



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

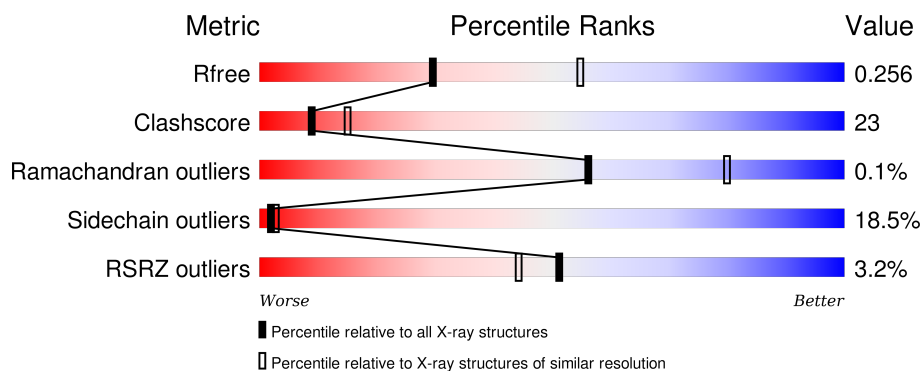
1 Overall quality at a glance

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}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	245	
1	C	245	
1	D	245	
1	E	245	

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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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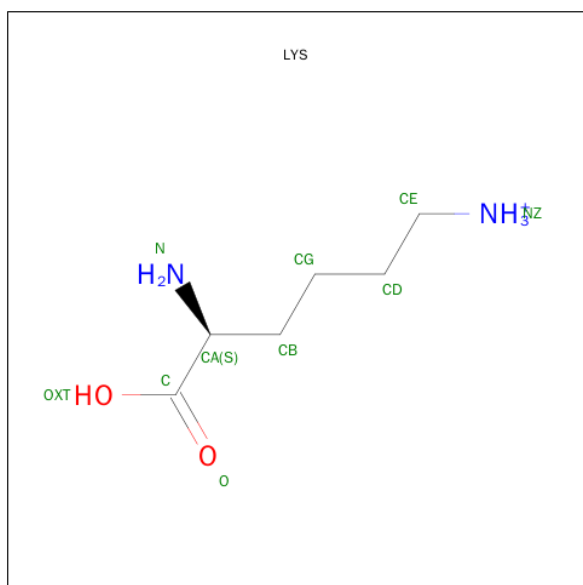
Chain	Residue	Modelled	Actual	Comment	Reference
B	239	HIS	-	expression tag	UNP Q7MAG0
B	240	HIS	-	expression tag	UNP Q7MAG0
B	241	HIS	-	expression tag	UNP Q7MAG0
B	242	HIS	-	expression tag	UNP Q7MAG0
B	243	HIS	-	expression tag	UNP Q7MAG0
C	-1	MSE	-	expression tag	UNP Q7MAG0
C	0	SER	-	expression tag	UNP 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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Chain A:

2% 49% 35% 10% 5%

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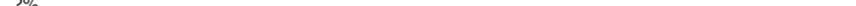
MSE SER L1 R2 G3 E4 L5 L9 E10 Y13 L14 P15 F16 E17 M18 K19 D20 K21 K22 G23 G24 Y25 I26 D29 L32 A33 R34 K38 A39 M40 G41 V42 K43 T49 S50 W51 L54 I55 P56 G57 L58 V59 T60 E61 K62 I65 I66 I67 S68 G69 M70 F71

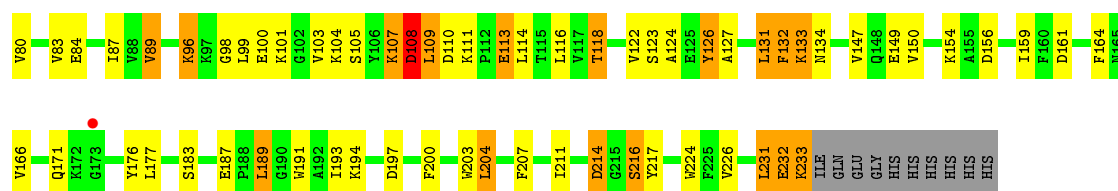
T72 N77 L78 R79 W80 M81 F82 G83 E84 V88 V89 G90 Q91 K96 K97 G98 L99 L100 K101 G102 V103 K104 S105 L109 E113 L114 T118 K119 V122 S123 A124 A128 L131 M134 L137 T142 E143 V147 Q148 E149 V150 L151 M152 G153 K154 A155 F156

M157 F158 D161 L162 P163 F164 M165 V166 M169 A170 Q171 K172 G173 Q174 G175 Y176 L177 V178 H179 L180 D181 T182 Y186 E187 P188 L189 G190 W191 A192 I193 K194 K195 F200 L201 L204 Q210 I211 D214 G215 S216 Y221 E222 R223 K229 E230 L231 E232 K233 ILE GLN

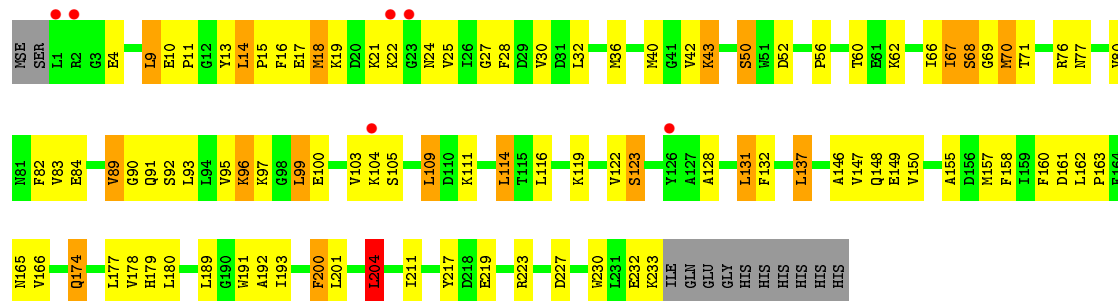
Chain B:

Category	Percentage
Green	59%
Yellow	31%
Orange	4%
Grey	5%

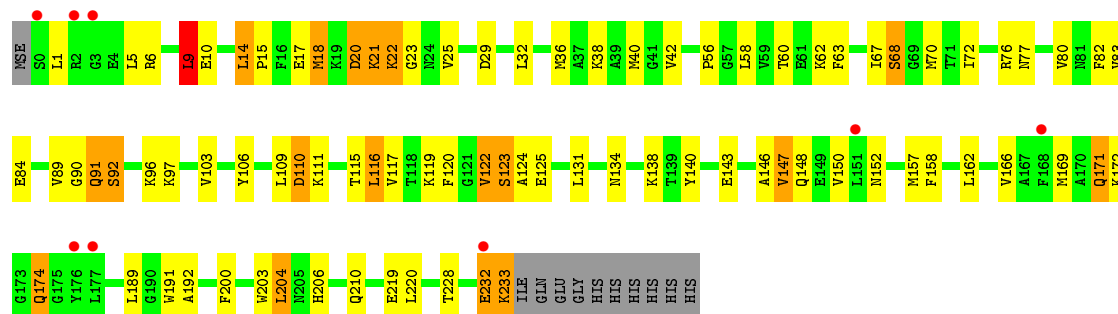
Chain C: 



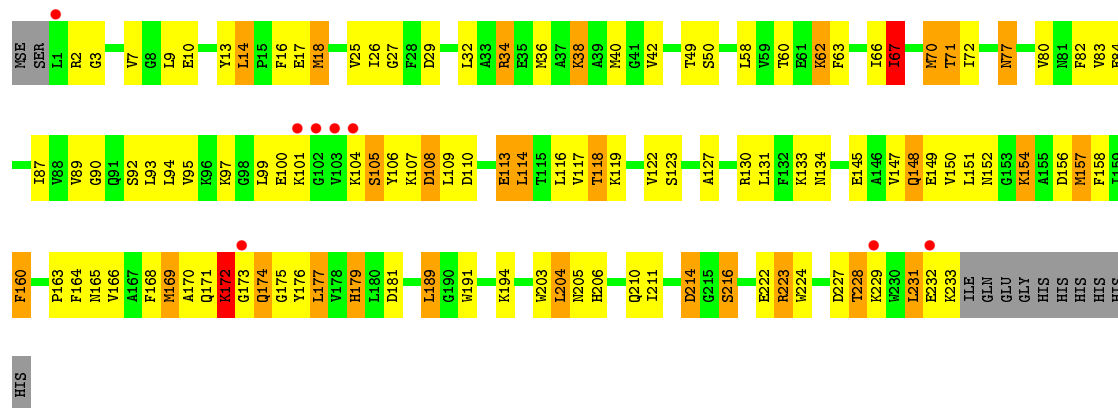
• Molecule 1: BINDING COMPONENT OF ABC TRANSPORTER



• 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 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
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.202 , 0.266 0.196 , 0.256	Depositor DCC
R_{free} test set	2657 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.6	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 51313 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:N	1:B:231:LEU:HD12	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:E:20:ASP:O	1:E:21:LYS:HB3	1.47	1.08
1:B:231:LEU:CD1	1:B:231:LEU:H	1.59	1.08
1:C:34:ARG:HH11	1:C:34:ARG:HG3	0.94	1.07
1:E:233:LYS:H	1:E:233:LYS:HD3	1.18	1.06
1:E:17:GLU:OE1	1:E:68:SER:HA	1.55	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:H	1:B:231:LEU:HD12	0.79	0.96
1:F:174:GLN:OE1	1:F:174:GLN:HA	1.63	0.96
1:B:40:MSE:HE1	1:B:200:PHE:CE1	2.01	0.95
1:E:21:LYS:C	1:E:21:LYS:HD2	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:C:118:THR:HG23	1:C:159:ILE:O	1.70	0.90
1:A:147:VAL:O	1:A:150:VAL:HG12	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:F:169:MSE:HA	1:F:173:GLY:N	1.87	0.89
1:D:21:LYS:HG2	1:D:233:LYS:HB2	1.54	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:HD3	1:C:233:LYS:H	1.42	0.84
1:F:97:LYS:HB2	1:F:176:TYR:O	1.77	0.84
1:F:95:VAL:HG12	1:F:157:MSE:HB2	1.59	0.84
1:F:60:THR:HG21	1:F:62:LYS:HE3	1.60	0.84
1:F:116:LEU:CD1	1:F:157:MSE:HG2	2.07	0.84
1:F:116:LEU:HD13	1:F:157:MSE:CG	2.07	0.84
1:B:60:THR:HG21	1:B:62:LYS:HE3	1.60	0.83
1:A:148:GLN:HA	1:A:148:GLN:HE21	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:N	1:F:38:LYS:HD2	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:E:21:LYS:CD	1:E:22:LYS:N	2.39	0.79
1:B:228:THR:O	1:B:231:LEU:CD1	2.30	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:F:171:GLN:CG	1:F:172:LYS:HD3	2.09	0.75
1:E:233:LYS:N	1:E:233:LYS:HD3	1.96	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:F:148:GLN:HA	1:F:148:GLN:NE2	2.02	0.72
1:D:71:THR:OG1	2:D:501:LYS:N	2.22	0.72
1:A:34:ARG:O	1:A:38:LYS:HD2	1.89	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:89:VAL:HG13	1:A:90:GLY:H	1.54	0.72
1:A:57:GLY:O	1:A:62:LYS:HB2	1.89	0.72
1:B:70:MSE:HE3	1:B:82:PHE:CE1	2.25	0.72
1:A:169:MSE:O	1:A:174:GLN:HG3	1.89	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:99:LEU:O	1:F:99:LEU:HD22	1.90	0.71
1:F:16:PHE:HB3	1:F:17:GLU:OE1	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:176:TYR:CD1	1:A:176:TYR:N	2.59	0.70
1:A:96:LYS:HD3	1:A:97:LYS:H	1.55	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:F:171:GLN:O	1:F:172:LYS:CG	2.36	0.69
1:F:127:ALA:O	1:F:131:LEU:HB2	1.92	0.69
1:D:66:ILE:HG21	1:D:70:MSE:HE2	1.75	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:C:110:ASP:O	1:C:134:ASN:HB2	1.93	0.67
1:A:1:LEU:HD11	1:A:5:LEU:HA	1.76	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:D:80:VAL:HG21	1:D:192:ALA:HB1	1.78	0.65
1:C:67:ILE:HG23	1:C:191:TRP:CD1	2.31	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:105:SER:OG	1:F:107:LYS:N	2.30	0.64
1:F:94:LEU:HD23	1:F:179:HIS:CB	2.27	0.64
1:E:20:ASP:OD2	1:E:21:LYS:N	2.29	0.64
1:F:105:SER:OG	1:F:106:TYR:N	2.30	0.64
1:F:10:GLU:OE1	1:F:119:LYS:NZ	2.30	0.64
1:F:113:GLU:HG3	1:F:114:LEU:HD23	1.79	0.64
1:A:60:THR:HG22	1:A:60:THR:O	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:F:173:GLY:O	1:F:174:GLN:C	2.34	0.63
1:F:18:MSE:HE3	1:F:26:ILE:O	1.98	0.63
1:E:70:MSE:HE3	1:E:82:PHE:CE1	2.33	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:F:18:MSE:HE3	1:F:27:GLY:HA3	1.82	0.61
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:E:21:LYS:HD2	1:E:22:LYS:H	1.58	0.61
1:B:231:LEU:O	1:B:232:GLU:C	2.33	0.61
1:A:147:VAL:O	1:A:150:VAL:CG1	2.46	0.61
1:F:94:LEU:HB3	1:F:177:LEU:HD23	1.82	0.61
1:F:58:LEU:HD22	1:F:66:ILE:HD12	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:F:60:THR:CG2	1:F:62:LYS:HE3	2.31	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: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:F:169:MSE:O	1:F:170:ALA:C	2.37	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:B:227:ASP:O	1:B:228:THR:OG1	2.11	0.58
1:F:17:GLU:C	1:F:18:MSE:HE2	2.23	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: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:HG22	1:F:60:THR:O	2.02	0.57
1:A:58:LEU:HD23	1:A:80:VAL:HG11	1.87	0.57
1:F:18:MSE:HE3	1:F:27:GLY:CA	2.35	0.57
1:B:89:VAL:HG11	1:B:161:ASP:HB3	1.86	0.57
1:A:118:THR:HG23	1:A:119:LYS:O	2.04	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:C:197:ASP:OD1	1:C:200:PHE:HB2	2.05	0.57
1:A:169:MSE:HE1	1:A:177:LEU:O	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:C:83:VAL:HG12	1:C:84:GLU:H	1.69	0.57
1:A:13:TYR:OH	1:A:161:ASP:HB2	2.05	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:E:232:GLU:O	1:E:233:LYS:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:SER:C	1:F:107:LYS:H	2.06	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: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:D:122:VAL:CG1	1:D:123:SER:N	2.70	0.55
1:B:82:PHE:O	1:E:206:HIS:HE1	1.89	0.55
1:D:128:ALA:HB1	1:D:137:LEU:HD13	1.88	0.55
1:B:152:ASN:OD1	1:B:154:LYS:HG2	2.07	0.55
1:F:97:LYS:NZ	1:F:175:GLY:O	2.36	0.55
1:C:110:ASP:OD2	1:C:132:PHE:O	2.25	0.55
1:C:108:ASP:O	1:C:109:LEU:HD13	2.06	0.55
1:A:79:ARG:NH2	3:A:505:HOH:O	2.38	0.55
1:D:60:THR:O	1:D:60:THR:CG2	2.55	0.54
1:A:210:GLN:O	1:A:214:ASP:HB2	2.07	0.54
1:A:174:GLN:H	1:A:174:GLN:CD	1.97	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:15:PRO:C	1:D:18:MSE:HE1	2.28	0.54
1:D:83:VAL:HG12	1:D:84:GLU:N	2.22	0.54
1:D:146:ALA:O	1:D:149:GLU:HB2	2.07	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: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:ND2	1:C:77:ASN:O	2.41	0.53
1:E:20:ASP:OD2	1:E:23:GLY:N	2.41	0.53
1:A:5:LEU:N	1:A:42:VAL:HG11	2.23	0.53
1:C:107:LYS:O	1:C:107:LYS:HD2	2.08	0.53
1:F:173:GLY:O	1:F:174:GLN:HB2	2.08	0.53
1:A:155:ALA:O	1:A:156:ASP:CG	2.47	0.53
1:A:66:ILE:CG2	1:A:70:MSE:HE1	2.31	0.53
1:F:106:TYR:C	1:F:106:TYR:CD2	2.79	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:B:160:PHE:CD2	1:B:161:ASP:N	2.76	0.52
1:A:195:LYS:HB3	1:B:199:ASP:OD2	2.08	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:D:132:PHE:CD1	1:D:132:PHE:N	2.74	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: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:D:42:VAL:HG12	1:D:43:LYS:N	2.25	0.51
1:C:14:LEU:HD22	1:C:164:PHE:CE1	2.46	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:C:83:VAL:CG1	1:C:84:GLU:H	2.23	0.51
1:D:111:LYS:HB2	1:D:114:LEU:CD1	2.41	0.51
1:D:14:LEU:HD12	1:D:18:MSE:SE	2.61	0.51
1:F:66:ILE:C	1:F:67:ILE:HG12	2.30	0.51
1:B:160:PHE:HZ	2:B:501:LYS:HD3	1.76	0.51
1:B:28:PHE:O	1:B:32:LEU:HB2	2.11	0.51
1:A:72:ILE:HD12	1:A:188:PRO:HB2	1.93	0.51
1:A:156:ASP:O	1:A:156:ASP:OD1	2.29	0.50
1:C:105:SER:O	1:C:108:ASP:OD1	2.29	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:B:96:LYS:HD3	1:B:97:LYS:N	2.27	0.50
1:C:110:ASP:O	1:C:134:ASN:CB	2.60	0.50
1:D:147:VAL:O	1:D:148:GLN:C	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HG11	1:A:186:TYR:CE1	2.45	0.50
1:E:96:LYS:HD3	1:E:97:LYS:H	1.77	0.50
1:F:18:MSE:CE	1:F:27:GLY:HA3	2.41	0.50
1:D:43:LYS:N	1:D:43:LYS:HD2	2.26	0.50
1:F:95:VAL:HG12	1:F:157:MSE:CB	2.38	0.50
1:A:171:GLN:HG3	1:A:172:LYS:N	2.27	0.50
1:A:100:GLU:O	1:A:103:VAL:HG13	2.12	0.50
1:C:4:GLU:HA	1:C:42:VAL:HG13	1.92	0.50
1:F:149:GLU:O	1:F:152:ASN:OD1	2.29	0.50
1:F:67:ILE:HG23	1:F:191:TRP:CD1	2.47	0.50
1:A:81:ASN:ND2	1:A:195:LYS:HA	2.27	0.49
1:F:94:LEU:HD21	1:F:165:ASN:HB3	1.94	0.49
1:A:229:LYS:O	1:A:232:GLU:HG3	2.12	0.49
1:F:229:LYS:O	1:F:232:GLU:HG2	2.12	0.49
1:C:56:PRO:O	1:C:60:THR:HB	2.11	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:211:ILE:HA	1:A:214:ASP:HB2	1.94	0.49
1:A:1:LEU:HD12	1:A:4:GLU:O	2.13	0.49
1:B:60:THR:O	1:B:60:THR:HG22	2.11	0.49
1:F:107:LYS:C	1:F:109:LEU:N	2.64	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:F:71:THR:HA	1:F:189:LEU:HD12	1.94	0.49
1:F:211:ILE:HA	1:F:214:ASP:HB2	1.95	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: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:233:LYS:HE3	1:A:233:LYS:HB2	1.67	0.48
1:A:60:THR:O	1:A:60:THR:CG2	2.60	0.48
1:E:169:MSE:HE3	1:E:174:GLN:HA	1.94	0.48
1:D:66:ILE:HG21	1:D:70:MSE:CE	2.43	0.48
1:B:9:LEU:HD21	1:B:46:LEU:HD22	1.95	0.48
1:F:170:ALA:O	1:F:171:GLN:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:THR:C	1:B:231:LEU:CD1	2.81	0.48
1:F:172:LYS:HA	1:F:174:GLN:NE2	2.28	0.48
1:C:233:LYS:N	1:C:233:LYS:HD3	2.10	0.48
1:A:42:VAL:HG13	1:A:43:LYS:N	2.29	0.48
1:D:67:ILE:HG23	1:D:191:TRP:CD1	2.49	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:F:40:MSE:HG2	1:F:203:TRP:CZ2	2.49	0.48
1:A:83:VAL:HG12	1:A:84:GLU:N	2.29	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:B:163:PRO:HA	1:B:166:VAL:HG22	1.96	0.47
1:A:55:ILE:HB	1:A:56:PRO:HD3	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:F:116:LEU:CD1	1:F:157:MSE:CG	2.82	0.47
1:A:122:VAL:HG12	1:A:124:ALA:H	1.80	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:C:9:LEU:HB2	1:C:17:GLU:HG2	1.96	0.47
1:B:114:LEU:HA	1:B:156:ASP:OD1	2.15	0.47
1:F:72:ILE:HG12	1:F:82:PHE:CD1	2.50	0.47
1:C:122:VAL:CG1	1:C:123:SER:N	2.77	0.47
1:F:172:LYS:HA	1:F:174:GLN:HE21	1.79	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:126:TYR:N	1:C:126:TYR:CD1	2.82	0.47
1:C:89:VAL:HG12	1:C:187:GLU:HB2	1.96	0.47
1:C:58:LEU:HD23	1:C:80:VAL:HG11	1.97	0.47
1:C:110:ASP:OD1	1:C:132:PHE:O	2.32	0.47
1:A:19:LYS:O	1:A:20:ASP:CB	2.60	0.47
1:D:36:MSE:HG2	1:D:40:MSE:CE	2.39	0.47
1:A:1:LEU:CD1	1:A:4:GLU:O	2.63	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:E:119:LYS:HD3	1:E:122:VAL:HG21	1.97	0.47
1:C:26:ILE:HD12	1:C:224:TRP:HH2	1.80	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:F:107:LYS:O	1:F:109:LEU:N	2.48	0.46
1:F:99:LEU:HD23	1:F:99:LEU:C	2.35	0.46
1:D:158:PHE:CZ	1:D:160:PHE:HB2	2.50	0.46
1:F:171:GLN:HG2	1:F:172:LYS:CG	2.41	0.46
1:B:117:VAL:HG12	1:B:138:LYS:HB2	1.98	0.46
1:D:230:TRP:O	1:D:232:GLU:O	2.34	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:B:105:SER:O	1:B:108:ASP:OD1	2.33	0.46
1:E:21:LYS:HG2	1:E:21:LYS:O	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: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:C:49:THR:HG22	1:C:50:SER:N	2.31	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:F:105:SER:C	1:F:107:LYS:N	2.69	0.45
1:D:91:GLN:OE1	1:D:160:PHE:CA	2.64	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: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:B:29:ASP:CG	1:B:67:ILE:HG22	2.37	0.45
1:E:20:ASP:OD2	1:E:20:ASP:C	2.48	0.45
1:F:83:VAL:HG12	1:F:84:GLU:N	2.31	0.45
1:E:83:VAL:O	1:E:84:GLU:C	2.55	0.45
1:F:26:ILE:HD12	1:F:224:TRP:HH2	1.81	0.45
1:D:77:ASN:ND2	1:D:77:ASN:O	2.50	0.45
1:A:162:LEU:N	1:A:163:PRO:CD	2.80	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:F:89:VAL:HG13	1:F:90:GLY:N	2.32	0.45
1:D:10:GLU:OE1	1:D:119:LYS:HE3	2.17	0.45
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
2:A:501:LYS:HE3	3:A:513:HOH:O	2.17	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:E:119:LYS:HA	1:E:140:TYR:O	2.17	0.44
1:D:50:SER:OG	1:D:52:ASP:OD2	2.34	0.44
1:A:22:LYS:HB2	1:A:24:ASN:ND2	2.33	0.44
1:F:164:PHE:O	1:F:168:PHE:HB2	2.17	0.44
1:D:200:PHE:O	1:D:204:LEU:HD22	2.17	0.44
1:B:109:LEU:O	1:B:157:MSE:HE1	2.17	0.44
1:A:19:LYS:O	1:A:20:ASP:HB2	2.17	0.44
1:D:60:THR:HG21	1:D:62:LYS:NZ	2.33	0.44
1:C:211:ILE:HG13	1:C:217:TYR:HB2	2.00	0.44
1:F:203:TRP:CE3	1:F:204:LEU:CD1	3.01	0.44
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.79	0.44
1:D:122:VAL:HG13	1:D:123:SER:H	1.81	0.43
1:D:56:PRO:O	1:D:60:THR:CB	2.64	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: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:A:51:TRP:CH2	2:A:501:LYS:HB3	2.52	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:E:72:ILE:HG23	1:E:82:PHE:CD2	2.53	0.43
1:C:108:ASP:O	1:C:109:LEU:CD1	2.66	0.43
1:E:122:VAL:O	1:E:123:SER:C	2.57	0.43
1:D:27:GLY:O	1:D:30:VAL:HB	2.18	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:54:LEU:HA	1:C:54:LEU:HD23	1.88	0.42
1:C:11:PRO:HA	1:C:17:GLU:HB2	2.01	0.42
1:A:3:GLY:O	1:A:43:LYS:HD2	2.19	0.42
1:E:21:LYS:O	1:E:21:LYS:CG	2.61	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:A:122:VAL:CG1	1:A:123:SER:N	2.83	0.42
1:E:92:SER:OG	1:E:162:LEU:HD12	2.19	0.42
1:E:10:GLU:OE1	2:E:501:LYS:NZ	2.47	0.42
1:B:187:GLU:HA	1:B:188:PRO:HD2	1.83	0.42
1:B:40:MSE:CE	1:B:200:PHE:CE1	2.90	0.42
1:A:231:LEU:CD1	1:A:231:LEU:H	2.17	0.42
1:D:91:GLN:OE1	1:D:160:PHE:HA	2.18	0.42
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.63	0.42
1:F:70:MSE:HE3	1:F:82:PHE:CZ	2.54	0.42
1:A:40:MSE:CE	1:A:200:PHE:HE1	2.32	0.42
1:C:104:LYS:HA	1:C:104:LYS:HD3	1.68	0.42
1:D:68:SER:O	1:D:69:GLY:C	2.56	0.42
1:D:96:LYS:O	1:D:99:LEU:HB2	2.20	0.42
1:A:152:ASN:C	1:A:152:ASN:OD1	2.57	0.42
1:F:94:LEU:HA	1:F:179:HIS:HB2	2.02	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: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:D:10:GLU:HA	1:D:11:PRO:HD2	1.96	0.42
1:C:207:PHE:O	1:C:207:PHE:CG	2.73	0.42
1:C:87:ILE:HG23	1:C:189:LEU:CD2	2.49	0.42
1:C:161:ASP:N	1:C:161:ASP:OD2	2.51	0.42
1:C:107:LYS:HA	1:C:107:LYS:HD3	1.81	0.42
1:B:17:GLU:OE1	1:B:29:ASP:OD1	2.38	0.42
1:B:100:GLU:N	1:B:100:GLU:OE1	2.43	0.42
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.89	0.42
1:E:171:GLN:HG3	1:E:172:LYS:N	2.35	0.42
1:D:16:PHE:HA	1:D:28:PHE:HB3	2.01	0.42
1:B:200:PHE:CD1	1:B:204:LEU:HD22	2.54	0.41
1:E:5:LEU:HD22	1:E:40:MSE:HE3	2.02	0.41
1:B:154:LYS:H	1:B:154:LYS:HG2	1.70	0.41
1:D:92:SER:OG	1:D:165:ASN:OD1	2.37	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:D:131:LEU:HB3	1:D:132:PHE:HD1	1.86	0.41
1:C:96:LYS:O	1:C:99:LEU:HD23	2.21	0.41
1:C:111:LYS:HD3	1:C:111:LYS:HA	1.72	0.41
1:E:70:MSE:CE	1:E:192:ALA:CB	2.98	0.41
1:A:50:SER:O	1:A:51:TRP:C	2.58	0.41
1:D:66:ILE:CG2	1:D:70:MSE:HE2	2.46	0.41
1:F:118:THR:HG23	1:F:119:LYS:N	2.34	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:C:149:GLU:O	1:C:154:LYS:N	2.53	0.41
1:A:154:LYS:H	1:A:154:LYS:HG3	1.27	0.41
1:C:9:LEU:HD22	1:C:17:GLU:CG	2.50	0.41
1:A:221:TYR:CE2	1:C:101:LYS:HB3	2.56	0.41
1:A:193:ILE:HD11	1:A:201:LEU:HG	2.03	0.41
1:B:40:MSE:CE	1:B:200:PHE:HE1	2.09	0.41
1:A:148:GLN:CA	1:A:148:GLN:NE2	2.82	0.41
1:A:5:LEU:N	1:A:42:VAL:CG1	2.84	0.41
1:E:174:GLN:H	1:E:174:GLN:HE21	1.69	0.41
1:C:114:LEU:HA	1:C:156:ASP:OD2	2.21	0.41
1:B:116:LEU:HD11	1:B:159:ILE:HB	2.02	0.41
1:B:230:TRP:O	1:B:233:LYS:HA	2.21	0.41
1:A:171:GLN:HE21	1:A:171:GLN:HB2	1.63	0.41
1:F:94:LEU:CD2	1:F:179:HIS:CB	2.99	0.41
1:C:211:ILE:HA	1:C:214:ASP:HB2	2.02	0.41
1:A:181:ASP:OD1	1:A:182:THR:N	2.54	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:F:87:ILE:HG23	1:F:189:LEU:HD22	2.03	0.41
1:E:143:GLU:O	1:E:146:ALA:HB3	2.20	0.41
1:B:83:VAL:HG12	1:B:84:GLU:H	1.86	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:100:GLU:OE2	1:A:101:LYS:CE	2.69	0.40
1:E:91:GLN:HE21	1:E:124:ALA:HA	1.87	0.40
1:B:55:ILE:HB	1:B:56:PRO:HD3	2.04	0.40
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.88	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%)	39	63
All	All	1387/1470 (94%)	1295 (93%)	91 (7%)	1 (0%)	56	80

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%)	2	2
1	B	200/204 (98%)	166 (83%)	34 (17%)	2	3
1	C	200/204 (98%)	162 (81%)	38 (19%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	200/204 (98%)	168 (84%)	32 (16%)	3	4
1	E	201/204 (98%)	166 (83%)	35 (17%)	2	3
1	F	200/204 (98%)	157 (78%)	43 (22%)	1	2
All	All	1201/1224 (98%)	980 (82%)	221 (18%)	2	3

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

Some 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 carbohydrates 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	A	501	-	6,9,9	0.38	0	4,10,10	0.69	0
2	LYS	B	501	-	6,9,9	0.28	0	4,10,10	0.87	0
2	LYS	C	501	-	6,9,9	0.55	0	4,10,10	0.68	0
2	LYS	D	501	-	6,9,9	0.60	0	4,10,10	0.50	0
2	LYS	E	501	-	6,9,9	0.47	0	4,10,10	0.46	0
2	LYS	F	501	-	6,9,9	0.59	0	4,10,10	0.49	0

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	A	501	-	-	0/5/9/9	0/0/0/0
2	LYS	B	501	-	-	0/5/9/9	0/0/0/0
2	LYS	C	501	-	-	0/5/9/9	0/0/0/0
2	LYS	D	501	-	-	0/5/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	E	501	-	-	0/5/9/9	0/0/0/0
2	LYS	F	501	-	-	0/5/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LYS	2	0
2	B	501	LYS	5	0
2	C	501	LYS	1	0
2	D	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, 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%)	0.11	6 (2%) 59 53	10, 27, 45, 62	0
1	B	227/245 (92%)	0.16	11 (4%) 34 27	13, 30, 50, 72	0
1	C	227/245 (92%)	0.04	4 (1%) 71 66	15, 30, 50, 67	0
1	D	227/245 (92%)	0.08	6 (2%) 59 53	15, 36, 53, 63	0
1	E	228/245 (93%)	0.07	8 (3%) 48 40	6, 25, 46, 65	0
1	F	227/245 (92%)	0.18	8 (3%) 48 40	13, 32, 62, 70	0
All	All	1363/1470 (92%)	0.11	43 (3%) 51 44	6, 30, 53, 72	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ARG	4.2
1	D	1	LEU	4.1
1	B	174	GLN	4.0
1	F	232	GLU	3.6
1	F	1	LEU	3.5
1	B	228	THR	3.5
1	F	101	LYS	3.4
1	A	1	LEU	3.3
1	A	114	LEU	3.1
1	B	115	THR	3.0
1	E	232	GLU	3.0
1	E	177	LEU	2.9
1	E	0	SER	2.9
1	F	104	LYS	2.9
1	C	3	GLY	2.9
1	A	147	VAL	2.9
1	B	173	GLY	2.8
1	E	168	PHE	2.8
1	B	2	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	2	ARG	2.6
1	E	151	LEU	2.5
1	F	229	LYS	2.4
1	B	155	ALA	2.4
1	B	25	VAL	2.4
1	F	102	GLY	2.3
1	F	173	GLY	2.3
1	B	138	LYS	2.3
1	D	104	LYS	2.3
1	C	173	GLY	2.3
1	A	232	GLU	2.3
1	D	23	GLY	2.3
1	B	147	VAL	2.2
1	B	150	VAL	2.2
1	E	176	TYR	2.2
1	A	176	TYR	2.1
1	C	23	GLY	2.1
1	F	103	VAL	2.1
1	D	22	LYS	2.1
1	E	3	GLY	2.1
1	D	126	TYR	2.0
1	A	26	ILE	2.0
1	B	229	LYS	2.0
1	C	20	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	LYS	D	501	10/10	0.97	0.20	1.93	29,36,37,37	0
2	LYS	A	501	10/10	0.95	0.20	1.50	21,23,24,25	0
2	LYS	E	501	10/10	0.97	0.18	1.07	24,30,30,31	0
2	LYS	F	501	10/10	0.94	0.20	0.93	24,24,26,27	0
2	LYS	B	501	10/10	0.96	0.17	0.52	22,26,28,28	0
2	LYS	C	501	10/10	0.96	0.17	0.08	25,33,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.