



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:39 PM EDT

PDB ID : 3K4U  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

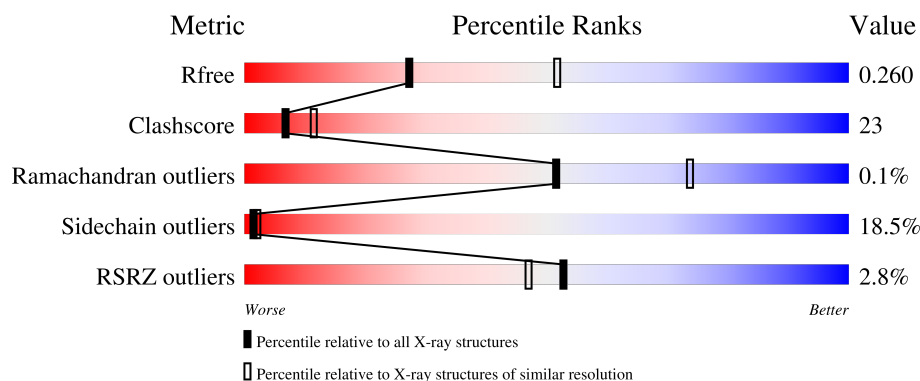
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>35%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	245	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	245	<div> <div>0%</div> <div> <div></div> <div>54%</div> <div>31%</div> <div>10%</div> <div>5%</div> </div> </div>
1	D	245	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>7%</div> <div>5%</div> </div> </div>
1	E	245	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>7%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	245	<div><div></div><div>3%</div><div>48%</div><div>35%</div><div>11%</div><div>5%</div></div>

## 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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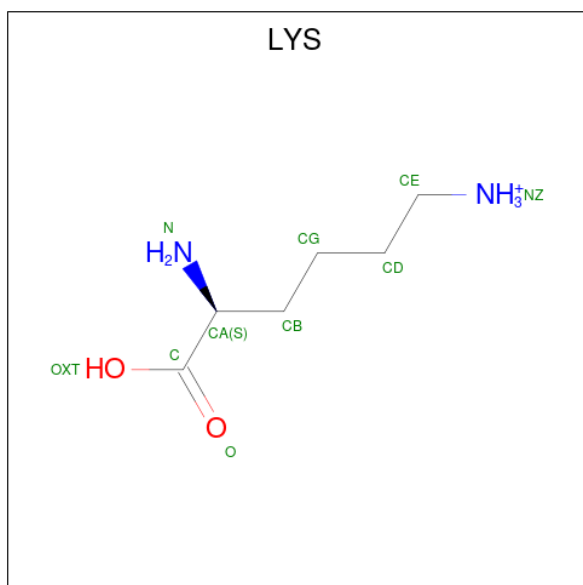
Chain	Residue	Modelled	Actual	Comment	Reference
B	239	HIS	-	expression tag	UNP Q7MAG0
B	240	HIS	-	expression tag	UNP Q7MAG0
B	241	HIS	-	expression tag	UNP Q7MAG0
B	242	HIS	-	expression tag	UNP Q7MAG0
B	243	HIS	-	expression tag	UNP Q7MAG0
C	-1	MSE	-	expression tag	UNP Q7MAG0
C	0	SER	-	expression tag	UNP 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 (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



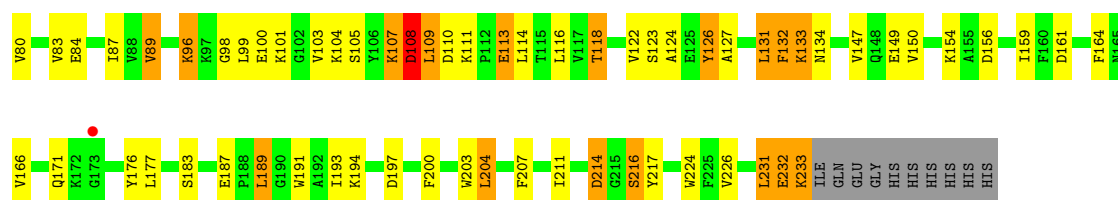
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		
2	E	1	Total	C	N	O	0	0
			10	6	2	2		
2	F	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is water.

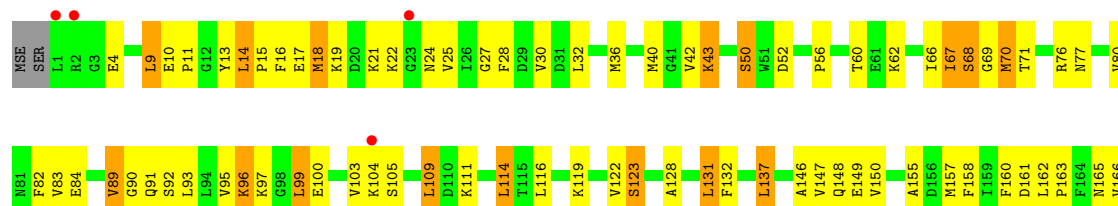
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	19	Total 19	O 19	0	0
3	C	19	Total 19	O 19	0	0
3	D	17	Total 17	O 17	0	0
3	E	22	Total 22	O 22	0	0
3	F	17	Total 17	O 17	0	0



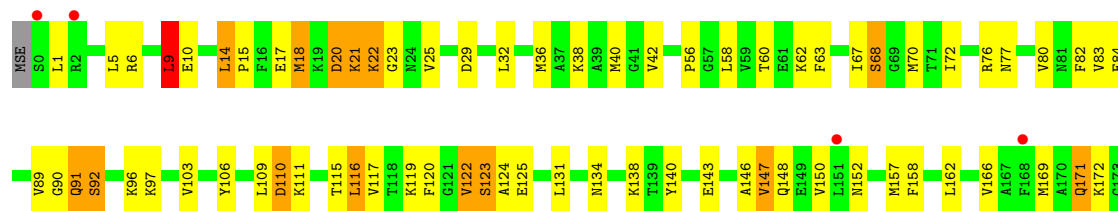




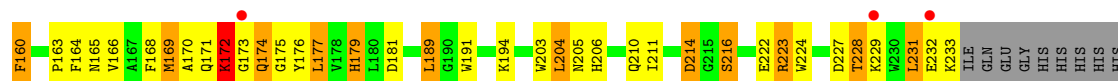
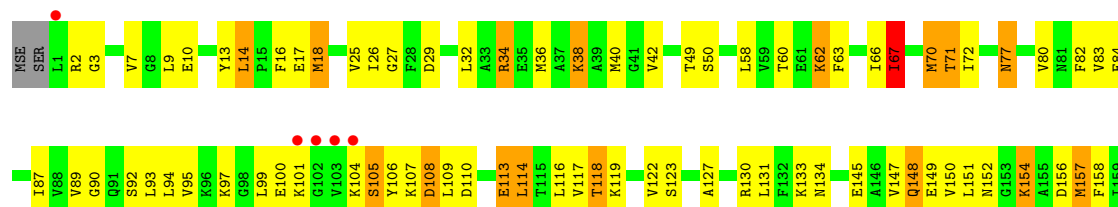
• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.41Å 149.15Å 81.97Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 42.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.6 (20.00-2.62) 99.5 (42.32-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.01	2/1909 (0.1%)	0.94	4/2566 (0.2%)
1	B	0.84	1/1909 (0.1%)	0.87	1/2566 (0.0%)
1	C	0.95	2/1909 (0.1%)	0.86	2/2566 (0.1%)
1	D	0.77	2/1909 (0.1%)	0.83	2/2566 (0.1%)
1	E	0.82	1/1915 (0.1%)	0.84	3/2574 (0.1%)
1	F	0.97	2/1909 (0.1%)	0.93	4/2566 (0.2%)
All	All	0.90	10/11460 (0.1%)	0.88	16/15404 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	TYR	CD1-CE1	-6.84	1.29	1.39
1	A	13	TYR	CD2-CE2	-5.86	1.30	1.39
1	C	132	PHE	CD1-CE1	-5.75	1.27	1.39
1	C	108	ASP	CB-CG	-5.22	1.40	1.51
1	D	70	MSE	CG-SE	-5.21	1.77	1.95
1	B	226	VAL	CB-CG1	-5.20	1.42	1.52
1	E	20	ASP	CB-CG	-5.19	1.40	1.51
1	F	70	MSE	CG-SE	-5.13	1.78	1.95
1	F	67	ILE	CA-CB	-5.04	1.43	1.54
1	D	67	ILE	CA-CB	-5.00	1.43	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	231	LEU	CB-CG-CD2	-7.63	98.03	111.00
1	A	176	TYR	N-CA-C	6.58	128.76	111.00
1	B	214	ASP	CB-CA-C	-5.88	98.63	110.40
1	C	116	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	156	ASP	N-CA-C	5.68	126.33	111.00
1	F	231	LEU	CA-CB-CG	-5.41	102.86	115.30
1	E	232	GLU	N-CA-C	-5.40	96.42	111.00
1	E	22	LYS	N-CA-C	-5.26	96.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	9	LEU	CA-CB-CG	5.24	127.35	115.30
1	C	108	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	D	204	LEU	CA-CB-CG	5.16	127.17	115.30
1	E	9	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	153	GLY	N-CA-C	5.05	125.74	113.10
1	F	172	LYS	C-N-CA	-5.04	111.71	122.30
1	D	76	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	19	LYS	CB-CA-C	-5.00	100.39	110.40

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	114	0
1	B	1872	0	1903	61	0
1	C	1872	0	1903	91	0
1	D	1872	0	1903	76	0
1	E	1878	0	1908	63	0
1	F	1872	0	1903	128	0
2	A	10	0	12	2	0
2	B	10	0	12	5	0
2	C	10	0	12	1	0
2	D	10	0	12	5	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	530	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 23.

All (530) 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
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: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	1.04
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:F:171:GLN:C	1:F:172:LYS:HG3	1.75	1.01
1:E:21:LYS:C	1:E:21:LYS:CD	2.28	0.96
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:E:21:LYS:HD2	1:E:21:LYS:C	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:83:VAL:HG12	1:C:84:GLU:N	1.94	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: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: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:148:GLN:NE2	1:F:148:GLN:HA	2.02	0.72
1:F:223:ARG:O	1:F:223:ARG:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:156:ASP:OD1	1:A:156:ASP:C	2.30	0.70
1:C:40:MSE:HE1	1:C:200:PHE:CE1	2.25	0.70
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:D:174:GLN:HA	1:D:174:GLN:NE2	2.07	0.69
1:C:36:MSE:HE3	1:C:204:LEU:HD11	1.76	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:F:231:LEU:HD23	1:F:231:LEU:C	2.14	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: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:C:87:ILE:HG23	1:C:189:LEU:HD22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ASP:OD2	1:E:22:LYS:N	2.30	0.65
1:E:232:GLU:O	1:E:233:LYS:C	2.35	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: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:18:MSE:HE3	1:F:26:ILE:O	1.98	0.63
1:F:173:GLY:O	1:F:174:GLN:C	2.34	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: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:E:70:MSE:HE1	1:E:192:ALA:CB	2.30	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:B:231:LEU:O	1:B:232:GLU:C	2.33	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:A:13:TYR:OH	1:A:161:ASP:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:SER:HB2	2:D:501:LYS:C	2.21	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:D:91:GLN:OE1	1:D:160:PHE:C	2.39	0.60
1:F:60:THR:CG2	1:F:62:LYS:HE3	2.31	0.60
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:F:169:MSE:O	1:F:170:ALA:C	2.37	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: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:F:17:GLU:C	1:F:18:MSE:HE2	2.23	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: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: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:169:MSE:C	1:F:173:GLY:H	2.07	0.57
1:F:107:LYS:C	1:F:109:LEU:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:GLU:O	1:E:233:LYS:O	2.23	0.56
1:F:105:SER:C	1:F:107:LYS:H	2.06	0.56
1:F:214:ASP:HB3	1:F:216:SER:H	1.70	0.56
1:C:108:ASP:OD1	1:C:108:ASP:N	2.30	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:B:231:LEU:C	1:B:233:LYS:N	2.53	0.56
1:D:80:VAL:CG2	1:D:192:ALA:HB1	2.37	0.55
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: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: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:A:174:GLN:CD	1:A:174:GLN:H	1.97	0.54
1:F:150:VAL:HG11	1:F:177:LEU:HD21	1.89	0.54
1:D:15:PRO:C	1:D:18:MSE:HE1	2.28	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: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:155:ALA:O	1:A:156:ASP:CG	2.47	0.53
1:F:106:TYR:CD2	1:F:106:TYR:C	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:171:GLN:HG3	1:A:172:LYS:H	1.76	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:F:66:ILE:C	1:F:67:ILE:HG12	2.30	0.51
1:A:156:ASP:OD1	1:A:156:ASP:O	2.29	0.50
1:C:105:SER:O	1:C:108:ASP:OD1	2.29	0.50
1:B:96:LYS:HD3	1:B:97:LYS:N	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:O	1:D:148:GLN:C	2.47	0.50
1:E:96:LYS:HD3	1:E:97:LYS:H	1.77	0.50
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: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: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: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:211:ILE:HA	1:A:214:ASP:HB2	1.94	0.49
1:C:50:SER:O	1:C:51:TRP:C	2.50	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:17:GLU:C	1:A:18:MSE:HE3	2.33	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:F:107:LYS:C	1:F:109:LEU:N	2.64	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:100:GLU:C	1:A:103:VAL:HG13	2.33	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:F:170:ALA:O	1:F:171:GLN:C	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG13	1:A:43:LYS:N	2.29	0.48
1:B:228:THR:C	1:B:231:LEU:CD1	2.81	0.48
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:C:15:PRO:C	1:C:18:MSE:HE1	2.34	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:A:83:VAL:HG12	1:A:84:GLU:N	2.29	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: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:A:231:LEU:C	1:A:233:LYS:H	2.18	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: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:A:19:LYS:O	1:A:20:ASP:CB	2.60	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
1:B:89:VAL:CG1	1:B:90:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:LEU:HD23	1:F:99:LEU:C	2.35	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: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: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:C:110:ASP:OD1	1:C:132:PHE:C	2.55	0.46
1:C:49:THR:HG22	1:C:50:SER:N	2.31	0.46
1:C:132:PHE:C	1:C:133:LYS:HG2	2.28	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:C:232:GLU:O	1:C:233:LYS:C	2.54	0.45
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: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:F:105:SER:C	1:F:107:LYS:N	2.69	0.45
1:B:29:ASP:CG	1:B:67:ILE:HG22	2.37	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:E:20:ASP:OD2	1:E:20:ASP:C	2.48	0.45
1:E:83:VAL:O	1:E:84:GLU:C	2.55	0.45
1:F:83:VAL:HG12	1:F:84:GLU:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:MSE:O	1:B:40:MSE:HB2	2.17	0.45
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: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: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: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: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: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: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:E:219:GLU:O	1:E:220:LEU:C	2.56	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:E:122:VAL:O	1:E:123:SER:C	2.57	0.43
1:A:4:GLU:HA	1:A:42:VAL:HG13	2.01	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:GLU:OE1	2:E:501:LYS:NZ	2.47	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:10:GLU:CD	1:F:119:LYS:HZ1	2.23	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:68:SER:O	1:D:69:GLY:C	2.56	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:D:96:LYS:O	1:D:99:LEU:HB2	2.20	0.42
1:A:152:ASN:OD1	1:A:152:ASN:C	2.57	0.42
1:B:51:TRP:CH2	2:B:501:LYS:HG3	2.55	0.42
1:D:89:VAL:CG1	1:D:90:GLY:N	2.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:H	1:A:42:VAL:HG11	1.85	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:A:50:SER:O	1:A:51:TRP:C	2.58	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: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: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:C:66:ILE:C	1:C:67:ILE:HG13	2.38	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: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%)	34	55
All	All	1387/1470 (94%)	1295 (93%)	91 (7%)	1 (0%)	51	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	108	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/204 (98%)	161 (80%)	39 (20%)	1	2
1	B	200/204 (98%)	166 (83%)	34 (17%)	2	3
1	C	200/204 (98%)	162 (81%)	38 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	200/204 (98%)	168 (84%)	32 (16%)	2	3
1	E	201/204 (98%)	166 (83%)	35 (17%)	2	2
1	F	200/204 (98%)	157 (78%)	43 (22%)	1	1
All	All	1201/1224 (98%)	980 (82%)	221 (18%)	1	2

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	9	LEU
1	A	13	TYR
1	A	18	MSE
1	A	20	ASP
1	A	32	LEU
1	A	38	LYS
1	A	42	VAL
1	A	43	LYS
1	A	62	LYS
1	A	70	MSE
1	A	77	ASN
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	131	LEU
1	A	134	ASN
1	A	137	LEU
1	A	147	VAL
1	A	148	GLN
1	A	149	GLU
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	179	HIS

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Mol	Chain	Res	Type
1	A	181	ASP
1	A	204	LEU
1	A	210	GLN
1	A	216	SER
1	A	222	GLU
1	A	223	ARG
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	34	ARG
1	B	38	LYS
1	B	42	VAL
1	B	43	LYS
1	B	62	LYS
1	B	77	ASN
1	B	86	TYR
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	174	GLN
1	B	176	TYR
1	B	177	LEU
1	B	189	LEU
1	B	204	LEU
1	B	214	ASP
1	B	216	SER
1	B	222	GLU
1	B	223	ARG
1	B	231	LEU
1	B	232	GLU
1	B	233	LYS
1	C	2	ARG
1	C	9	LEU

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Mol	Chain	Res	Type
1	C	13	TYR
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	62	LYS
1	C	63	PHE
1	C	68	SER
1	C	77	ASN
1	C	89	VAL
1	C	96	LYS
1	C	107	LYS
1	C	108	ASP
1	C	109	LEU
1	C	113	GLU
1	C	118	THR
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	176	TYR
1	C	177	LEU
1	C	183	SER
1	C	189	LEU
1	C	194	LYS
1	C	204	LEU
1	C	214	ASP
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	13	TYR
1	D	14	LEU
1	D	18	MSE
1	D	19	LYS
1	D	25	VAL

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Mol	Chain	Res	Type
1	D	32	LEU
1	D	43	LYS
1	D	50	SER
1	D	68	SER
1	D	89	VAL
1	D	96	LYS
1	D	99	LEU
1	D	104	LYS
1	D	105	SER
1	D	109	LEU
1	D	114	LEU
1	D	123	SER
1	D	131	LEU
1	D	137	LEU
1	D	150	VAL
1	D	161	ASP
1	D	166	VAL
1	D	174	GLN
1	D	177	LEU
1	D	180	LEU
1	D	189	LEU
1	D	200	PHE
1	D	204	LEU
1	D	219	GLU
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	63	PHE
1	E	68	SER
1	E	77	ASN
1	E	91	GLN
1	E	92	SER
1	E	103	VAL
1	E	106	TYR

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Mol	Chain	Res	Type
1	E	109	LEU
1	E	110	ASP
1	E	111	LYS
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	171	GLN
1	E	174	GLN
1	E	189	LEU
1	E	204	LEU
1	E	210	GLN
1	E	228	THR
1	E	233	LYS
1	F	14	LEU
1	F	18	MSE
1	F	25	VAL
1	F	32	LEU
1	F	34	ARG
1	F	38	LYS
1	F	42	VAL
1	F	62	LYS
1	F	63	PHE
1	F	67	ILE
1	F	71	THR
1	F	77	ASN
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

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Mol	Chain	Res	Type
1	F	148	GLN
1	F	154	LYS
1	F	156	ASP
1	F	157	MSE
1	F	160	PHE
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	214	ASP
1	F	216	SER
1	F	222	GLU
1	F	223	ARG
1	F	227	ASP
1	F	228	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	148	GLN
1	A	165	ASN
1	A	171	GLN
1	A	179	HIS
1	A	210	GLN
1	C	24	ASN
1	D	77	ASN
1	D	152	ASN
1	D	165	ASN
1	D	174	GLN
1	E	171	GLN
1	E	174	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 monosaccharides 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	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%)
2	LYS	C	501	-	8,9,9	0.87	0	7,10,10	1.04	0
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%)

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	D	501	-	-	2/9/9/9	-
2	LYS	A	501	-	-	6/9/9/9	-

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

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 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	LYS	5	0
2	A	501	LYS	2	0
2	C	501	LYS	1	0
2	B	501	LYS	5	0
2	E	501	LYS	1	0
2	F	501	LYS	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/245 (92%)	0.08	6 (2%) 56 50	10, 27, 45, 62	0
1	B	227/245 (92%)	0.12	10 (4%) 34 28	13, 30, 50, 72	0
1	C	227/245 (92%)	0.01	3 (1%) 77 73	15, 30, 50, 67	0
1	D	227/245 (92%)	0.05	4 (1%) 68 64	15, 36, 53, 63	0
1	E	228/245 (93%)	0.03	7 (3%) 49 42	6, 25, 46, 65	0
1	F	227/245 (92%)	0.14	8 (3%) 44 37	13, 32, 62, 70	0
All	All	1363/1470 (92%)	0.07	38 (2%) 53 47	6, 30, 53, 72	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	LEU	4.1
1	D	2	ARG	4.1
1	B	174	GLN	3.8
1	F	232	GLU	3.5
1	F	1	LEU	3.4
1	B	228	THR	3.4
1	F	101	LYS	3.3
1	A	1	LEU	3.3
1	A	114	LEU	3.0
1	B	115	THR	3.0
1	E	232	GLU	2.9
1	E	177	LEU	2.9
1	E	0	SER	2.9
1	C	3	GLY	2.9
1	A	147	VAL	2.8
1	F	104	LYS	2.8
1	B	173	GLY	2.8
1	E	168	PHE	2.7
1	E	2	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	2	ARG	2.5
1	E	151	LEU	2.4
1	B	155	ALA	2.4
1	F	229	LYS	2.4
1	B	25	VAL	2.3
1	F	102	GLY	2.3
1	F	173	GLY	2.3
1	B	138	LYS	2.3
1	D	23	GLY	2.2
1	D	104	LYS	2.2
1	C	173	GLY	2.2
1	A	232	GLU	2.2
1	B	147	VAL	2.2
1	B	150	VAL	2.1
1	E	176	TYR	2.1
1	A	176	TYR	2.1
1	F	103	VAL	2.0
1	C	23	GLY	2.0
1	A	26	ILE	2.0

## 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 monosaccharides 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, 95<sup>th</sup> 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	0.94	0.20	24,24,26,27	0
2	LYS	A	501	10/10	0.95	0.20	21,23,24,25	0
2	LYS	C	501	10/10	0.96	0.18	25,33,33,34	0
2	LYS	B	501	10/10	0.96	0.17	22,26,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LYS	E	501	10/10	0.97	0.18	24,30,30,31	0
2	LYS	D	501	10/10	0.97	0.20	29,36,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.