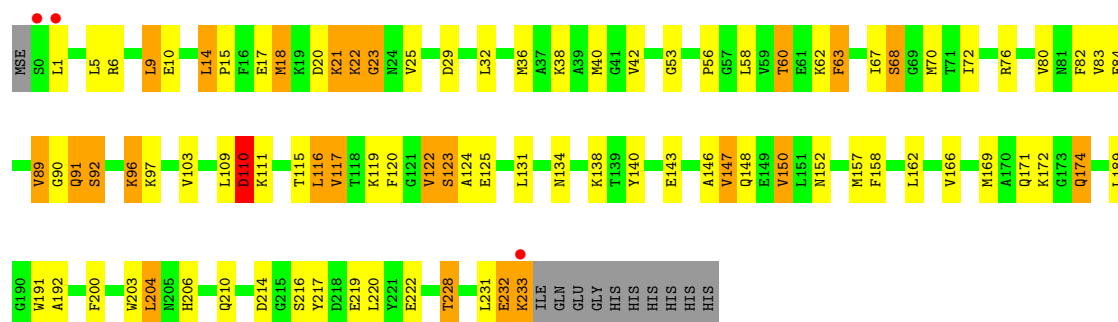
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	19	Total 19	O 19	0	0
3	C	19	Total 19	O 19	0	0
3	D	17	Total 17	O 17	0	0
3	E	22	Total 22	O 22	0	0
3	F	17	Total 17	O 17	0	0



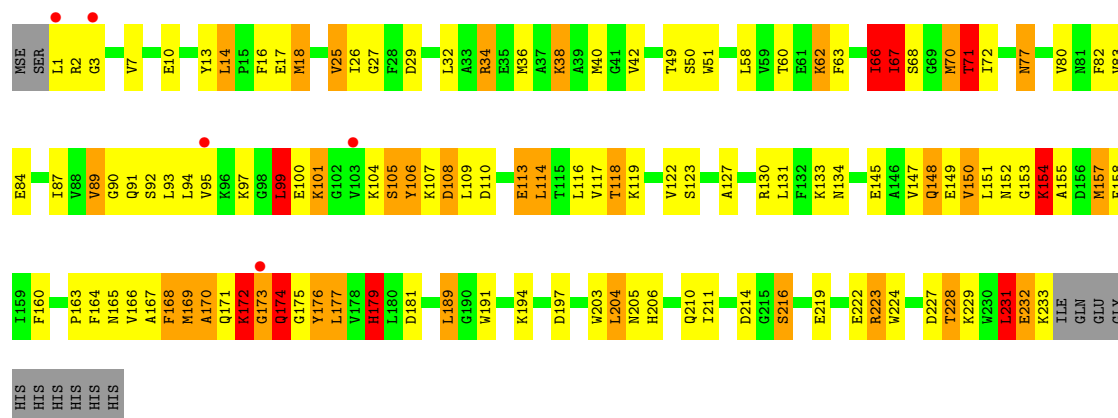
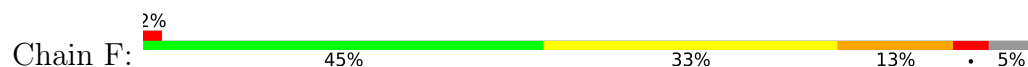
• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.41Å 149.15Å 81.97Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 20.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	90.6 (20.00-2.62) 99.2 (20.00-2.62)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.202 , 0.266 0.197 , 0.260	Depositor DCC
R_{free} test set	2663 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11414	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	1.29	13/1909 (0.7%)	1.33	20/2566 (0.8%)
1	B	1.05	9/1909 (0.5%)	1.19	11/2566 (0.4%)
1	C	1.21	12/1909 (0.6%)	1.18	8/2566 (0.3%)
1	D	0.99	7/1909 (0.4%)	1.13	8/2566 (0.3%)
1	E	1.00	1/1915 (0.1%)	1.19	11/2574 (0.4%)
1	F	1.27	17/1909 (0.9%)	1.28	20/2566 (0.8%)
All	All	1.14	59/11460 (0.5%)	1.22	78/15404 (0.5%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	VAL	CA-CB	-9.39	1.46	1.54
1	B	68	SER	C-O	-8.82	1.14	1.24
1	F	67	ILE	CA-CB	-8.23	1.43	1.54
1	C	70	MSE	SE-CE	-8.18	1.71	1.95
1	D	67	ILE	CA-CB	-8.17	1.43	1.54
1	D	55	ILE	CA-CB	-7.90	1.50	1.54
1	C	67	ILE	CA-CB	-7.84	1.43	1.54
1	B	70	MSE	SE-CE	-7.78	1.72	1.95
1	F	70	MSE	SE-CE	-7.67	1.72	1.95
1	A	70	MSE	SE-CE	-7.51	1.73	1.95
1	A	14	LEU	CA-C	-7.47	1.44	1.52
1	C	166	VAL	CA-CB	7.32	1.64	1.54
1	F	150	VAL	CA-CB	-6.96	1.45	1.54
1	F	170	ALA	N-CA	-6.81	1.38	1.46
1	B	68	SER	N-CA	-6.81	1.40	1.46
1	F	67	ILE	C-O	-6.78	1.16	1.24
1	F	66	ILE	C-O	-6.77	1.16	1.24
1	A	156	ASP	CA-C	6.74	1.61	1.52
1	A	19	LYS	CA-C	-6.70	1.44	1.52
1	F	66	ILE	CA-CB	-6.66	1.45	1.54
1	F	68	SER	C-O	-6.64	1.14	1.23
1	B	66	ILE	C-O	-6.54	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	VAL	CA-CB	-6.53	1.46	1.54
1	A	67	ILE	C-O	-6.47	1.16	1.24
1	C	47	VAL	N-CA	-6.43	1.40	1.46
1	A	69	GLY	C-O	-6.32	1.17	1.24
1	A	72	ILE	CA-C	-6.28	1.47	1.53
1	C	47	VAL	C-O	-6.25	1.17	1.23
1	B	68	SER	CA-C	-6.24	1.45	1.53
1	D	70	MSE	SE-CE	-6.17	1.76	1.95
1	B	67	ILE	C-O	-6.17	1.16	1.24
1	B	65	ILE	CA-CB	6.13	1.61	1.55
1	C	46	LEU	C-O	-6.04	1.16	1.23
1	A	14	LEU	C-O	-6.03	1.17	1.24
1	C	70	MSE	C-O	-6.00	1.16	1.24
1	D	70	MSE	CG-SE	-5.91	1.77	1.95
1	B	70	MSE	C-O	-5.90	1.17	1.24
1	F	70	MSE	CG-SE	-5.81	1.78	1.95
1	F	155	ALA	CA-CB	-5.78	1.43	1.53
1	F	170	ALA	CA-CB	-5.51	1.44	1.53
1	A	19	LYS	C-O	-5.45	1.17	1.24
1	A	178	VAL	CA-CB	-5.35	1.47	1.54
1	C	109	LEU	N-CA	-5.32	1.40	1.46
1	D	67	ILE	C-O	-5.32	1.17	1.24
1	F	167	ALA	CA-CB	-5.31	1.45	1.53
1	F	66	ILE	N-CA	-5.30	1.39	1.46
1	C	135	ALA	CA-CB	-5.28	1.44	1.53
1	D	71	THR	C-O	-5.28	1.17	1.24
1	F	174	GLN	CA-C	-5.27	1.48	1.53
1	B	226	VAL	C-O	-5.25	1.17	1.24
1	F	231	LEU	N-CA	-5.24	1.39	1.46
1	A	152	ASN	CA-C	-5.21	1.46	1.53
1	C	69	GLY	C-O	-5.20	1.18	1.24
1	F	71	THR	CA-CB	-5.19	1.45	1.53
1	D	166	VAL	CA-CB	5.18	1.60	1.54
1	C	48	PRO	CA-CB	-5.15	1.47	1.53
1	A	10	GLU	C-O	-5.09	1.18	1.25
1	F	170	ALA	CA-C	-5.08	1.46	1.52
1	E	22	LYS	N-CA	-5.00	1.39	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	TYR	N-CA-C	16.04	128.76	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	VAL	N-CA-C	14.07	122.74	111.62
1	E	22	LYS	N-CA-C	-13.20	96.80	113.16
1	A	154	LYS	N-CA-C	10.73	122.97	111.28
1	F	170	ALA	N-CA-C	-10.03	100.34	111.07
1	C	131	LEU	N-CA-C	9.56	121.78	111.36
1	F	154	LYS	N-CA-C	9.55	121.69	111.28
1	F	101	LYS	N-CA-C	9.48	124.22	109.52
1	B	226	VAL	CB-CA-C	-9.23	102.83	111.05
1	A	152	ASN	N-CA-C	-8.93	99.43	110.41
1	B	227	ASP	N-CA-C	8.49	120.53	111.28
1	B	232	GLU	N-CA-C	-8.45	100.94	111.75
1	A	20	ASP	N-CA-C	7.92	121.27	108.76
1	C	109	LEU	N-CA-C	-7.76	100.92	113.19
1	F	172	LYS	CA-C-N	-7.54	111.71	120.00
1	F	172	LYS	C-N-CA	-7.54	111.71	120.00
1	A	174	GLN	N-CA-C	7.35	119.29	111.28
1	A	156	ASP	N-CA-C	7.29	126.33	110.80
1	D	133	LYS	N-CA-C	7.13	119.14	111.36
1	D	57	GLY	N-CA-C	-7.09	103.91	112.49
1	E	232	GLU	N-CA-C	-6.96	96.42	108.52
1	C	200	PHE	N-CA-C	-6.89	103.70	111.14
1	F	176	TYR	N-CA-C	6.75	118.30	111.07
1	A	175	GLY	CA-C-N	6.70	129.26	120.28
1	A	175	GLY	C-N-CA	6.70	129.26	120.28
1	B	173	GLY	N-CA-C	6.60	122.22	113.37
1	B	214	ASP	CB-CA-C	-6.59	98.63	110.70
1	D	227	ASP	N-CA-C	6.52	119.21	111.71
1	F	174	GLN	N-CA-C	-6.47	98.47	108.31
1	D	68	SER	N-CA-C	6.43	120.77	112.41
1	D	131	LEU	N-CA-C	6.42	118.36	111.36
1	A	22	LYS	N-CA-C	-6.41	105.21	113.16
1	F	106	TYR	N-CA-C	-6.39	105.54	113.15
1	A	70	MSE	N-CA-C	6.35	119.59	109.24
1	A	150	VAL	N-CA-C	6.31	117.06	110.62
1	F	99	LEU	N-CA-C	-6.28	103.01	111.87
1	D	134	ASN	N-CA-C	6.24	121.03	113.17
1	E	231	LEU	N-CA-C	6.22	120.47	113.01
1	F	170	ALA	CA-C-N	-6.17	112.41	120.44
1	F	170	ALA	C-N-CA	-6.17	112.41	120.44
1	E	214	ASP	N-CA-C	6.16	118.00	111.28
1	F	172	LYS	N-CA-C	6.12	122.84	112.99
1	E	23	GLY	N-CA-C	6.02	123.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	THR	N-CA-C	6.00	120.60	113.16
1	E	117	VAL	N-CA-C	5.96	117.06	108.48
1	B	229	LYS	CA-C-N	5.93	128.81	120.28
1	B	229	LYS	C-N-CA	5.93	128.81	120.28
1	A	153	GLY	N-CA-C	5.92	125.74	115.62
1	F	197	ASP	CA-C-N	-5.90	113.67	120.04
1	F	197	ASP	C-N-CA	-5.90	113.67	120.04
1	F	25	VAL	CB-CA-C	5.87	118.82	110.84
1	D	132	PHE	N-CA-C	5.87	118.66	107.75
1	C	231	LEU	N-CA-C	5.86	118.44	111.71
1	F	153	GLY	N-CA-C	5.79	119.69	112.73
1	E	63	PHE	N-CA-C	5.71	116.62	108.74
1	E	110	ASP	N-CA-C	5.69	119.48	112.54
1	A	19	LYS	CB-CA-C	-5.67	100.39	109.75
1	E	150	VAL	CB-CA-C	5.63	119.78	112.24
1	C	70	MSE	N-CA-C	5.54	117.77	108.96
1	E	214	ASP	CB-CA-C	-5.37	101.87	110.79
1	A	213	HIS	N-CA-C	-5.34	105.60	113.61
1	C	25	VAL	CB-CA-C	5.33	117.52	110.91
1	D	135	ALA	N-CA-C	5.33	118.16	109.59
1	A	76	ARG	N-CA-C	-5.31	105.53	112.23
1	C	197	ASP	CA-C-N	5.29	124.79	119.19
1	C	197	ASP	C-N-CA	5.29	124.79	119.19
1	A	210	GLN	N-CA-C	-5.26	105.24	110.97
1	F	173	GLY	N-CA-C	-5.25	106.06	112.77
1	A	87	ILE	CA-C-N	-5.19	116.75	123.19
1	A	87	ILE	C-N-CA	-5.19	116.75	123.19
1	F	168	PHE	N-CA-C	5.17	116.91	111.28
1	A	7	VAL	N-CA-C	5.16	116.40	108.71
1	A	159	ILE	N-CA-C	5.11	115.26	108.11
1	B	25	VAL	N-CA-C	5.08	115.60	108.89
1	F	179	HIS	N-CA-C	5.06	116.66	108.26
1	B	213	HIS	CA-C-N	5.04	129.20	120.58
1	B	213	HIS	C-N-CA	5.04	129.20	120.58
1	F	51	TRP	N-CA-C	5.04	117.43	111.33

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	1872	0	1903	119	0
1	B	1872	0	1903	65	0
1	C	1872	0	1903	95	0
1	D	1872	0	1903	77	0
1	E	1878	0	1908	66	0
1	F	1872	0	1903	130	0
2	A	10	0	12	2	0
2	B	10	0	12	6	0
2	C	10	0	12	1	0
2	D	10	0	12	6	0
2	E	10	0	12	1	0
2	F	10	0	12	1	0
3	A	22	0	0	5	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	17	0	0	0	0
3	E	22	0	0	1	0
3	F	17	0	0	1	0
All	All	11414	0	11495	549	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (549) 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:F:148:GLN:NE2	1:F:151:LEU:HD12	1.48	1.26
1:E:21:LYS:HD2	1:E:22:LYS:N	1.59	1.17
1:B:231:LEU:HD12	1:B:231:LEU:N	1.51	1.15
1:F:171:GLN:HG2	1:F:172:LYS:HD3	1.16	1.14
1:F:148:GLN:HE22	1:F:151:LEU:CD1	1.60	1.14
1:F:171:GLN:O	1:F:172:LYS:HG3	1.49	1.12
1:C:132:PHE:O	1:C:133:LYS:HG2	1.47	1.11
1:B:228:THR:O	1:B:231:LEU:HD13	1.49	1.11
1:F:169:MSE:HG3	1:F:173:GLY:HA3	1.24	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:LEU:HD13	1:F:157:MSE:HG2	1.33	1.08
1:B:231:LEU:H	1:B:231:LEU:CD1	1.59	1.08
1:E:20:ASP:O	1:E:21:LYS:HB3	1.47	1.08
1:C:34:ARG:HG3	1:C:34:ARG:HH11	0.94	1.07
1:F:171:GLN:C	1:F:172:LYS:HG3	1.75	1.07
1:E:17:GLU:OE1	1:E:68:SER:HA	1.55	1.06
1:E:233:LYS:H	1:E:233:LYS:HD3	1.18	1.06
1:A:155:ALA:O	1:A:156:ASP:HB3	1.54	1.06
1:B:40:MSE:HE1	1:B:200:PHE:HE1	1.19	1.06
1:D:71:THR:HG1	2:D:501:LYS:N	1.55	1.03
1:F:169:MSE:HA	1:F:173:GLY:H	1.24	1.03
1:F:171:GLN:HG2	1:F:172:LYS:CD	1.90	1.02
1:E:21:LYS:C	1:E:21:LYS:CD	2.28	1.01
1:E:21:LYS:HD2	1:E:21:LYS:C	1.80	0.99
1:C:34:ARG:HG3	1:C:34:ARG:NH1	1.67	0.96
1:B:231:LEU:HD12	1:B:231:LEU:H	0.79	0.96
1:F:174:GLN:HA	1:F:174:GLN:OE1	1.63	0.96
1:B:40:MSE:HE1	1:B:200:PHE:CE1	2.01	0.95
1:F:169:MSE:CG	1:F:173:GLY:HA3	1.96	0.93
1:A:66:ILE:HG21	1:A:70:MSE:HE1	1.50	0.92
1:D:174:GLN:HE21	1:D:174:GLN:HA	1.32	0.91
1:C:100:GLU:O	1:C:103:VAL:HG22	1.71	0.91
1:A:155:ALA:O	1:A:156:ASP:CB	2.10	0.91
1:A:147:VAL:O	1:A:150:VAL:HG12	1.70	0.90
1:C:118:THR:HG23	1:C:159:ILE:O	1.70	0.90
1:F:169:MSE:HG3	1:F:173:GLY:CA	2.02	0.90
1:F:148:GLN:HE22	1:F:151:LEU:HD12	0.77	0.90
1:A:231:LEU:H	1:A:231:LEU:HD12	1.38	0.89
1:F:97:LYS:HD2	1:F:175:GLY:O	1.73	0.89
1:D:21:LYS:HG2	1:D:233:LYS:HB2	1.54	0.89
1:F:169:MSE:HA	1:F:173:GLY:N	1.87	0.89
1:F:169:MSE:CA	1:F:173:GLY:H	1.87	0.88
1:C:118:THR:CG2	1:C:159:ILE:O	2.24	0.85
1:C:40:MSE:HE1	1:C:200:PHE:HE1	1.40	0.85
1:A:21:LYS:HD3	3:A:521:HOH:O	1.77	0.85
1:C:233:LYS:H	1:C:233:LYS:HD3	1.42	0.84
1:F:60:THR:HG21	1:F:62:LYS:HE3	1.60	0.84
1:F:95:VAL:HG12	1:F:157:MSE:HB2	1.59	0.84
1:F:97:LYS:HB2	1:F:176:TYR:O	1.77	0.84
1:F:116:LEU:HD13	1:F:157:MSE:CG	2.07	0.84
1:F:116:LEU:CD1	1:F:157:MSE:HG2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:THR:HG21	1:B:62:LYS:HE3	1.60	0.83
1:A:148:GLN:HE21	1:A:148:GLN:HA	1.43	0.82
1:C:55:ILE:HD11	1:C:70:MSE:HE1	1.59	0.82
1:A:21:LYS:CD	3:A:521:HOH:O	2.26	0.81
1:C:83:VAL:HG12	1:C:84:GLU:N	1.94	0.81
1:E:110:ASP:O	1:E:134:ASN:HB2	1.79	0.81
1:F:38:LYS:HD2	1:F:38:LYS:N	1.93	0.81
1:F:106:TYR:CD2	1:F:106:TYR:O	2.34	0.80
1:F:99:LEU:O	1:F:99:LEU:CD2	2.30	0.80
1:F:174:GLN:OE1	1:F:174:GLN:CA	2.29	0.80
1:A:103:VAL:HB	1:A:109:LEU:HD11	1.62	0.80
1:E:200:PHE:O	1:E:204:LEU:HD22	1.82	0.79
1:B:228:THR:O	1:B:231:LEU:CD1	2.30	0.79
1:E:21:LYS:CD	1:E:22:LYS:N	2.39	0.79
1:C:132:PHE:O	1:C:133:LYS:CG	2.30	0.78
1:C:10:GLU:HB2	1:C:49:THR:O	1.84	0.77
1:A:66:ILE:HG21	1:A:70:MSE:CE	2.13	0.77
1:D:36:MSE:HG2	1:D:40:MSE:HE3	1.66	0.76
1:A:14:LEU:HD12	1:A:18:MSE:HE2	1.68	0.76
1:F:13:TYR:HB3	1:F:17:GLU:OE2	1.87	0.75
1:E:233:LYS:HD3	1:E:233:LYS:N	1.96	0.75
1:F:171:GLN:CG	1:F:172:LYS:HD3	2.09	0.75
1:E:36:MSE:HG2	1:E:40:MSE:HE3	1.69	0.74
1:A:156:ASP:OD1	1:A:156:ASP:C	2.30	0.74
1:F:134:ASN:HB2	3:F:510:HOH:O	1.87	0.74
1:C:34:ARG:HH11	1:C:34:ARG:CG	1.84	0.73
1:A:34:ARG:O	1:A:38:LYS:HD2	1.89	0.72
1:D:71:THR:OG1	2:D:501:LYS:N	2.22	0.72
1:F:223:ARG:O	1:F:223:ARG:HG3	1.88	0.72
1:F:152:ASN:OD1	1:F:154:LYS:HG3	1.89	0.72
1:A:57:GLY:O	1:A:62:LYS:HB2	1.89	0.72
1:A:89:VAL:HG13	1:A:90:GLY:H	1.54	0.72
1:A:169:MSE:O	1:A:174:GLN:HG3	1.89	0.72
1:B:70:MSE:HE3	1:B:82:PHE:CE1	2.25	0.72
1:C:20:ASP:HB2	1:C:24:ASN:O	1.90	0.72
1:C:36:MSE:HE1	1:C:65:ILE:HD12	1.72	0.72
1:E:20:ASP:O	1:E:21:LYS:CB	2.30	0.72
1:F:231:LEU:O	1:F:231:LEU:HD23	1.89	0.72
1:F:16:PHE:HB3	1:F:17:GLU:OE1	1.90	0.71
1:F:99:LEU:O	1:F:99:LEU:HD22	1.90	0.71
1:F:231:LEU:HD23	1:F:231:LEU:C	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:CG1	1:A:90:GLY:N	2.53	0.71
1:D:56:PRO:O	1:D:60:THR:HB	1.91	0.71
1:A:18:MSE:O	1:A:18:MSE:HG2	1.90	0.70
1:B:150:VAL:HG13	1:B:177:LEU:HD11	1.73	0.70
1:A:96:LYS:HD3	1:A:97:LYS:H	1.55	0.70
1:A:176:TYR:CD1	1:A:176:TYR:N	2.59	0.70
1:C:40:MSE:HE1	1:C:200:PHE:CE1	2.25	0.70
1:F:148:GLN:NE2	1:F:148:GLN:HA	2.02	0.70
1:E:232:GLU:O	1:E:233:LYS:C	2.35	0.69
1:E:58:LEU:HD23	1:E:80:VAL:HG11	1.74	0.69
1:E:9:LEU:HD22	1:E:17:GLU:HG2	1.75	0.69
1:D:66:ILE:HG21	1:D:70:MSE:HE2	1.75	0.69
1:F:127:ALA:O	1:F:131:LEU:HB2	1.92	0.69
1:F:171:GLN:O	1:F:172:LYS:CG	2.36	0.69
1:C:36:MSE:HE3	1:C:204:LEU:HD11	1.76	0.68
1:F:173:GLY:O	1:F:174:GLN:C	2.34	0.68
1:F:168:PHE:O	1:F:172:LYS:N	2.21	0.68
1:E:203:TRP:HE3	1:E:204:LEU:HD13	1.59	0.68
1:F:169:MSE:SE	1:F:173:GLY:HA3	2.43	0.68
1:A:1:LEU:HD11	1:A:5:LEU:HA	1.76	0.67
1:C:110:ASP:O	1:C:134:ASN:HB2	1.93	0.67
1:C:111:LYS:HB3	1:C:113:GLU:OE1	1.95	0.66
1:D:122:VAL:HG13	1:D:123:SER:N	2.11	0.66
1:D:91:GLN:OE1	1:D:160:PHE:C	2.39	0.66
1:B:231:LEU:O	1:B:232:GLU:C	2.33	0.66
1:D:96:LYS:HD3	1:D:97:LYS:H	1.59	0.66
1:E:70:MSE:HE1	1:E:192:ALA:HB3	1.77	0.66
1:A:143:GLU:O	1:A:147:VAL:HG22	1.95	0.65
1:C:67:ILE:HG23	1:C:191:TRP:CD1	2.31	0.65
1:D:80:VAL:HG21	1:D:192:ALA:HB1	1.78	0.65
1:A:149:GLU:OE2	1:A:149:GLU:N	2.30	0.65
1:D:123:SER:HB2	2:D:501:LYS:C	2.21	0.65
1:C:87:ILE:HG23	1:C:189:LEU:HD22	1.79	0.65
1:E:20:ASP:OD2	1:E:22:LYS:N	2.30	0.65
1:F:228:THR:O	1:F:231:LEU:HB2	1.96	0.65
1:F:99:LEU:O	1:F:99:LEU:HD23	1.96	0.65
1:F:93:LEU:O	1:F:179:HIS:HB2	1.96	0.64
1:C:83:VAL:CG1	1:C:84:GLU:N	2.60	0.64
1:F:94:LEU:HD23	1:F:179:HIS:CB	2.27	0.64
1:F:105:SER:OG	1:F:107:LYS:N	2.30	0.64
1:F:169:MSE:O	1:F:170:ALA:C	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ASP:OD2	1:E:21:LYS:N	2.29	0.64
1:F:10:GLU:OE1	1:F:119:LYS:NZ	2.30	0.64
1:F:105:SER:OG	1:F:106:TYR:N	2.30	0.64
1:F:113:GLU:HG3	1:F:114:LEU:HD23	1.79	0.64
1:A:60:THR:O	1:A:60:THR:HG22	1.96	0.64
1:A:128:ALA:HB1	1:A:137:LEU:HD13	1.80	0.64
1:D:95:VAL:HG12	1:D:157:MSE:HB3	1.80	0.64
1:D:123:SER:HB2	2:D:501:LYS:HA	1.79	0.63
1:D:116:LEU:HD12	1:D:157:MSE:O	1.97	0.63
1:E:70:MSE:HE3	1:E:82:PHE:CE1	2.33	0.63
1:F:17:GLU:C	1:F:18:MSE:HE2	2.23	0.63
1:F:18:MSE:HE3	1:F:26:ILE:O	1.98	0.63
1:F:97:LYS:CD	1:F:175:GLY:O	2.46	0.63
1:F:145:GLU:O	1:F:149:GLU:HG2	1.98	0.63
1:D:123:SER:HB2	2:D:501:LYS:CA	2.27	0.63
1:D:149:GLU:O	1:D:155:ALA:N	2.30	0.63
1:D:4:GLU:HA	1:D:42:VAL:CG1	2.28	0.63
1:D:174:GLN:HA	1:D:174:GLN:NE2	2.07	0.63
1:B:49:THR:HG22	1:B:50:SER:O	1.98	0.62
1:A:149:GLU:OE2	1:A:149:GLU:CA	2.46	0.62
1:E:15:PRO:HA	1:E:18:MSE:HE1	1.81	0.62
1:A:96:LYS:HD3	1:A:97:LYS:N	2.14	0.62
1:A:21:LYS:HD2	3:A:521:HOH:O	1.94	0.62
1:A:174:GLN:CD	1:A:174:GLN:H	1.97	0.62
1:E:70:MSE:HE1	1:E:192:ALA:CB	2.30	0.62
1:F:107:LYS:C	1:F:109:LEU:H	2.07	0.62
1:F:169:MSE:C	1:F:173:GLY:H	2.07	0.62
1:A:89:VAL:CG1	1:A:90:GLY:H	2.13	0.61
1:C:127:ALA:O	1:C:131:LEU:HB2	1.99	0.61
1:F:18:MSE:HE3	1:F:27:GLY:HA3	1.82	0.61
1:A:147:VAL:O	1:A:150:VAL:CG1	2.46	0.61
1:E:21:LYS:HD2	1:E:22:LYS:H	1.58	0.61
1:F:58:LEU:HD22	1:F:66:ILE:HD12	1.82	0.61
1:F:94:LEU:HB3	1:F:177:LEU:HD23	1.82	0.61
1:C:70:MSE:HG3	1:C:76:ARG:NH1	2.15	0.61
1:F:105:SER:C	1:F:107:LYS:H	2.06	0.61
1:A:13:TYR:OH	1:A:161:ASP:CB	2.49	0.60
1:B:231:LEU:C	1:B:233:LYS:N	2.53	0.60
1:F:94:LEU:HD23	1:F:179:HIS:HB2	1.82	0.60
1:C:70:MSE:CE	1:C:76:ARG:HD3	2.31	0.60
1:F:60:THR:CG2	1:F:62:LYS:HE3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:OE2	1:A:101:LYS:HE2	2.01	0.60
1:D:96:LYS:HD3	1:D:97:LYS:N	2.16	0.60
1:D:9:LEU:HD22	1:D:17:GLU:HG2	1.83	0.60
1:B:60:THR:HG21	1:B:62:LYS:CE	2.30	0.59
1:F:10:GLU:OE1	2:F:501:LYS:NZ	2.33	0.59
1:B:70:MSE:HE3	1:B:82:PHE:CZ	2.38	0.59
1:D:100:GLU:HB3	1:D:178:VAL:HG11	1.83	0.59
1:A:210:GLN:HG2	3:E:505:HOH:O	2.02	0.59
1:D:15:PRO:C	1:D:18:MSE:HE1	2.28	0.59
1:B:227:ASP:O	1:B:228:THR:OG1	2.11	0.58
1:F:7:VAL:HG13	1:F:67:ILE:HG13	1.84	0.58
1:A:10:GLU:HB2	1:A:49:THR:O	2.02	0.58
1:A:214:ASP:HB3	1:A:216:SER:H	1.68	0.58
1:D:100:GLU:O	1:D:103:VAL:HG22	2.04	0.58
1:A:155:ALA:O	1:A:156:ASP:CG	2.47	0.58
1:C:40:MSE:CE	1:C:200:PHE:HE1	2.13	0.58
1:D:43:LYS:H	1:D:43:LYS:HD2	1.69	0.58
1:F:106:TYR:CD2	1:F:106:TYR:C	2.79	0.58
1:F:60:THR:O	1:F:60:THR:HG22	2.02	0.57
1:A:58:LEU:HD23	1:A:80:VAL:HG11	1.87	0.57
1:A:118:THR:HG23	1:A:119:LYS:O	2.04	0.57
1:B:89:VAL:HG11	1:B:161:ASP:HB3	1.86	0.57
1:F:18:MSE:HE3	1:F:27:GLY:CA	2.35	0.57
1:A:17:GLU:OE1	1:A:29:ASP:OD1	2.21	0.57
1:F:171:GLN:C	1:F:172:LYS:CG	2.63	0.57
1:A:169:MSE:HE1	1:A:177:LEU:O	2.05	0.57
1:C:197:ASP:OD1	1:C:200:PHE:HB2	2.05	0.57
1:F:110:ASP:OD1	1:F:133:LYS:N	2.35	0.57
1:C:70:MSE:HE3	1:C:76:ARG:HD3	1.87	0.57
1:A:13:TYR:OH	1:A:161:ASP:HB2	2.05	0.57
1:C:83:VAL:HG12	1:C:84:GLU:H	1.69	0.57
1:A:66:ILE:CG2	1:A:70:MSE:CE	2.82	0.56
1:F:105:SER:OG	1:F:107:LYS:HB2	2.04	0.56
1:B:123:SER:OG	2:B:501:LYS:HA	2.05	0.56
1:D:22:LYS:HD3	1:D:24:ASN:OD1	2.05	0.56
1:B:25:VAL:HG13	1:B:46:LEU:HD13	1.88	0.56
1:F:214:ASP:HB3	1:F:216:SER:H	1.70	0.56
1:E:232:GLU:O	1:E:233:LYS:O	2.23	0.56
1:D:66:ILE:HD13	1:D:70:MSE:HE1	1.88	0.56
1:F:210:GLN:O	1:F:214:ASP:HB2	2.06	0.56
1:D:80:VAL:CG2	1:D:192:ALA:HB1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:LEU:HB2	1:E:157:MSE:HE3	1.89	0.55
1:D:132:PHE:N	1:D:132:PHE:HD1	2.05	0.55
1:B:82:PHE:O	1:E:206:HIS:HE1	1.89	0.55
1:D:122:VAL:CG1	1:D:123:SER:N	2.70	0.55
1:F:66:ILE:C	1:F:67:ILE:HG12	2.30	0.55
1:B:152:ASN:OD1	1:B:154:LYS:HG2	2.07	0.55
1:D:128:ALA:HB1	1:D:137:LEU:HD13	1.88	0.55
1:A:79:ARG:NH2	3:A:505:HOH:O	2.38	0.55
1:C:108:ASP:O	1:C:109:LEU:HD13	2.06	0.55
1:C:110:ASP:OD2	1:C:132:PHE:O	2.25	0.55
1:D:147:VAL:O	1:D:148:GLN:C	2.47	0.55
1:F:97:LYS:NZ	1:F:175:GLY:O	2.36	0.55
1:A:210:GLN:O	1:A:214:ASP:HB2	2.07	0.54
1:D:60:THR:CG2	1:D:60:THR:O	2.55	0.54
1:F:150:VAL:HG11	1:F:177:LEU:HD21	1.89	0.54
1:F:60:THR:CG2	1:F:60:THR:O	2.55	0.54
1:D:83:VAL:HG12	1:D:84:GLU:N	2.22	0.54
1:B:143:GLU:OE1	2:B:501:LYS:NZ	2.40	0.54
1:B:176:TYR:N	1:B:176:TYR:CD2	2.75	0.54
1:D:146:ALA:O	1:D:149:GLU:HB2	2.07	0.54
1:A:17:GLU:C	1:A:18:MSE:HE3	2.33	0.54
1:E:6:ARG:NH2	1:E:62:LYS:O	2.41	0.54
1:A:148:GLN:HA	1:A:148:GLN:NE2	2.15	0.54
1:A:58:LEU:HD22	1:A:66:ILE:CD1	2.38	0.53
1:C:77:ASN:O	1:C:77:ASN:ND2	2.41	0.53
1:A:5:LEU:N	1:A:42:VAL:HG11	2.23	0.53
1:C:107:LYS:HD2	1:C:107:LYS:O	2.08	0.53
1:E:20:ASP:OD2	1:E:23:GLY:N	2.41	0.53
1:A:66:ILE:CG2	1:A:70:MSE:HE1	2.31	0.53
1:A:100:GLU:C	1:A:103:VAL:HG13	2.33	0.53
1:B:228:THR:C	1:B:231:LEU:CD1	2.81	0.53
1:F:173:GLY:O	1:F:174:GLN:HB2	2.08	0.53
1:D:116:LEU:O	1:D:137:LEU:HA	2.08	0.53
1:A:89:VAL:HG12	1:A:90:GLY:N	2.24	0.53
1:C:15:PRO:C	1:C:18:MSE:HE1	2.34	0.53
1:D:82:PHE:O	1:F:206:HIS:HE1	1.92	0.53
1:A:119:LYS:HE2	1:A:142:THR:HA	1.92	0.52
1:A:195:LYS:HB3	1:B:199:ASP:OD2	2.08	0.52
1:B:160:PHE:CD2	1:B:161:ASP:N	2.76	0.52
1:C:34:ARG:NH1	1:C:34:ARG:CG	2.50	0.52
1:D:193:ILE:HD11	1:D:201:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:C	1:A:233:LYS:H	2.18	0.52
1:C:1:LEU:HD23	1:C:2:ARG:N	2.24	0.52
1:A:67:ILE:HG23	1:A:191:TRP:CD1	2.45	0.52
1:B:214:ASP:HB3	1:B:216:SER:H	1.74	0.52
1:D:132:PHE:N	1:D:132:PHE:CD1	2.74	0.52
1:D:42:VAL:CG1	1:D:43:LYS:N	2.73	0.52
1:B:228:THR:HA	1:B:231:LEU:HD11	1.92	0.52
1:F:173:GLY:O	1:F:176:TYR:N	2.41	0.52
1:F:233:LYS:O	1:F:233:LYS:HG3	2.10	0.52
1:C:15:PRO:HA	1:C:18:MSE:HE1	1.92	0.52
1:C:171:GLN:HB3	1:C:231:LEU:CD2	2.39	0.52
1:E:70:MSE:HE3	1:E:82:PHE:HE1	1.76	0.51
1:A:58:LEU:HD22	1:A:66:ILE:HD12	1.91	0.51
1:A:5:LEU:H	1:A:42:VAL:CG1	2.24	0.51
1:F:203:TRP:HE3	1:F:204:LEU:HD13	1.75	0.51
1:D:103:VAL:HG11	1:D:109:LEU:HD22	1.92	0.51
1:C:55:ILE:HD11	1:C:70:MSE:CE	2.36	0.51
1:F:99:LEU:HD23	1:F:99:LEU:C	2.35	0.51
1:A:171:GLN:HG3	1:A:172:LYS:H	1.76	0.51
1:C:50:SER:O	1:C:51:TRP:C	2.50	0.51
1:C:14:LEU:HD22	1:C:164:PHE:CE1	2.46	0.51
1:D:42:VAL:HG12	1:D:43:LYS:N	2.25	0.51
1:C:83:VAL:CG1	1:C:84:GLU:H	2.23	0.51
1:C:118:THR:HG21	1:C:124:ALA:CB	2.39	0.51
1:C:118:THR:HG21	1:C:124:ALA:HB3	1.92	0.51
1:D:14:LEU:HD12	1:D:18:MSE:SE	2.61	0.51
1:D:111:LYS:HB2	1:D:114:LEU:CD1	2.41	0.51
1:A:72:ILE:HD12	1:A:188:PRO:HB2	1.93	0.51
1:B:28:PHE:O	1:B:32:LEU:HB2	2.11	0.51
1:B:160:PHE:HZ	2:B:501:LYS:HD3	1.76	0.51
1:C:110:ASP:OD1	1:C:132:PHE:C	2.55	0.50
1:C:105:SER:O	1:C:108:ASP:OD1	2.29	0.50
1:C:132:PHE:C	1:C:133:LYS:HG2	2.28	0.50
1:B:96:LYS:HD3	1:B:97:LYS:N	2.27	0.50
1:C:232:GLU:O	1:C:233:LYS:C	2.54	0.50
1:E:17:GLU:OE1	1:E:29:ASP:OD1	2.29	0.50
1:F:89:VAL:CG1	1:F:90:GLY:N	2.73	0.50
1:A:88:VAL:HG11	1:A:186:TYR:CE1	2.45	0.50
1:C:110:ASP:O	1:C:134:ASN:CB	2.60	0.50
1:E:96:LYS:HD3	1:E:97:LYS:H	1.77	0.50
1:B:29:ASP:CG	1:B:67:ILE:HG22	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:LYS:HD2	1:D:43:LYS:N	2.26	0.50
1:F:18:MSE:CE	1:F:27:GLY:HA3	2.41	0.50
1:F:170:ALA:O	1:F:171:GLN:C	2.46	0.50
1:F:95:VAL:HG12	1:F:157:MSE:CB	2.38	0.50
1:A:100:GLU:O	1:A:103:VAL:HG13	2.12	0.50
1:A:171:GLN:HG3	1:A:172:LYS:N	2.27	0.50
1:C:4:GLU:HA	1:C:42:VAL:HG13	1.92	0.50
1:E:20:ASP:OD2	1:E:20:ASP:C	2.48	0.50
1:E:83:VAL:O	1:E:84:GLU:C	2.55	0.50
1:B:118:THR:OG1	1:B:159:ILE:O	2.26	0.50
1:F:67:ILE:HG23	1:F:191:TRP:CD1	2.47	0.50
1:F:149:GLU:O	1:F:152:ASN:OD1	2.29	0.50
1:A:81:ASN:ND2	1:A:195:LYS:HA	2.27	0.49
1:C:108:ASP:OD1	1:C:108:ASP:N	2.30	0.49
1:A:229:LYS:O	1:A:232:GLU:HG3	2.12	0.49
1:F:94:LEU:HD21	1:F:165:ASN:HB3	1.94	0.49
1:C:56:PRO:O	1:C:60:THR:HB	2.11	0.49
1:F:229:LYS:O	1:F:232:GLU:HG2	2.12	0.49
1:A:156:ASP:OD1	1:A:156:ASP:O	2.29	0.49
1:A:211:ILE:HA	1:A:214:ASP:HB2	1.94	0.49
1:F:14:LEU:HD12	1:F:18:MSE:SE	2.62	0.49
1:A:1:LEU:HD12	1:A:4:GLU:O	2.13	0.49
1:A:149:GLU:HA	1:A:152:ASN:OD1	2.13	0.49
1:B:60:THR:HG22	1:B:60:THR:O	2.11	0.49
1:F:71:THR:HA	1:F:189:LEU:HD12	1.94	0.49
1:C:1:LEU:HD21	1:C:4:GLU:O	2.13	0.49
1:D:89:VAL:HG13	1:D:90:GLY:N	2.27	0.49
1:F:211:ILE:HA	1:F:214:ASP:HB2	1.95	0.49
1:A:18:MSE:HE3	1:A:18:MSE:N	2.28	0.49
1:B:118:THR:HG23	1:B:119:LYS:N	2.28	0.49
1:C:214:ASP:HB3	1:C:216:SER:OG	2.12	0.49
1:C:171:GLN:HB3	1:C:231:LEU:HD23	1.94	0.49
1:A:60:THR:O	1:A:60:THR:CG2	2.60	0.48
1:A:233:LYS:HB2	1:A:233:LYS:HE3	1.67	0.48
1:E:169:MSE:HE3	1:E:174:GLN:HA	1.94	0.48
1:B:9:LEU:HD21	1:B:46:LEU:HD22	1.95	0.48
1:D:66:ILE:HG21	1:D:70:MSE:CE	2.43	0.48
1:A:165:ASN:O	1:A:169:MSE:HB2	2.13	0.48
1:F:84:GLU:HG2	1:F:205:ASN:OD1	2.13	0.48
1:F:163:PRO:HA	1:F:166:VAL:HG22	1.94	0.48
1:A:42:VAL:HG13	1:A:43:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LYS:HD3	1:C:233:LYS:N	2.10	0.48
1:D:67:ILE:HG23	1:D:191:TRP:CD1	2.49	0.48
1:F:172:LYS:HA	1:F:174:GLN:NE2	2.28	0.48
1:E:117:VAL:HG12	1:E:138:LYS:HB2	1.95	0.48
1:A:9:LEU:HB3	1:A:68:SER:HB3	1.94	0.48
1:D:15:PRO:HA	1:D:18:MSE:HE1	1.96	0.48
1:F:36:MSE:O	1:F:40:MSE:HG3	2.13	0.48
1:E:56:PRO:O	1:E:60:THR:HB	2.13	0.48
1:B:147:VAL:O	1:B:150:VAL:HG12	2.12	0.48
1:E:219:GLU:O	1:E:220:LEU:C	2.56	0.48
1:A:83:VAL:HG12	1:A:84:GLU:N	2.29	0.48
1:E:122:VAL:O	1:E:123:SER:C	2.57	0.48
1:F:40:MSE:HG2	1:F:203:TRP:CZ2	2.49	0.48
1:F:49:THR:HG22	1:F:50:SER:O	2.14	0.48
1:F:169:MSE:O	1:F:173:GLY:N	2.47	0.48
1:A:16:PHE:HB3	1:A:17:GLU:OE1	2.12	0.47
1:A:55:ILE:HB	1:A:56:PRO:HD3	1.96	0.47
1:B:163:PRO:HA	1:B:166:VAL:HG22	1.96	0.47
1:C:126:TYR:N	1:C:126:TYR:HD1	2.12	0.47
1:E:67:ILE:HG23	1:E:191:TRP:CD1	2.49	0.47
1:A:122:VAL:HG12	1:A:124:ALA:H	1.80	0.47
1:F:116:LEU:CD1	1:F:157:MSE:CG	2.82	0.47
1:D:211:ILE:O	1:D:217:TYR:HB3	2.14	0.47
1:B:231:LEU:O	1:B:233:LYS:N	2.46	0.47
1:F:107:LYS:C	1:F:109:LEU:N	2.64	0.47
1:B:114:LEU:HA	1:B:156:ASP:OD1	2.15	0.47
1:C:9:LEU:HB2	1:C:17:GLU:HG2	1.96	0.47
1:C:122:VAL:CG1	1:C:123:SER:N	2.77	0.47
1:F:72:ILE:HG12	1:F:82:PHE:CD1	2.50	0.47
1:A:231:LEU:HD12	1:A:231:LEU:N	2.19	0.47
1:C:58:LEU:HD23	1:C:80:VAL:HG11	1.97	0.47
1:C:89:VAL:HG12	1:C:187:GLU:HB2	1.96	0.47
1:C:126:TYR:N	1:C:126:TYR:CD1	2.82	0.47
1:D:68:SER:O	1:D:69:GLY:C	2.56	0.47
1:F:10:GLU:CD	1:F:119:LYS:HZ1	2.23	0.47
1:F:105:SER:C	1:F:107:LYS:N	2.69	0.47
1:F:172:LYS:HA	1:F:174:GLN:HE21	1.79	0.47
1:A:1:LEU:CD1	1:A:4:GLU:O	2.63	0.47
1:C:110:ASP:OD1	1:C:132:PHE:O	2.32	0.47
1:D:36:MSE:HG2	1:D:40:MSE:CE	2.39	0.47
1:A:42:VAL:CG1	1:A:43:LYS:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:CG1	1:B:90:GLY:N	2.77	0.47
1:C:26:ILE:HD12	1:C:224:TRP:HH2	1.80	0.47
1:E:119:LYS:HD3	1:E:122:VAL:HG21	1.97	0.47
1:C:65:ILE:HG13	1:C:193:ILE:CG2	2.44	0.47
1:C:40:MSE:HG3	1:C:203:TRP:CZ2	2.50	0.46
1:D:158:PHE:CZ	1:D:160:PHE:HB2	2.50	0.46
1:F:107:LYS:O	1:F:109:LEU:N	2.48	0.46
1:B:117:VAL:HG12	1:B:138:LYS:HB2	1.98	0.46
1:F:171:GLN:HG2	1:F:172:LYS:CG	2.41	0.46
1:D:230:TRP:O	1:D:232:GLU:O	2.34	0.46
1:B:105:SER:O	1:B:108:ASP:OD1	2.33	0.46
1:C:66:ILE:C	1:C:67:ILE:HG13	2.38	0.46
1:E:70:MSE:HG3	1:E:76:ARG:NH1	2.30	0.46
1:F:77:ASN:ND2	1:F:80:VAL:O	2.47	0.46
1:E:21:LYS:O	1:E:21:LYS:HG2	2.16	0.46
1:A:152:ASN:OD1	1:A:152:ASN:C	2.57	0.46
1:C:118:THR:HG23	1:C:159:ILE:HG23	1.97	0.46
1:B:60:THR:O	1:B:61:GLU:HB2	2.16	0.46
1:F:17:GLU:OE1	1:F:29:ASP:OD1	2.33	0.46
1:F:158:PHE:CE2	1:F:160:PHE:HB2	2.51	0.46
1:A:50:SER:O	1:A:51:TRP:C	2.58	0.46
1:C:49:THR:HG22	1:C:50:SER:N	2.31	0.46
1:F:116:LEU:HD12	1:F:157:MSE:O	2.16	0.46
1:A:17:GLU:OE1	1:A:68:SER:HA	2.16	0.46
1:A:89:VAL:HB	1:A:189:LEU:HD13	1.98	0.46
1:F:203:TRP:HE3	1:F:204:LEU:CD1	2.29	0.46
1:D:4:GLU:HA	1:D:42:VAL:HG13	1.97	0.45
1:E:89:VAL:CG1	1:E:90:GLY:N	2.79	0.45
1:A:19:LYS:O	1:A:20:ASP:CB	2.60	0.45
1:C:60:THR:O	1:C:61:GLU:HB2	2.16	0.45
1:C:98:GLY:O	1:C:101:LYS:HG2	2.16	0.45
1:D:91:GLN:OE1	1:D:160:PHE:CA	2.64	0.45
1:E:18:MSE:HE2	1:E:18:MSE:HB3	1.86	0.45
1:F:66:ILE:O	1:F:66:ILE:HG22	2.13	0.45
1:F:83:VAL:HG12	1:F:84:GLU:N	2.31	0.45
1:A:147:VAL:C	1:A:150:VAL:HG12	2.38	0.45
1:F:26:ILE:HD12	1:F:224:TRP:HH2	1.81	0.45
1:A:162:LEU:N	1:A:163:PRO:CD	2.80	0.45
1:D:77:ASN:O	1:D:77:ASN:ND2	2.50	0.45
1:A:232:GLU:O	1:A:233:LYS:C	2.60	0.45
1:B:36:MSE:O	1:B:40:MSE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:GLU:OE1	1:D:119:LYS:HE3	2.17	0.45
1:F:89:VAL:HG13	1:F:90:GLY:N	2.32	0.45
2:A:501:LYS:HE3	3:A:513:HOH:O	2.17	0.44
1:C:110:ASP:CG	1:C:132:PHE:O	2.60	0.44
1:E:70:MSE:CE	1:E:192:ALA:HB2	2.47	0.44
1:F:2:ARG:HG2	1:F:3:GLY:H	1.82	0.44
1:E:36:MSE:O	1:E:40:MSE:HG3	2.17	0.44
1:C:51:TRP:CH2	2:C:501:LYS:HG2	2.53	0.44
1:D:162:LEU:N	1:D:163:PRO:CD	2.80	0.44
1:A:22:LYS:HB2	1:A:24:ASN:ND2	2.33	0.44
1:B:228:THR:C	1:B:231:LEU:HD13	2.28	0.44
1:D:50:SER:OG	1:D:52:ASP:OD2	2.34	0.44
1:E:119:LYS:HA	1:E:140:TYR:O	2.17	0.44
1:B:109:LEU:O	1:B:157:MSE:HE1	2.17	0.44
1:D:76:ARG:HH22	2:D:501:LYS:C	2.26	0.44
1:D:200:PHE:O	1:D:204:LEU:HD22	2.17	0.44
1:F:164:PHE:O	1:F:168:PHE:HB2	2.17	0.44
1:A:19:LYS:O	1:A:20:ASP:HB2	2.17	0.44
1:B:152:ASN:OD1	1:B:152:ASN:C	2.60	0.44
1:C:211:ILE:HG13	1:C:217:TYR:HB2	2.00	0.44
1:D:60:THR:HG21	1:D:62:LYS:NZ	2.33	0.44
1:B:201:LEU:HD23	1:B:201:LEU:HA	1.79	0.44
1:F:203:TRP:CE3	1:F:204:LEU:CD1	3.01	0.44
1:D:56:PRO:O	1:D:60:THR:CB	2.64	0.43
1:D:122:VAL:HG13	1:D:123:SER:H	1.81	0.43
1:F:203:TRP:CE3	1:F:204:LEU:HD13	2.53	0.43
1:A:34:ARG:O	1:A:38:LYS:CD	2.63	0.43
1:A:51:TRP:CH2	2:A:501:LYS:HB3	2.52	0.43
1:B:123:SER:HG	2:B:501:LYS:HA	1.82	0.43
1:C:65:ILE:HG13	1:C:193:ILE:HG22	2.00	0.43
1:D:90:GLY:O	1:D:162:LEU:HB2	2.17	0.43
1:D:93:LEU:O	1:D:179:HIS:HD2	2.00	0.43
1:F:34:ARG:O	1:F:38:LYS:HD3	2.19	0.43
1:A:197:ASP:OD2	1:A:197:ASP:C	2.61	0.43
1:C:181:ASP:O	1:C:182:THR:C	2.62	0.43
1:E:9:LEU:CD2	1:E:17:GLU:HG2	2.47	0.43
1:E:14:LEU:HD12	1:E:18:MSE:HB3	1.99	0.43
1:C:108:ASP:O	1:C:109:LEU:CD1	2.66	0.43
1:D:27:GLY:O	1:D:30:VAL:HB	2.18	0.43
1:E:72:ILE:HG23	1:E:82:PHE:CD2	2.53	0.43
1:A:4:GLU:HA	1:A:42:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:HG13	1:A:158:PHE:CD2	2.53	0.43
1:B:176:TYR:N	1:B:176:TYR:HD2	2.17	0.43
1:E:10:GLU:OE1	2:E:501:LYS:NZ	2.47	0.43
1:F:92:SER:O	1:F:93:LEU:HD23	2.19	0.43
1:F:104:LYS:N	1:F:108:ASP:OD1	2.51	0.43
1:A:226:VAL:O	1:A:227:ASP:C	2.61	0.42
1:C:11:PRO:HA	1:C:17:GLU:HB2	2.01	0.42
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.88	0.42
1:A:3:GLY:O	1:A:43:LYS:HD2	2.19	0.42
1:A:122:VAL:CG1	1:A:123:SER:N	2.83	0.42
1:E:21:LYS:O	1:E:21:LYS:CG	2.61	0.42
1:E:92:SER:OG	1:E:162:LEU:HD12	2.19	0.42
1:F:89:VAL:HG13	1:F:90:GLY:H	1.83	0.42
1:B:187:GLU:HA	1:B:188:PRO:HD2	1.83	0.42
1:A:40:MSE:CE	1:A:200:PHE:HE1	2.32	0.42
1:A:231:LEU:H	1:A:231:LEU:CD1	2.17	0.42
1:B:40:MSE:CE	1:B:200:PHE:CE1	2.90	0.42
1:C:104:LYS:HD3	1:C:104:LYS:HA	1.68	0.42
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.63	0.42
1:D:91:GLN:OE1	1:D:160:PHE:HA	2.18	0.42
1:F:70:MSE:HE3	1:F:82:PHE:CZ	2.54	0.42
1:C:217:TYR:C	1:C:217:TYR:CD2	2.96	0.42
1:D:96:LYS:O	1:D:99:LEU:HB2	2.20	0.42
1:B:51:TRP:CH2	2:B:501:LYS:HG3	2.55	0.42
1:C:91:GLN:HG3	1:C:160:PHE:C	2.45	0.42
1:D:89:VAL:CG1	1:D:90:GLY:N	2.82	0.42
1:E:110:ASP:O	1:E:111:LYS:C	2.62	0.42
1:E:146:ALA:HB3	1:E:158:PHE:HE1	1.85	0.42
1:F:94:LEU:HA	1:F:179:HIS:HB2	2.02	0.42
1:A:20:ASP:OD1	1:A:233:LYS:NZ	2.35	0.42
1:A:65:ILE:HD11	1:A:191:TRP:HB3	2.02	0.42
1:B:16:PHE:HB3	1:B:17:GLU:OE1	2.19	0.42
1:C:207:PHE:O	1:C:207:PHE:CG	2.73	0.42
1:D:10:GLU:HA	1:D:11:PRO:HD2	1.96	0.42
1:C:87:ILE:HG23	1:C:189:LEU:CD2	2.49	0.42
1:C:161:ASP:OD2	1:C:161:ASP:N	2.51	0.42
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.89	0.42
1:B:17:GLU:OE1	1:B:29:ASP:OD1	2.38	0.42
1:B:100:GLU:OE1	1:B:100:GLU:N	2.43	0.42
1:C:107:LYS:HA	1:C:107:LYS:HD3	1.81	0.42
1:D:16:PHE:HA	1:D:28:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:GLN:HG3	1:E:172:LYS:N	2.35	0.42
1:B:154:LYS:HG2	1:B:154:LYS:H	1.70	0.41
1:B:200:PHE:CD1	1:B:204:LEU:HD22	2.54	0.41
1:D:92:SER:OG	1:D:165:ASN:OD1	2.37	0.41
1:E:5:LEU:HD22	1:E:40:MSE:HE3	2.02	0.41
1:A:5:LEU:H	1:A:42:VAL:HG11	1.85	0.41
1:A:164:PHE:CD2	1:A:164:PHE:C	2.99	0.41
1:E:119:LYS:HG2	1:E:120:PHE:N	2.34	0.41
1:A:98:GLY:O	1:A:101:LYS:HG3	2.20	0.41
1:B:51:TRP:CE3	2:B:501:LYS:HE3	2.55	0.41
1:C:96:LYS:O	1:C:99:LEU:HD23	2.21	0.41
1:D:131:LEU:HB3	1:D:132:PHE:HD1	1.86	0.41
1:C:111:LYS:HA	1:C:111:LYS:HD3	1.72	0.41
1:E:70:MSE:CE	1:E:192:ALA:CB	2.98	0.41
1:E:216:SER:O	1:E:217:TYR:C	2.63	0.41
1:C:149:GLU:O	1:C:154:LYS:N	2.53	0.41
1:D:66:ILE:CG2	1:D:70:MSE:HE2	2.46	0.41
1:D:114:LEU:HB2	1:D:157:MSE:HE2	2.02	0.41
1:E:147:VAL:HG13	1:E:158:PHE:CG	2.55	0.41
1:F:118:THR:HG23	1:F:119:LYS:N	2.34	0.41
1:A:154:LYS:H	1:A:154:LYS:HG3	1.27	0.41
1:A:193:ILE:HD11	1:A:201:LEU:HG	2.03	0.41
1:A:221:TYR:CE2	1:C:101:LYS:HB3	2.56	0.41
1:C:9:LEU:HD22	1:C:17:GLU:CG	2.50	0.41
1:A:5:LEU:N	1:A:42:VAL:CG1	2.84	0.41
1:A:148:GLN:NE2	1:A:148:GLN:CA	2.82	0.41
1:B:40:MSE:CE	1:B:200:PHE:HE1	2.09	0.41
1:C:114:LEU:HA	1:C:156:ASP:OD2	2.21	0.41
1:E:174:GLN:H	1:E:174:GLN:HE21	1.69	0.41
1:B:116:LEU:HD11	1:B:159:ILE:HB	2.02	0.41
1:A:171:GLN:HE21	1:A:171:GLN:HB2	1.63	0.41
1:A:181:ASP:OD1	1:A:182:THR:N	2.54	0.41
1:B:230:TRP:O	1:B:233:LYS:HA	2.21	0.41
1:C:211:ILE:HA	1:C:214:ASP:HB2	2.02	0.41
1:F:13:TYR:C	1:F:13:TYR:CD2	2.98	0.41
1:F:94:LEU:CD2	1:F:179:HIS:CB	2.99	0.41
1:B:83:VAL:HG12	1:B:84:GLU:H	1.86	0.41
1:C:51:TRP:HA	1:C:54:LEU:HD12	2.03	0.41
1:E:143:GLU:O	1:E:146:ALA:HB3	2.20	0.41
1:F:87:ILE:HG23	1:F:189:LEU:HD22	2.03	0.41
1:E:53:GLY:C	1:E:56:PRO:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLN:O	1:E:152:ASN:N	2.51	0.40
1:A:171:GLN:HB3	1:A:231:LEU:HD23	2.03	0.40
1:A:152:ASN:HD21	1:A:154:LYS:HD2	1.85	0.40
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.88	0.40
1:A:100:GLU:OE2	1:A:101:LYS:CE	2.69	0.40
1:B:55:ILE:HB	1:B:56:PRO:HD3	2.04	0.40
1:E:91:GLN:HE21	1:E:124:ALA:HA	1.87	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	231/245 (94%)	212 (92%)	19 (8%)	0	100	100
1	B	231/245 (94%)	216 (94%)	15 (6%)	0	100	100
1	C	231/245 (94%)	217 (94%)	14 (6%)	0	100	100
1	D	231/245 (94%)	217 (94%)	14 (6%)	0	100	100
1	E	232/245 (95%)	217 (94%)	15 (6%)	0	100	100
1	F	231/245 (94%)	216 (94%)	14 (6%)	1 (0%)	30	49
All	All	1387/1470 (94%)	1295 (93%)	91 (7%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	108	ASP

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	200/204 (98%)	165 (82%)	35 (18%)	2	3
1	B	200/204 (98%)	161 (80%)	39 (20%)	1	2
1	C	200/204 (98%)	161 (80%)	39 (20%)	1	2
1	D	200/204 (98%)	163 (82%)	37 (18%)	1	2
1	E	201/204 (98%)	166 (83%)	35 (17%)	2	3
1	F	200/204 (98%)	152 (76%)	48 (24%)	1	1
All	All	1201/1224 (98%)	968 (81%)	233 (19%)	1	2

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	18	MSE
1	A	20	ASP
1	A	32	LEU
1	A	38	LYS
1	A	42	VAL
1	A	62	LYS
1	A	77	ASN
1	A	89	VAL
1	A	91	GLN
1	A	96	LYS
1	A	97	LYS
1	A	103	VAL
1	A	105	SER
1	A	113	GLU
1	A	118	THR
1	A	122	VAL
1	A	131	LEU
1	A	137	LEU
1	A	147	VAL
1	A	148	GLN
1	A	149	GLU

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Mol	Chain	Res	Type
1	A	154	LYS
1	A	156	ASP
1	A	166	VAL
1	A	171	GLN
1	A	174	GLN
1	A	176	TYR
1	A	177	LEU
1	A	204	LEU
1	A	210	GLN
1	A	216	SER
1	A	222	GLU
1	A	223	ARG
1	A	231	LEU
1	B	1	LEU
1	B	2	ARG
1	B	18	MSE
1	B	19	LYS
1	B	21	LYS
1	B	24	ASN
1	B	38	LYS
1	B	40	MSE
1	B	42	VAL
1	B	43	LYS
1	B	55	ILE
1	B	62	LYS
1	B	86	TYR
1	B	95	VAL
1	B	96	LYS
1	B	97	LYS
1	B	99	LEU
1	B	103	VAL
1	B	108	ASP
1	B	113	GLU
1	B	118	THR
1	B	122	VAL
1	B	131	LEU
1	B	156	ASP
1	B	174	GLN
1	B	176	TYR
1	B	177	LEU
1	B	189	LEU
1	B	194	LYS

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Mol	Chain	Res	Type
1	B	204	LEU
1	B	214	ASP
1	B	216	SER
1	B	219	GLU
1	B	222	GLU
1	B	223	ARG
1	B	226	VAL
1	B	231	LEU
1	B	232	GLU
1	B	233	LYS
1	C	2	ARG
1	C	9	LEU
1	C	14	LEU
1	C	18	MSE
1	C	25	VAL
1	C	32	LEU
1	C	34	ARG
1	C	42	VAL
1	C	50	SER
1	C	62	LYS
1	C	65	ILE
1	C	68	SER
1	C	89	VAL
1	C	96	LYS
1	C	97	LYS
1	C	99	LEU
1	C	100	GLU
1	C	107	LYS
1	C	109	LEU
1	C	113	GLU
1	C	118	THR
1	C	122	VAL
1	C	126	TYR
1	C	131	LEU
1	C	133	LYS
1	C	147	VAL
1	C	150	VAL
1	C	166	VAL
1	C	177	LEU
1	C	178	VAL
1	C	183	SER
1	C	189	LEU

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Mol	Chain	Res	Type
1	C	194	LYS
1	C	204	LEU
1	C	216	SER
1	C	226	VAL
1	C	231	LEU
1	C	232	GLU
1	C	233	LYS
1	D	9	LEU
1	D	14	LEU
1	D	17	GLU
1	D	18	MSE
1	D	19	LYS
1	D	25	VAL
1	D	32	LEU
1	D	50	SER
1	D	60	THR
1	D	68	SER
1	D	80	VAL
1	D	89	VAL
1	D	91	GLN
1	D	93	LEU
1	D	96	LYS
1	D	99	LEU
1	D	104	LYS
1	D	105	SER
1	D	108	ASP
1	D	109	LEU
1	D	114	LEU
1	D	122	VAL
1	D	123	SER
1	D	131	LEU
1	D	133	LYS
1	D	137	LEU
1	D	150	VAL
1	D	166	VAL
1	D	174	GLN
1	D	177	LEU
1	D	178	VAL
1	D	180	LEU
1	D	189	LEU
1	D	204	LEU
1	D	219	GLU

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Mol	Chain	Res	Type
1	D	223	ARG
1	D	227	ASP
1	E	1	LEU
1	E	9	LEU
1	E	14	LEU
1	E	18	MSE
1	E	21	LYS
1	E	25	VAL
1	E	32	LEU
1	E	38	LYS
1	E	42	VAL
1	E	60	THR
1	E	63	PHE
1	E	68	SER
1	E	89	VAL
1	E	91	GLN
1	E	92	SER
1	E	96	LYS
1	E	103	VAL
1	E	109	LEU
1	E	110	ASP
1	E	115	THR
1	E	116	LEU
1	E	122	VAL
1	E	123	SER
1	E	125	GLU
1	E	131	LEU
1	E	147	VAL
1	E	150	VAL
1	E	166	VAL
1	E	174	GLN
1	E	189	LEU
1	E	204	LEU
1	E	210	GLN
1	E	222	GLU
1	E	228	THR
1	E	233	LYS
1	F	1	LEU
1	F	14	LEU
1	F	18	MSE
1	F	25	VAL
1	F	32	LEU

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Mol	Chain	Res	Type
1	F	34	ARG
1	F	38	LYS
1	F	42	VAL
1	F	62	LYS
1	F	63	PHE
1	F	66	ILE
1	F	67	ILE
1	F	71	THR
1	F	77	ASN
1	F	89	VAL
1	F	91	GLN
1	F	99	LEU
1	F	100	GLU
1	F	101	LYS
1	F	105	SER
1	F	113	GLU
1	F	114	LEU
1	F	117	VAL
1	F	118	THR
1	F	122	VAL
1	F	123	SER
1	F	130	ARG
1	F	147	VAL
1	F	148	GLN
1	F	154	LYS
1	F	157	MSE
1	F	169	MSE
1	F	172	LYS
1	F	174	GLN
1	F	177	LEU
1	F	179	HIS
1	F	181	ASP
1	F	189	LEU
1	F	194	LYS
1	F	204	LEU
1	F	216	SER
1	F	219	GLU
1	F	222	GLU
1	F	223	ARG
1	F	227	ASP
1	F	228	THR
1	F	231	LEU

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Mol	Chain	Res	Type
1	F	232	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	91	GLN
1	A	148	GLN
1	A	165	ASN
1	A	171	GLN
1	A	179	HIS
1	A	210	GLN
1	B	77	ASN
1	B	81	ASN
1	B	165	ASN
1	C	24	ASN
1	D	77	ASN
1	D	152	ASN
1	D	165	ASN
1	D	174	GLN
1	E	81	ASN
1	E	165	ASN
1	E	171	GLN
1	E	206	HIS
1	E	210	GLN
1	F	77	ASN
1	F	148	GLN
1	F	206	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LYS	B	501	-	8,9,9	1.01	1 (12%)	7,10,10	1.46	1 (14%)
2	LYS	E	501	-	8,9,9	0.91	1 (12%)	7,10,10	0.93	1 (14%)
2	LYS	F	501	-	8,9,9	0.95	1 (12%)	7,10,10	1.25	1 (14%)
2	LYS	C	501	-	8,9,9	0.87	0	7,10,10	1.04	0
2	LYS	D	501	-	8,9,9	0.97	1 (12%)	7,10,10	1.38	1 (14%)
2	LYS	A	501	-	8,9,9	0.84	1 (12%)	7,10,10	1.41	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	B	501	-	-	2/9/9/9	-
2	LYS	E	501	-	-	1/9/9/9	-
2	LYS	F	501	-	-	0/9/9/9	-
2	LYS	C	501	-	-	3/9/9/9	-
2	LYS	D	501	-	-	2/9/9/9	-
2	LYS	A	501	-	-	6/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LYS	OXT-C	-2.76	1.21	1.30
2	D	501	LYS	OXT-C	-2.42	1.22	1.30
2	E	501	LYS	OXT-C	-2.29	1.23	1.30
2	F	501	LYS	OXT-C	-2.21	1.23	1.30
2	A	501	LYS	OXT-C	-2.03	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LYS	OXT-C-O	-3.44	116.27	124.08
2	D	501	LYS	OXT-C-O	-3.22	116.78	124.08
2	B	501	LYS	OXT-C-O	-3.18	116.87	124.08
2	F	501	LYS	OXT-C-O	-3.07	117.12	124.08
2	E	501	LYS	OXT-C-O	-2.21	119.06	124.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LYS	N-CA-CB-CG
2	A	501	LYS	C-CA-CB-CG
2	C	501	LYS	N-CA-CB-CG
2	C	501	LYS	C-CA-CB-CG
2	D	501	LYS	C-CA-CB-CG
2	A	501	LYS	CE-CD-CG-CB
2	A	501	LYS	CA-CB-CG-CD
2	B	501	LYS	O-C-CA-CB
2	D	501	LYS	N-CA-CB-CG
2	B	501	LYS	OXT-C-CA-CB
2	C	501	LYS	CE-CD-CG-CB
2	A	501	LYS	O-C-CA-N
2	A	501	LYS	OXT-C-CA-N
2	E	501	LYS	CA-CB-CG-CD

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	LYS	6	0
2	E	501	LYS	1	0
2	F	501	LYS	1	0
2	C	501	LYS	1	0
2	D	501	LYS	6	0
2	A	501	LYS	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/245 (92%)	-0.23	2 (0%) 81 78	10, 27, 45, 62	0
1	B	227/245 (92%)	-0.29	2 (0%) 81 78	13, 30, 50, 72	0
1	C	227/245 (92%)	-0.30	0 100 100	15, 30, 50, 67	0
1	D	227/245 (92%)	-0.25	2 (0%) 81 78	15, 36, 53, 63	0
1	E	228/245 (93%)	-0.27	3 (1%) 75 71	6, 25, 46, 65	0
1	F	227/245 (92%)	-0.07	5 (2%) 62 57	13, 32, 62, 70	0
All	All	1363/1470 (92%)	-0.24	14 (1%) 79 76	6, 30, 53, 72	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	0	SER	3.8
1	F	173	GLY	3.1
1	F	1	LEU	2.9
1	D	1	LEU	2.8
1	B	1	LEU	2.4
1	F	3	GLY	2.4
1	E	1	LEU	2.3
1	F	103	VAL	2.2
1	A	176	TYR	2.1
1	F	95	VAL	2.1
1	E	233	LYS	2.1
1	D	2	ARG	2.0
1	A	114	LEU	2.0
1	B	173	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LYS	F	501	10/10	0.93	0.07	24,24,26,27	0
2	LYS	A	501	10/10	0.94	0.07	21,23,24,25	0
2	LYS	C	501	10/10	0.95	0.07	25,33,33,34	0
2	LYS	D	501	10/10	0.95	0.08	29,36,37,37	0
2	LYS	B	501	10/10	0.95	0.07	22,26,28,28	0
2	LYS	E	501	10/10	0.96	0.11	24,30,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.