



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GU9
Title : CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS
ALKYLPEROXIDASE AHPD
Authors : Nunn, C.M.; Djordjevic, S.; Hillas, P.J.; Nishida, C.; De Montellano, P.R.O.
Deposited on : 2002-01-24
Resolution : 1.90 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

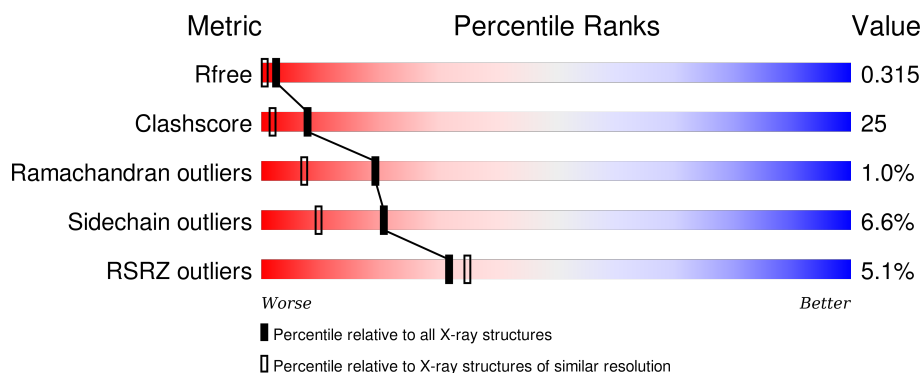
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	177	<div> <div>3%</div> <div>67% 25% 5%</div> </div>
1	B	177	<div> <div>5%</div> <div>67% 27% 5%</div> </div>
1	C	177	<div> <div>2%</div> <div>65% 25% 5% 5%</div> </div>
1	D	177	<div> <div>3%</div> <div>63% 29% 5%</div> </div>
1	E	177	<div> <div>7%</div> <div>54% 37% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	177	<div><div></div><div>3%</div><div>67%</div><div>25%</div><div>5%</div></div>
1	G	177	<div><div></div><div>3%</div><div>63%</div><div>28%</div><div>5%</div></div>
1	H	177	<div><div></div><div>6%</div><div>63%</div><div>31%</div><div></div></div>
1	I	177	<div><div></div><div>7%</div><div>61%</div><div>32%</div><div>5%</div></div>
1	J	177	<div><div></div><div>7%</div><div>62%</div><div>32%</div><div></div></div>
1	K	177	<div><div></div><div>3%</div><div>58%</div><div>36%</div><div></div></div>
1	L	177	<div><div></div><div>7%</div><div>57%</div><div>33%</div><div>5%</div><div>5%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16174 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 ALKYLHYDROPEROXIDASE D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	Se	0	0	0
			1284	808	232	239	3	2			
1	B	173	Total	C	N	O	S	Se	8	0	0
			1292	814	233	240	3	2			
1	C	168	Total	C	N	O	S	Se	0	0	0
			1256	791	228	232	3	2			
1	D	172	Total	C	N	O	S	Se	0	0	0
			1284	808	232	239	3	2			
1	E	173	Total	C	N	O	S	Se	8	0	0
			1292	814	233	240	3	2			
1	F	169	Total	C	N	O	S	Se	0	0	0
			1264	797	229	233	3	2			
1	G	168	Total	C	N	O	S	Se	11	0	0
			1256	791	228	232	3	2			
1	H	171	Total	C	N	O	S	Se	0	0	0
			1275	803	231	236	3	2			
1	I	173	Total	C	N	O	S	Se	0	0	0
			1292	814	233	240	3	2			
1	J	172	Total	C	N	O	S	Se	0	0	0
			1284	808	232	239	3	2			
1	K	173	Total	C	N	O	S	Se	0	0	0
			1292	814	233	240	3	2			
1	L	168	Total	C	N	O	S	Se	11	0	0
			1256	791	228	232	3	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	78	Total	O	0	0
			78	78		

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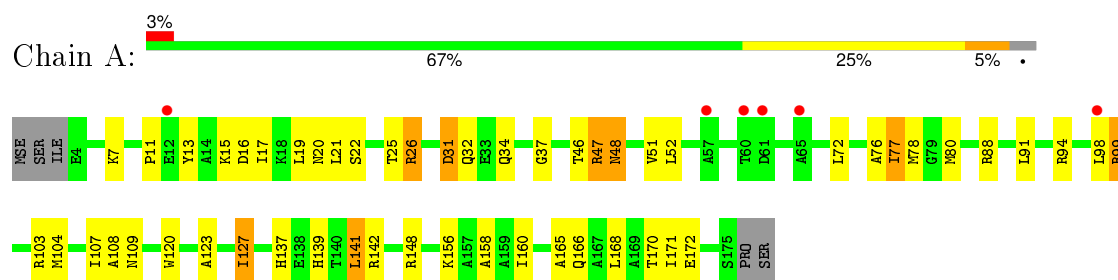
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	88	Total 88	O 88	0	0
2	D	70	Total 70	O 70	0	0
2	E	53	Total 53	O 53	0	0
2	F	108	Total 108	O 108	0	0
2	G	66	Total 66	O 66	0	0
2	H	65	Total 65	O 65	0	0
2	I	57	Total 57	O 57	0	0
2	J	76	Total 76	O 76	0	0
2	K	58	Total 58	O 58	0	0
2	L	67	Total 67	O 67	0	0

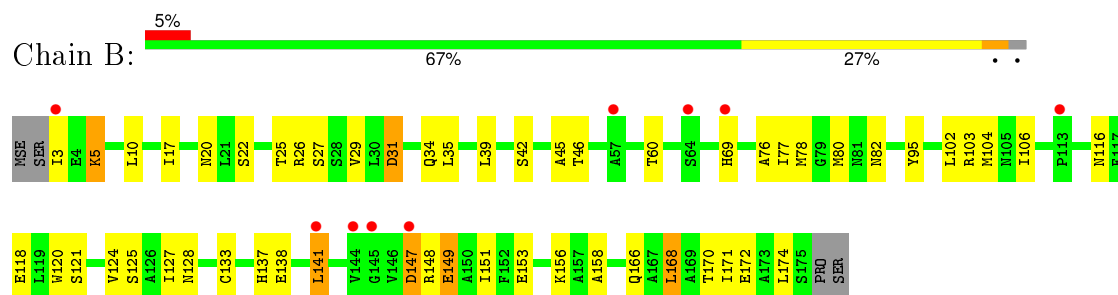
3 Residue-property plots

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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

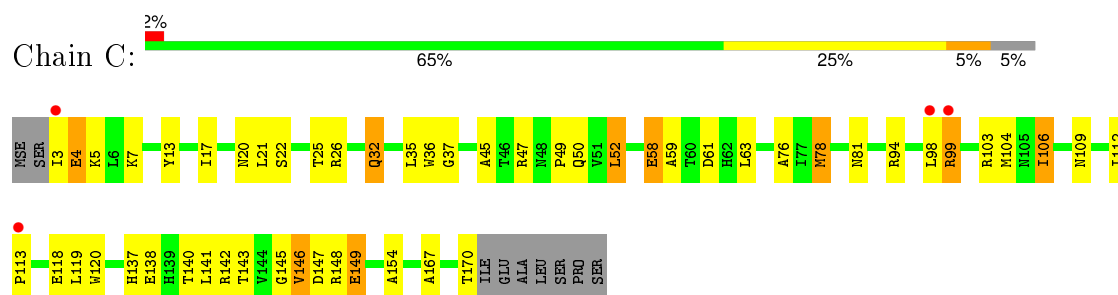
• Molecule 1: ALKYLHYDROPEROXIDASE D



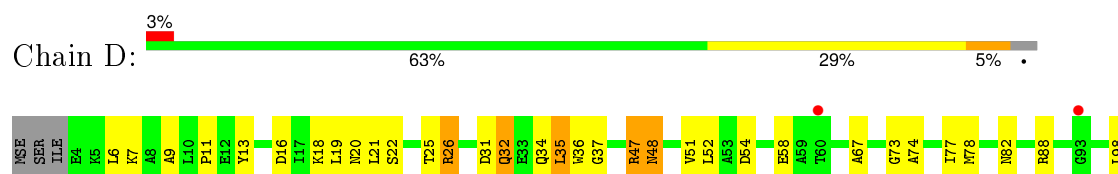
• Molecule 1: ALKYLHYDROPEROXIDASE D



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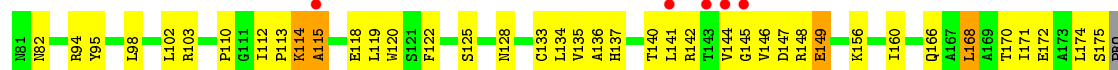
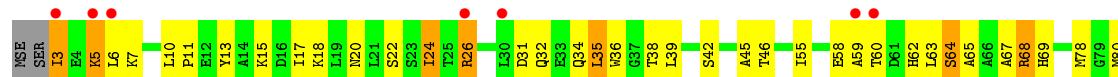


• Molecule 1: ALKYLHYDROPEROXIDASE D





• Molecule 1: ALKYLHYDROPEROXIDASE D

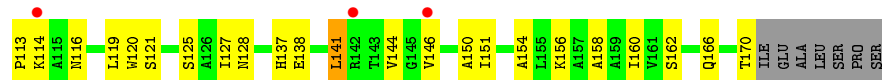
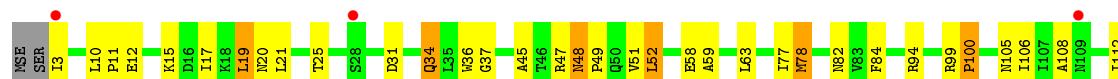


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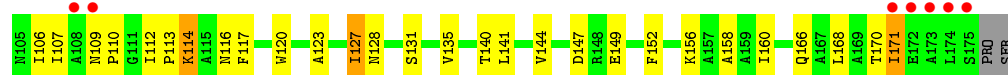
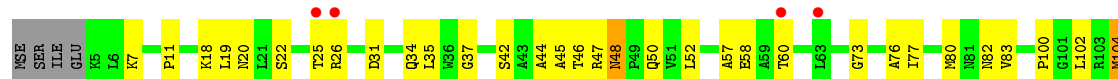
• Molecule 1: ALKYLHYDROPEROXIDASE D



• Molecule 1: ALKYLHYDROPEROXIDASE D

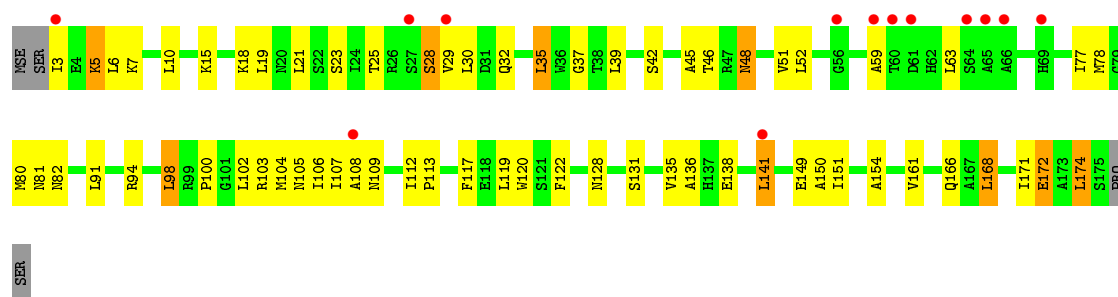


• Molecule 1: ALKYLHYDROPEROXIDASE D

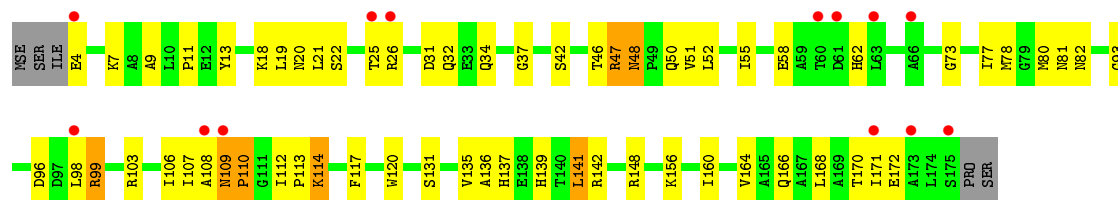


• Molecule 1: ALKYLHYDROPEROXIDASE D

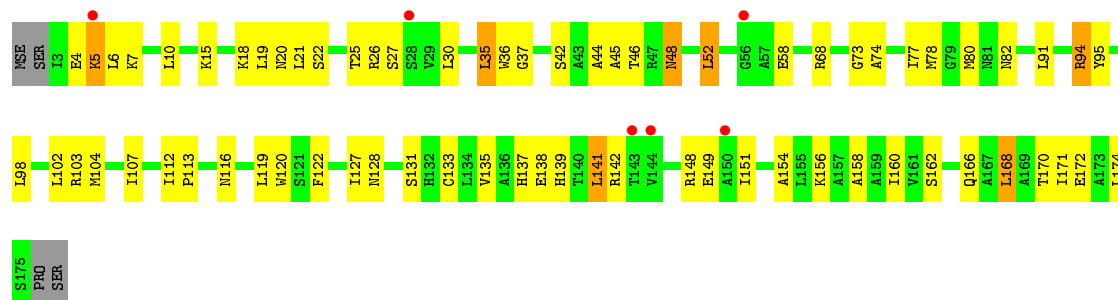




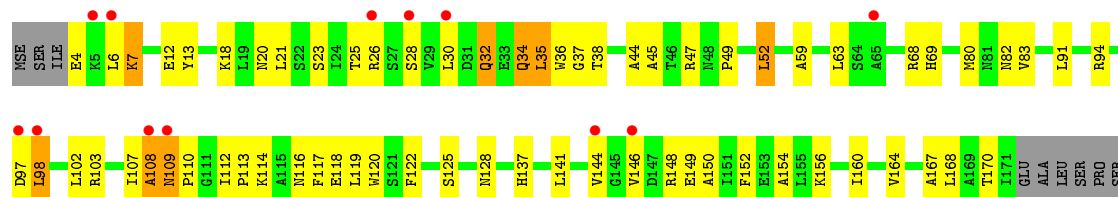
• Molecule 1: ALKYLHYDROPEROXIDASE D



• Molecule 1: ALKYLHYDROPEROXIDASE D



• Molecule 1: ALKYLHYDROPEROXIDASE D



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.38 Å 117.28 Å 88.99 Å 90.00° 113.97° 90.00°	Depositor
Resolution (Å)	29.60 – 1.90 29.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.60-1.90) 99.4 (29.59-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.91 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.313 0.245 , 0.315	Depositor DCC
R_{free} test set	13616 reflections (9.98%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	14 of 136434 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16174	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.34 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0701e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.45	0/1303	0.65	0/1764
1	B	0.44	0/1311	0.64	0/1775
1	C	0.46	0/1275	0.66	0/1726
1	D	0.47	0/1303	0.64	0/1764
1	E	0.44	0/1311	0.64	0/1775
1	F	0.45	0/1283	0.65	0/1737
1	G	0.47	0/1275	0.66	1/1726 (0.1%)
1	H	0.45	0/1294	0.65	1/1752 (0.1%)
1	I	0.41	0/1311	0.66	0/1775
1	J	0.44	0/1303	0.63	0/1764
1	K	0.43	0/1311	0.64	0/1775
1	L	0.43	0/1275	0.64	0/1726
All	All	0.45	0/15555	0.65	2/21059 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	104	MET	CG-SD-CE	-5.99	90.62	100.20
1	G	78	MSE	CG-SE-CE	-5.94	85.84	98.90

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	1284	0	1296	75	0
1	B	1292	0	1307	59	0
1	C	1256	0	1269	66	0
1	D	1284	0	1296	75	0
1	E	1292	0	1307	81	0
1	F	1264	0	1280	56	0
1	G	1256	0	1269	59	0
1	H	1275	0	1290	74	0
1	I	1292	0	1307	79	0
1	J	1284	0	1296	84	0
1	K	1292	0	1307	72	0
1	L	1256	0	1269	79	0
2	A	61	0	0	4	0
2	B	78	0	0	6	0
2	C	88	0	0	6	0
2	D	70	0	0	3	0
2	E	53	0	0	4	0
2	F	108	0	0	2	0
2	G	66	0	0	2	0
2	H	65	0	0	6	0
2	I	57	0	0	7	0
2	J	76	0	0	3	0
2	K	58	0	0	5	0
2	L	67	0	0	5	0
All	All	16174	0	15493	769	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (769) 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:J:78:MSE:HE2	1:J:82:ASN:ND2	1.58	1.19
1:G:78:MSE:HE2	1:G:121:SER:HB3	1.15	1.14
1:K:5:LYS:HA	1:K:5:LYS:HE3	1.32	1.10
1:C:3:ILE:HG22	1:C:4:GLU:H	1.16	1.10
1:F:99:ARG:HD2	1:F:99:ARG:H	1.07	1.10
1:D:78:MSE:HE1	1:D:137:HIS:CD2	1.88	1.09
1:H:127:ILE:HD11	1:H:158:ALA:HB1	1.36	1.05
1:J:78:MSE:HE3	1:J:78:MSE:HA	1.41	1.03
1:G:78:MSE:HE2	1:G:121:SER:CB	1.87	1.02
1:A:31:ASP:H	1:A:34:GLN:NE2	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ILE:HG12	1:F:113:PRO:HD2	1.38	1.02
1:A:31:ASP:N	1:A:34:GLN:HE21	1.59	1.01
1:C:78:MSE:HE2	1:C:81:ASN:HB2	1.41	1.00
1:A:127:ILE:HD11	1:A:158:ALA:HB1	1.40	1.00
1:A:11:PRO:HB3	1:A:171:ILE:HD11	1.38	0.99
1:A:25:THR:HG23	1:A:26:ARG:HD2	1.45	0.98
1:D:31:ASP:H	1:D:34:GLN:HE21	1.05	0.97
1:C:78:MSE:CE	1:C:81:ASN:HB2	1.94	0.96
1:B:82:ASN:HD22	1:B:128:ASN:HD22	1.05	0.96
1:I:82:ASN:HD22	1:I:128:ASN:HD22	1.12	0.96
1:C:99:ARG:HE	1:C:99:ARG:H	1.11	0.95
1:H:127:ILE:CD1	1:H:158:ALA:HB1	1.96	0.94
1:D:78:MSE:HE3	1:D:125:SER:OG	1.65	0.94
1:C:112:ILE:HB	1:C:113:PRO:HD2	1.50	0.94
1:I:112:ILE:HB	1:I:113:PRO:HD2	1.51	0.92
1:K:91:LEU:O	1:K:94:ARG:HG3	1.68	0.92
1:A:127:ILE:CD1	1:A:158:ALA:HB1	1.99	0.92
1:D:82:ASN:HD22	1:D:128:ASN:HD22	1.19	0.91
1:K:82:ASN:HD22	1:K:128:ASN:HD22	1.19	0.91
1:J:77:ILE:HG13	1:J:106:ILE:HG21	1.53	0.91
1:E:82:ASN:HD22	1:E:128:ASN:HD22	1.16	0.91
1:J:160:ILE:HD11	1:K:102:LEU:HD22	1.50	0.90
1:I:104:MET:CE	1:I:107:ILE:HD12	2.01	0.89
1:J:20:ASN:HB3	1:J:160:ILE:HD12	1.53	0.89
1:H:20:ASN:HB3	1:H:160:ILE:HD12	1.54	0.89
1:J:106:ILE:HG23	1:J:107:ILE:HD12	1.55	0.89
1:F:99:ARG:CD	1:F:99:ARG:H	1.81	0.88
1:H:82:ASN:HD22	1:H:128:ASN:HD22	1.20	0.88
1:F:82:ASN:HD22	1:F:128:ASN:HD22	1.19	0.88
1:G:78:MSE:CE	1:G:121:SER:HB3	1.99	0.88
1:A:20:ASN:HB3	1:A:160:ILE:HD12	1.56	0.87
1:F:99:ARG:HD2	1:F:99:ARG:N	1.90	0.87
1:K:112:ILE:HB	1:K:113:PRO:HD2	1.57	0.86
1:L:167:ALA:O	1:L:170:THR:HG22	1.75	0.86
1:G:20:ASN:HB3	1:G:160:ILE:HD12	1.56	0.86
1:D:78:MSE:HE2	1:D:121:SER:HB2	1.57	0.86
1:C:3:ILE:HG22	1:C:4:GLU:N	1.92	0.85
1:D:160:ILE:HD11	1:E:102:LEU:HD22	1.55	0.85
1:G:78:MSE:HE1	1:G:137:HIS:CD2	2.12	0.85
1:D:103:ARG:H	1:F:20:ASN:HD21	1.26	0.84
1:E:78:MSE:HE1	1:E:133:CYS:HB3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ALA:HB1	1:E:63:LEU:HD12	1.57	0.84
1:I:91:LEU:O	1:I:94:ARG:HG3	1.78	0.83
1:E:5:LYS:HE3	1:E:5:LYS:HA	1.59	0.83
1:J:78:MSE:HE2	1:J:82:ASN:HD21	1.40	0.82
1:H:160:ILE:HD11	1:I:102:LEU:HD22	1.60	0.82
1:H:168:LEU:HD12	1:H:171:ILE:HD11	1.62	0.82
1:J:20:ASN:HD21	1:K:103:ARG:H	1.28	0.82
1:I:104:MET:HE3	1:I:107:ILE:HD12	1.61	0.82
1:H:22:SER:O	1:H:25:THR:HG22	1.78	0.82
1:C:78:MSE:HE2	1:C:78:MSE:HA	1.61	0.81
1:J:78:MSE:HE3	1:J:81:ASN:HB2	1.63	0.81
1:C:3:ILE:N	1:C:58:GLU:HG3	1.95	0.81
1:B:78:MSE:HE1	1:B:133:CYS:HB3	1.64	0.80
1:J:112:ILE:HB	1:J:113:PRO:HD2	1.64	0.80
1:G:127:ILE:HD12	1:G:162:SER:OG	1.81	0.80
1:A:160:ILE:HD11	1:B:102:LEU:HD22	1.64	0.80
1:E:171:ILE:HD12	1:E:172:GLU:N	1.97	0.80
1:F:112:ILE:CG1	1:F:113:PRO:HD2	2.10	0.80
1:L:141:LEU:HB3	1:L:146:VAL:CG1	2.11	0.80
1:C:21:LEU:O	1:C:25:THR:HG22	1.81	0.80
1:B:78:MSE:CE	1:B:125:SER:HB3	2.11	0.80
1:C:167:ALA:O	1:C:170:THR:HG22	1.82	0.80
1:J:77:ILE:HG13	1:J:106:ILE:CG2	2.11	0.79
1:H:31:ASP:H	1:H:34:GLN:HE21	1.26	0.79
1:F:67:ALA:HA	1:F:112:ILE:HD12	1.65	0.79
1:J:103:ARG:H	1:L:20:ASN:HD21	1.31	0.79
1:J:108:ALA:O	1:J:109:ASN:HB2	1.82	0.79
1:K:142:ARG:NH1	1:K:148:ARG:HB3	1.98	0.79
1:K:171:ILE:HD12	1:K:172:GLU:N	1.98	0.78
1:A:11:PRO:HD3	1:A:171:ILE:HG13	1.64	0.78
1:D:31:ASP:H	1:D:34:GLN:NE2	1.79	0.77
1:D:168:LEU:O	1:D:172:GLU:HG3	1.84	0.77
1:D:74:ALA:HA	1:D:77:ILE:HD11	1.66	0.77
1:J:98:LEU:HD11	1:L:148:ARG:HH22	1.50	0.77
1:K:127:ILE:HD12	1:K:162:SER:OG	1.85	0.77
1:J:98:LEU:HD11	1:L:148:ARG:NH2	1.99	0.76
1:A:103:ARG:H	1:C:20:ASN:HD21	1.31	0.76
1:D:48:ASN:HD22	1:D:51:VAL:H	1.32	0.76
1:J:31:ASP:H	1:J:34:GLN:HE21	1.32	0.75
1:J:78:MSE:HA	1:J:78:MSE:CE	2.16	0.75
1:L:112:ILE:HB	1:L:113:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD13	1:B:80:MSE:SE	2.36	0.75
1:D:131:SER:O	1:D:135:VAL:HG12	1.87	0.75
1:B:3:ILE:HD13	1:B:25:THR:HG21	1.67	0.75
1:D:22:SER:O	1:D:26:ARG:HD2	1.88	0.74
1:K:73:GLY:O	1:K:77:ILE:HG13	1.87	0.74
1:D:106:ILE:HG23	1:D:107:ILE:HD12	1.70	0.74
1:G:48:ASN:HD22	1:G:51:VAL:H	1.35	0.74
1:L:82:ASN:HD22	1:L:128:ASN:HD22	1.36	0.74
1:E:59:ALA:O	1:E:63:LEU:HB2	1.88	0.74
1:G:82:ASN:HD22	1:G:128:ASN:HD22	1.36	0.74
1:K:156:LYS:O	1:K:160:ILE:HG12	1.87	0.74
1:D:20:ASN:HB3	1:D:160:ILE:HD12	1.71	0.73
1:G:160:ILE:HD11	1:H:102:LEU:HD22	1.71	0.73
1:C:3:ILE:CG2	1:C:4:GLU:H	1.96	0.73
1:K:104:MET:HE3	1:K:107:ILE:HD12	1.70	0.73
1:L:7:LYS:HD2	1:L:7:LYS:H	1.54	0.73
1:H:104:MET:CE	1:H:107:ILE:HD12	2.18	0.73
1:B:31:ASP:HB2	1:B:34:GLN:HG3	1.69	0.73
1:J:78:MSE:CE	1:J:82:ASN:ND2	2.46	0.72
1:H:112:ILE:HB	1:H:113:PRO:HD2	1.71	0.72
1:F:112:ILE:HG12	1:F:113:PRO:CD	2.19	0.72
1:C:78:MSE:CE	1:C:78:MSE:HA	2.19	0.72
1:L:141:LEU:HB3	1:L:146:VAL:HG11	1.71	0.72
1:H:77:ILE:HD13	1:H:106:ILE:HG23	1.71	0.72
1:G:15:LYS:O	1:G:19:LEU:HD22	1.89	0.71
1:E:26:ARG:HB2	1:E:26:ARG:NH1	2.05	0.71
1:J:7:LYS:O	1:J:18:LYS:HD3	1.90	0.71
1:B:148:ARG:HG3	2:B:2072:HOH:O	1.90	0.71
1:G:48:ASN:ND2	1:G:51:VAL:H	1.89	0.71
1:F:167:ALA:O	1:F:170:THR:HG22	1.90	0.71
1:F:3:ILE:N	1:F:58:GLU:HG3	2.06	0.71
1:I:103:ARG:HH21	1:I:105:ASN:ND2	1.88	0.71
1:B:20:ASN:HD21	1:C:103:ARG:H	1.38	0.71
1:H:131:SER:O	1:H:135:VAL:HG12	1.90	0.71
1:G:52:LEU:HD22	1:I:174:LEU:HD11	1.71	0.71
1:K:20:ASN:HB3	1:K:160:ILE:HD12	1.73	0.70
1:L:4:GLU:HA	1:L:7:LYS:HD3	1.72	0.70
1:C:3:ILE:CG2	1:C:7:LYS:HG3	2.21	0.70
1:C:78:MSE:CE	1:C:81:ASN:CB	2.70	0.70
1:K:141:LEU:HB3	1:K:151:ILE:HD11	1.74	0.70
1:K:36:TRP:CH2	1:K:58:GLU:HG2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:MSE:CE	1:J:81:ASN:HB2	2.22	0.70
1:C:13:TYR:OH	1:C:170:THR:HG23	1.92	0.70
1:D:166:GLN:HE22	1:E:45:ALA:HA	1.56	0.70
1:G:77:ILE:HG21	1:G:106:ILE:CG2	2.22	0.69
1:E:78:MSE:CE	1:E:125:SER:HB3	2.23	0.69
1:H:11:PRO:HG3	1:H:171:ILE:CG2	2.23	0.69
1:L:98:LEU:HD22	1:L:98:LEU:H	1.58	0.69
1:G:77:ILE:HG21	1:G:106:ILE:HG21	1.74	0.69
1:C:98:LEU:HA	1:C:99:ARG:HH21	1.56	0.69
1:H:170:THR:HG21	2:I:2025:HOH:O	1.92	0.69
1:D:48:ASN:ND2	1:D:51:VAL:H	1.90	0.69
1:H:127:ILE:HD11	1:H:158:ALA:CB	2.20	0.68
1:F:7:LYS:HB2	1:F:7:LYS:NZ	2.08	0.68
1:J:168:LEU:O	1:J:172:GLU:HG3	1.92	0.68
1:K:77:ILE:HD12	1:K:78:MSE:N	2.09	0.68
1:C:99:ARG:NE	1:C:99:ARG:H	1.87	0.68
1:D:78:MSE:HE1	1:D:137:HIS:HD2	1.54	0.68
1:K:131:SER:O	1:K:135:VAL:HG22	1.93	0.68
1:D:98:LEU:O	1:D:99:ARG:HB3	1.94	0.68
1:A:98:LEU:O	1:A:99:ARG:CB	2.42	0.68
1:J:51:VAL:O	1:J:55:ILE:HD13	1.94	0.68
1:B:78:MSE:HE3	1:B:125:SER:HB3	1.76	0.67
1:C:50:GLN:HG2	2:C:2006:HOH:O	1.93	0.67
1:G:108:ALA:O	1:G:114:LYS:NZ	2.27	0.67
1:I:77:ILE:HG21	1:I:106:ILE:HG21	1.75	0.67
1:D:106:ILE:HD13	2:F:2004:HOH:O	1.93	0.67
1:F:94:ARG:HG2	1:F:94:ARG:HH11	1.59	0.67
1:J:48:ASN:HD22	1:J:51:VAL:H	1.41	0.67
1:E:20:ASN:HD21	1:F:103:ARG:H	1.41	0.67
1:C:118:GLU:OE1	1:C:137:HIS:HD2	1.76	0.67
1:E:137:HIS:O	1:E:141:LEU:HD23	1.95	0.67
1:E:5:LYS:HA	1:E:5:LYS:CE	2.24	0.66
1:A:91:LEU:O	1:A:94:ARG:HD3	1.96	0.66
1:B:82:ASN:ND2	1:B:128:ASN:HD22	1.88	0.66
1:J:170:THR:HG21	2:J:2075:HOH:O	1.96	0.66
1:A:166:GLN:HE22	1:B:45:ALA:HA	1.59	0.66
1:F:118:GLU:OE1	1:F:137:HIS:HD2	1.77	0.66
1:D:78:MSE:CE	1:D:137:HIS:CD2	2.74	0.66
1:E:119:LEU:O	1:E:122:PHE:HB3	1.96	0.66
1:D:31:ASP:N	1:D:34:GLN:HE21	1.88	0.66
1:A:98:LEU:O	1:A:99:ARG:HB3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:HD22	1:C:98:LEU:N	2.11	0.66
1:D:104:MET:HB2	1:D:107:ILE:HD13	1.77	0.66
1:H:160:ILE:HD13	1:I:80:MSE:SE	2.45	0.66
1:B:118:GLU:HB3	1:B:141:LEU:HD13	1.78	0.66
1:L:152:PHE:CE2	1:L:156:LYS:HD3	2.30	0.66
1:J:166:GLN:HE22	1:K:45:ALA:HA	1.61	0.66
1:D:16:ASP:HB3	1:E:103:ARG:O	1.96	0.65
1:H:166:GLN:HE22	1:I:45:ALA:HA	1.61	0.65
1:A:11:PRO:HB3	1:A:171:ILE:CD1	2.20	0.65
1:D:82:ASN:ND2	1:D:128:ASN:HD22	1.93	0.65
1:F:132:HIS:HB2	2:F:2091:HOH:O	1.95	0.65
1:L:37:GLY:HA3	1:L:120:TRP:CZ2	2.32	0.65
1:F:144:VAL:HG12	1:F:144:VAL:O	1.96	0.65
1:K:166:GLN:HE22	1:L:45:ALA:HA	1.61	0.65
1:F:21:LEU:O	1:F:25:THR:HG22	1.97	0.64
1:I:5:LYS:HE2	1:I:5:LYS:HA	1.79	0.64
1:A:137:HIS:O	1:A:141:LEU:HD22	1.97	0.64
1:K:127:ILE:HD13	1:L:83:VAL:HG11	1.78	0.64
1:H:57:ALA:O	1:H:60:THR:HG22	1.98	0.64
1:H:77:ILE:HG21	1:H:106:ILE:CG2	2.27	0.64
1:L:26:ARG:HG3	1:L:26:ARG:O	1.98	0.64
1:A:11:PRO:CB	1:A:171:ILE:HD11	2.22	0.64
1:G:78:MSE:HE2	1:G:121:SER:CA	2.28	0.64
1:A:127:ILE:HD11	1:A:158:ALA:CB	2.23	0.64
1:G:156:LYS:O	1:G:160:ILE:HG12	1.96	0.64
1:B:77:ILE:HD11	1:B:104:MET:CB	2.28	0.64
1:B:77:ILE:HD12	1:B:106:ILE:CG2	2.27	0.64
1:A:31:ASP:HB2	1:A:34:GLN:H	1.62	0.63
1:J:11:PRO:HB3	1:J:171:ILE:CG2	2.28	0.63
1:D:98:LEU:O	1:D:99:ARG:CB	2.44	0.63
1:J:137:HIS:O	1:J:141:LEU:HD22	1.97	0.63
1:A:32:GLN:HA	1:A:32:GLN:NE2	2.13	0.63
1:J:160:ILE:HD11	1:K:102:LEU:CD2	2.26	0.63
1:I:131:SER:O	1:I:135:VAL:HG22	1.98	0.63
1:A:156:LYS:O	1:A:160:ILE:HG12	1.99	0.63
1:I:37:GLY:HA3	1:I:120:TRP:CE2	2.33	0.63
1:K:21:LEU:O	1:K:25:THR:HG22	1.98	0.63
1:J:107:ILE:HG13	1:J:117:PHE:HE2	1.64	0.63
1:B:77:ILE:HD12	1:B:106:ILE:HG22	1.80	0.62
1:J:114:LYS:HB2	1:J:114:LYS:NZ	2.13	0.62
1:C:78:MSE:HE1	2:C:2042:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASN:HD22	1:B:128:ASN:ND2	1.88	0.62
1:H:22:SER:O	1:H:26:ARG:HD2	1.98	0.62
1:E:144:VAL:HG12	1:E:144:VAL:O	1.98	0.62
1:K:48:ASN:C	1:K:48:ASN:HD22	2.03	0.62
1:B:166:GLN:HE22	1:C:45:ALA:HA	1.65	0.62
1:C:106:ILE:HD13	1:C:106:ILE:O	2.00	0.62
1:K:160:ILE:HD11	1:L:102:LEU:HD22	1.81	0.62
1:G:78:MSE:HE3	1:G:121:SER:O	2.00	0.62
1:G:166:GLN:HE22	1:H:45:ALA:HA	1.65	0.62
1:L:32:GLN:CA	1:L:32:GLN:HE21	2.11	0.62
1:E:156:LYS:HE2	2:E:2048:HOH:O	1.98	0.61
1:H:156:LYS:O	1:H:160:ILE:HG12	2.00	0.61
1:E:166:GLN:HE22	1:F:45:ALA:HA	1.64	0.61
1:D:13:TYR:HB3	1:E:69:HIS:CE1	2.36	0.61
1:A:19:LEU:HD12	1:B:103:ARG:HG3	1.83	0.61
1:A:25:THR:HG23	1:A:26:ARG:CD	2.27	0.61
1:E:42:SER:O	1:E:46:THR:HG23	2.01	0.61
1:H:20:ASN:HB3	1:H:160:ILE:CD1	2.30	0.61
1:J:26:ARG:HG2	1:J:26:ARG:HH11	1.65	0.61
1:D:114:LYS:HG2	2:D:2055:HOH:O	2.01	0.61
1:I:77:ILE:HG21	1:I:106:ILE:CG2	2.30	0.60
1:E:26:ARG:HB2	1:E:26:ARG:CZ	2.30	0.60
1:G:45:ALA:HA	1:I:166:GLN:HE22	1.66	0.60
1:D:160:ILE:HD13	1:E:80:MSE:SE	2.51	0.60
1:I:103:ARG:HE	1:I:105:ASN:HD22	1.50	0.60
1:H:168:LEU:HA	1:H:171:ILE:HD11	1.84	0.60
1:H:123:ALA:O	1:H:127:ILE:HD13	2.01	0.60
1:I:7:LYS:NZ	1:I:7:LYS:HB3	2.17	0.60
1:D:171:ILE:HG13	1:D:172:GLU:N	2.17	0.60
1:F:13:TYR:OH	1:F:170:THR:HG23	2.01	0.60
1:I:30:LEU:HB2	2:I:2015:HOH:O	2.02	0.60
1:J:160:ILE:HD13	1:K:80:MSE:SE	2.52	0.59
1:I:15:LYS:HD2	1:I:18:LYS:NZ	2.17	0.59
1:C:22:SER:O	1:C:26:ARG:HG2	2.01	0.59
1:D:78:MSE:HE2	1:D:121:SER:CB	2.31	0.59
1:H:31:ASP:H	1:H:34:GLN:NE2	1.98	0.59
1:C:3:ILE:O	1:C:5:LYS:N	2.36	0.59
1:G:20:ASN:CB	1:G:160:ILE:HD12	2.31	0.59
1:A:19:LEU:CD1	1:B:103:ARG:HG3	2.32	0.59
1:B:17:ILE:CD1	1:C:76:ALA:HB1	2.33	0.59
1:H:77:ILE:HD11	1:H:117:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ARG:HG2	1:E:142:ARG:HH11	1.67	0.58
1:H:20:ASN:CB	1:H:160:ILE:HD12	2.31	0.58
1:D:11:PRO:HD3	1:D:171:ILE:HG21	1.85	0.58
1:L:49:PRO:HG2	2:L:2018:HOH:O	2.02	0.58
1:I:112:ILE:HB	1:I:113:PRO:CD	2.30	0.58
1:B:77:ILE:HD11	1:B:104:MET:HB2	1.86	0.58
1:E:67:ALA:C	1:E:69:HIS:H	2.05	0.58
1:L:98:LEU:CD2	1:L:98:LEU:H	2.15	0.58
1:K:174:LEU:HD21	1:L:52:LEU:HD22	1.84	0.58
1:J:73:GLY:O	1:J:77:ILE:HG12	2.04	0.58
1:I:42:SER:O	1:I:46:THR:HG23	2.03	0.58
1:H:11:PRO:HG3	1:H:171:ILE:HG23	1.85	0.58
1:K:5:LYS:HE2	2:K:2002:HOH:O	2.04	0.57
1:H:77:ILE:HD13	1:H:106:ILE:CG2	2.34	0.57
1:A:98:LEU:HD11	1:C:148:ARG:CZ	2.33	0.57
1:K:5:LYS:HA	1:K:5:LYS:CE	2.14	0.57
1:H:82:ASN:ND2	1:H:128:ASN:HD22	1.99	0.57
1:D:73:GLY:O	1:D:77:ILE:HG13	2.05	0.57
1:B:116:ASN:HB2	2:B:2057:HOH:O	2.04	0.57
1:D:9:ALA:O	1:D:171:ILE:HD13	2.04	0.57
1:D:36:TRP:CH2	1:D:58:GLU:HG2	2.40	0.57
1:D:82:ASN:HD22	1:D:128:ASN:ND2	1.97	0.57
1:G:78:MSE:HE3	1:G:125:SER:OG	2.05	0.57
1:A:170:THR:HG21	2:B:2032:HOH:O	2.04	0.57
1:I:48:ASN:HD22	1:I:48:ASN:C	2.08	0.57
1:C:112:ILE:HB	1:C:113:PRO:CD	2.31	0.57
1:J:32:GLN:NE2	1:J:62:HIS:HD2	2.02	0.57
1:E:15:LYS:HB2	1:E:15:LYS:NZ	2.20	0.57
1:A:98:LEU:HD11	1:C:148:ARG:NH2	2.19	0.57
1:L:32:GLN:HE21	1:L:32:GLN:N	2.03	0.57
1:G:112:ILE:HB	1:G:113:PRO:HD2	1.87	0.57
1:J:156:LYS:O	1:J:160:ILE:HG12	2.05	0.57
1:D:37:GLY:HA3	1:D:120:TRP:CE2	2.40	0.57
1:E:7:LYS:HE2	1:E:22:SER:HB3	1.86	0.57
1:D:78:MSE:HE1	1:D:137:HIS:NE2	2.20	0.56
1:D:135:VAL:HG13	2:D:2065:HOH:O	2.03	0.56
1:B:29:VAL:HG13	1:B:153:GLU:HG2	1.87	0.56
1:J:77:ILE:CG1	1:J:106:ILE:HG21	2.32	0.56
1:J:20:ASN:CB	1:J:160:ILE:HD12	2.32	0.56
1:A:22:SER:O	1:A:25:THR:HG22	2.05	0.56
1:J:31:ASP:H	1:J:34:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:MET:HE3	1:H:107:ILE:HD12	1.87	0.56
1:H:77:ILE:HD11	1:H:117:PHE:HZ	1.70	0.56
1:H:25:THR:HG23	1:H:26:ARG:HH11	1.70	0.56
1:J:48:ASN:ND2	1:J:51:VAL:H	2.03	0.56
1:I:82:ASN:ND2	1:I:128:ASN:HD22	1.95	0.56
1:G:160:ILE:HD13	1:H:80:MSE:SE	2.55	0.56
1:F:22:SER:O	1:F:26:ARG:HG2	2.06	0.56
1:G:52:LEU:HD22	1:I:174:LEU:CD1	2.35	0.56
1:D:7:LYS:HG2	1:D:21:LEU:HD23	1.88	0.56
1:B:35:LEU:O	1:B:39:LEU:HD13	2.06	0.56
1:I:21:LEU:O	1:I:25:THR:HG22	2.06	0.56
1:G:77:ILE:HG23	2:I:2006:HOH:O	2.04	0.56
1:G:49:PRO:HG2	2:G:2014:HOH:O	2.06	0.56
1:H:48:ASN:HD22	1:H:48:ASN:C	2.10	0.56
1:L:23:SER:HB3	1:L:26:ARG:HH12	1.71	0.55
1:D:106:ILE:HD12	1:D:110:PRO:HA	1.88	0.55
1:B:31:ASP:HB2	1:B:34:GLN:CG	2.36	0.55
1:D:166:GLN:NE2	1:E:45:ALA:HA	2.20	0.55
1:D:148:ARG:NH2	1:E:98:LEU:HD21	2.21	0.55
1:F:11:PRO:HD3	1:F:171:ILE:HD11	1.88	0.55
1:J:131:SER:O	1:J:135:VAL:HG12	2.06	0.55
1:J:22:SER:O	1:J:26:ARG:HG3	2.06	0.55
1:K:137:HIS:O	1:K:141:LEU:HD22	2.07	0.55
1:J:22:SER:O	1:J:25:THR:HG22	2.06	0.55
1:E:32:GLN:NE2	1:E:62:HIS:ND1	2.54	0.55
1:L:146:VAL:HG22	1:L:150:ALA:HB3	1.87	0.55
1:G:48:ASN:ND2	1:G:51:VAL:HG23	2.20	0.55
1:E:156:LYS:CE	2:E:2048:HOH:O	2.55	0.55
1:L:91:LEU:O	1:L:94:ARG:HD3	2.07	0.55
1:I:104:MET:HE3	1:I:107:ILE:CD1	2.36	0.54
1:H:73:GLY:O	1:H:77:ILE:HG12	2.07	0.54
1:J:166:GLN:NE2	1:K:45:ALA:HA	2.22	0.54
1:L:98:LEU:HD22	1:L:98:LEU:N	2.22	0.54
1:G:105:ASN:HA	2:G:2034:HOH:O	2.07	0.54
1:L:7:LYS:HB2	1:L:18:LYS:HE2	1.89	0.54
1:H:147:ASP:OD1	1:H:149:GLU:HB2	2.08	0.54
1:A:48:ASN:C	1:A:48:ASN:HD22	2.11	0.54
1:I:103:ARG:HE	1:I:105:ASN:ND2	2.04	0.54
1:G:36:TRP:CH2	1:G:58:GLU:HG2	2.43	0.54
1:D:166:GLN:O	1:D:170:THR:HG23	2.08	0.54
1:J:58:GLU:HB2	2:J:2027:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HD3	1:A:171:ILE:CG1	2.37	0.54
1:E:17:ILE:CD1	1:F:76:ALA:HB1	2.38	0.54
1:H:50:GLN:HG3	2:H:2065:HOH:O	2.07	0.54
1:J:135:VAL:HG13	2:J:2063:HOH:O	2.07	0.54
1:C:145:GLY:O	1:C:146:VAL:O	2.25	0.54
1:L:12:GLU:OE1	1:L:12:GLU:HA	2.07	0.54
1:A:31:ASP:HB2	1:A:34:GLN:HG3	1.90	0.53
1:D:98:LEU:HD11	1:F:148:ARG:NH2	2.23	0.53
1:E:15:LYS:HA	1:E:18:LYS:HE2	1.90	0.53
1:H:58:GLU:OE1	1:H:58:GLU:HA	2.08	0.53
1:H:37:GLY:HA3	1:H:120:TRP:CE2	2.44	0.53
1:J:171:ILE:HG13	1:J:172:GLU:N	2.22	0.53
1:L:141:LEU:HB3	1:L:146:VAL:HG12	1.90	0.53
1:J:11:PRO:HG3	1:J:13:TYR:CE1	2.43	0.53
1:G:78:MSE:HE1	1:G:137:HIS:NE2	2.22	0.53
1:G:94:ARG:HH22	1:I:138:GLU:CD	2.11	0.53
1:I:104:MET:HE2	1:I:107:ILE:HD12	1.86	0.53
1:I:35:LEU:HG	2:I:2015:HOH:O	2.07	0.53
1:F:17:ILE:HD12	1:F:17:ILE:N	2.23	0.53
1:F:118:GLU:OE1	1:F:137:HIS:CD2	2.60	0.53
1:F:7:LYS:HB2	1:F:7:LYS:HZ3	1.72	0.53
1:C:138:GLU:OE2	1:C:142:ARG:HD2	2.09	0.53
1:K:138:GLU:OE1	1:K:138:GLU:C	2.47	0.52
1:D:7:LYS:O	1:D:18:LYS:HD3	2.09	0.52
1:A:37:GLY:HA3	1:A:120:TRP:CE2	2.44	0.52
1:E:3:ILE:N	1:E:3:ILE:HD13	2.24	0.52
1:H:127:ILE:HD13	1:H:158:ALA:HB1	1.87	0.52
1:L:4:GLU:N	2:L:2001:HOH:O	2.42	0.52
1:L:107:ILE:O	1:L:109:ASN:N	2.43	0.52
1:L:141:LEU:O	1:L:144:VAL:HG12	2.10	0.52
1:C:99:ARG:N	1:C:99:ARG:HE	1.93	0.52
1:C:49:PRO:HG2	2:C:2027:HOH:O	2.09	0.52
1:D:139:HIS:CD2	1:D:142:ARG:HH21	2.27	0.52
1:L:119:LEU:O	1:L:122:PHE:HB3	2.10	0.52
1:K:35:LEU:HG	2:K:2016:HOH:O	2.09	0.52
1:K:160:ILE:HD13	1:L:80:MSE:SE	2.59	0.51
1:A:148:ARG:HB2	1:B:95:TYR:CE2	2.45	0.51
1:J:112:ILE:CB	1:J:113:PRO:HD2	2.39	0.51
1:K:77:ILE:HD12	1:K:78:MSE:HG2	1.93	0.51
1:J:148:ARG:NH2	1:K:98:LEU:HD21	2.25	0.51
1:A:22:SER:O	1:A:26:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:SER:O	1:B:46:THR:HG23	2.10	0.51
1:F:32:GLN:NE2	1:F:32:GLN:HA	2.25	0.51
1:C:36:TRP:CB	1:C:63:LEU:HD21	2.40	0.51
1:E:15:LYS:HB2	1:E:15:LYS:HZ2	1.75	0.51
1:L:68:ARG:HH21	1:L:69:HIS:HE1	1.59	0.51
1:B:120:TRP:O	1:B:124:VAL:HG23	2.09	0.51
1:J:20:ASN:HB3	1:J:160:ILE:CD1	2.34	0.51
1:K:77:ILE:HD12	1:K:78:MSE:H	1.76	0.51
1:K:138:GLU:OE1	1:K:139:HIS:N	2.44	0.51
1:I:81:ASN:HD21	1:I:104:MET:CE	2.23	0.51
1:E:64:SER:OG	1:E:65:ALA:N	2.43	0.51
1:J:37:GLY:HA3	1:J:120:TRP:CE2	2.46	0.51
1:L:30:LEU:HB3	1:L:34:GLN:HE21	1.75	0.51
1:F:104:MET:CE	1:F:107:ILE:HD12	2.40	0.51
1:K:77:ILE:HD13	1:K:78:MSE:HE2	1.93	0.51
1:C:142:ARG:NH1	2:C:2080:HOH:O	2.43	0.51
1:L:32:GLN:CA	1:L:32:GLN:NE2	2.73	0.51
1:E:15:LYS:HA	1:E:18:LYS:HG3	1.93	0.51
1:C:149:GLU:CD	1:C:149:GLU:H	2.14	0.51
1:A:88:ARG:HG2	2:A:2040:HOH:O	2.10	0.50
1:H:127:ILE:N	1:H:127:ILE:CD1	2.74	0.50
1:A:127:ILE:CD1	1:A:127:ILE:N	2.73	0.50
1:K:42:SER:O	1:K:46:THR:HG23	2.11	0.50
1:G:77:ILE:HG13	1:G:78:MSE:N	2.27	0.50
1:B:116:ASN:ND2	2:B:2058:HOH:O	2.44	0.50
1:B:118:GLU:OE2	1:B:137:HIS:HD2	1.95	0.50
1:E:36:TRP:CZ3	1:E:58:GLU:HB2	2.47	0.50
2:H:2002:HOH:O	1:I:77:ILE:HG23	2.11	0.50
1:G:127:ILE:HD13	1:H:83:VAL:HG11	1.94	0.50
1:L:59:ALA:HB1	1:L:63:LEU:HD22	1.93	0.50
1:A:104:MET:HB2	1:A:107:ILE:HD12	1.92	0.50
1:J:78:MSE:HE3	1:J:78:MSE:CA	2.28	0.49
1:K:6:LEU:HD12	1:K:168:LEU:HD21	1.94	0.49
1:I:77:ILE:HD13	1:I:106:ILE:CG2	2.42	0.49
1:G:127:ILE:HD12	1:G:162:SER:HG	1.77	0.49
1:K:15:LYS:NZ	2:K:2011:HOH:O	2.44	0.49
1:K:170:THR:HG21	1:L:44:ALA:HB1	1.93	0.49
1:I:77:ILE:HD11	1:I:117:PHE:CZ	2.48	0.49
1:C:59:ALA:HB1	1:C:63:LEU:HD23	1.94	0.49
1:A:46:THR:O	1:A:47:ARG:HB2	2.12	0.49
1:J:80:MSE:HE1	1:L:20:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:GLY:HA3	1:K:120:TRP:CE2	2.48	0.49
1:J:107:ILE:HD12	1:J:107:ILE:N	2.28	0.49
1:K:148:ARG:CZ	1:L:98:LEU:HD21	2.43	0.49
1:J:11:PRO:HB3	1:J:171:ILE:HG21	1.93	0.49
1:A:99:ARG:HH11	1:A:99:ARG:HG2	1.77	0.49
1:E:60:THR:C	1:E:62:HIS:H	2.14	0.49
1:L:30:LEU:HB3	1:L:34:GLN:NE2	2.28	0.49
1:K:4:GLU:OE1	1:K:7:LYS:HD3	2.12	0.49
1:K:127:ILE:HD13	1:L:83:VAL:CG1	2.42	0.49
1:B:138:GLU:OE1	1:C:94:ARG:NH2	2.46	0.49
1:G:20:ASN:HB3	1:G:160:ILE:CD1	2.36	0.49
1:D:74:ALA:O	1:D:77:ILE:HD12	2.12	0.49
1:E:64:SER:HB3	1:E:67:ALA:HB3	1.94	0.49
1:A:37:GLY:HA3	1:A:120:TRP:CZ2	2.48	0.49
1:I:171:ILE:HG13	1:I:172:GLU:N	2.28	0.49
1:K:112:ILE:CB	1:K:113:PRO:HD2	2.37	0.49
1:F:32:GLN:HE21	1:F:32:GLN:CA	2.26	0.49
1:D:107:ILE:N	1:D:107:ILE:HD12	2.28	0.48
1:L:141:LEU:C	1:L:146:VAL:HG12	2.33	0.48
1:L:37:GLY:HA3	1:L:120:TRP:CE2	2.48	0.48
1:B:127:ILE:HD11	1:B:158:ALA:O	2.13	0.48
1:I:141:LEU:HD23	1:I:151:ILE:HG12	1.94	0.48
1:C:147:ASP:N	1:C:147:ASP:OD2	2.37	0.48
1:A:127:ILE:HD13	1:A:158:ALA:HB1	1.89	0.48
1:A:22:SER:O	1:A:25:THR:CG2	2.62	0.48
1:H:77:ILE:HG21	1:H:106:ILE:HG21	1.93	0.48
1:A:166:GLN:NE2	1:B:45:ALA:HA	2.26	0.48
1:C:119:LEU:HD11	1:C:154:ALA:HB2	1.95	0.48
1:I:6:LEU:HD12	1:I:168:LEU:HD21	1.96	0.48
1:K:171:ILE:HD12	1:K:171:ILE:C	2.33	0.48
1:J:135:VAL:HG13	1:J:136:ALA:N	2.29	0.48
1:B:60:THR:HA	2:B:2027:HOH:O	2.14	0.48
1:E:174:LEU:O	1:E:175:SER:HB3	2.14	0.48
1:L:6:LEU:HD11	1:L:168:LEU:HD21	1.95	0.48
1:C:98:LEU:HD12	2:C:2056:HOH:O	2.13	0.48
1:I:112:ILE:CB	1:I:113:PRO:HD2	2.34	0.48
1:L:13:TYR:HE1	1:L:170:THR:HG21	1.79	0.48
1:L:13:TYR:OH	1:L:170:THR:HG23	2.14	0.48
1:D:148:ARG:CZ	1:E:98:LEU:HD21	2.44	0.48
1:A:48:ASN:ND2	1:A:51:VAL:H	2.11	0.48
1:H:100:PRO:HB2	2:H:2035:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:ILE:O	1:F:4:GLU:CB	2.62	0.48
1:I:10:LEU:HD23	1:I:168:LEU:HD13	1.95	0.48
1:A:76:ALA:HB1	1:C:17:ILE:HD12	1.95	0.48
1:H:25:THR:HG23	1:H:26:ARG:NH1	2.28	0.48
1:A:32:GLN:CA	1:A:32:GLN:NE2	2.76	0.48
1:I:81:ASN:HD21	1:I:104:MET:HE3	1.79	0.47
1:I:119:LEU:HD11	1:I:154:ALA:HB2	1.96	0.47
1:L:21:LEU:O	1:L:25:THR:HG22	2.13	0.47
1:A:160:ILE:CD1	1:B:80:MSE:SE	3.10	0.47
1:L:112:ILE:HD11	1:L:117:PHE:HB2	1.96	0.47
1:A:32:GLN:HE21	1:A:32:GLN:CA	2.27	0.47
1:F:3:ILE:N	1:F:58:GLU:CG	2.76	0.47
1:J:166:GLN:O	1:J:170:THR:HG23	2.14	0.47
1:C:119:LEU:HA	1:C:141:LEU:HD11	1.96	0.47
1:I:5:LYS:HE2	1:I:5:LYS:CA	2.43	0.47
1:A:51:VAL:HG21	1:A:165:ALA:HA	1.96	0.47
1:G:31:ASP:OD1	1:G:34:GLN:HB2	2.13	0.47
1:D:156:LYS:O	1:D:160:ILE:HG12	2.15	0.47
1:A:47:ARG:N	1:A:47:ARG:HD3	2.30	0.47
1:A:108:ALA:C	1:A:109:ASN:HD22	2.18	0.47
1:F:144:VAL:CG1	1:F:144:VAL:O	2.61	0.47
1:A:13:TYR:HB3	1:B:69:HIS:CE1	2.49	0.47
1:E:78:MSE:HE3	1:E:82:ASN:OD1	2.15	0.47
1:K:127:ILE:CD1	1:L:83:VAL:HG11	2.45	0.47
1:H:77:ILE:HD12	1:H:107:ILE:CG1	2.45	0.47
1:H:7:LYS:O	1:H:18:LYS:HD3	2.14	0.47
1:H:47:ARG:NH2	2:H:2013:HOH:O	2.31	0.47
1:I:107:ILE:HA	1:I:117:PHE:CE2	2.50	0.47
1:H:166:GLN:NE2	1:I:45:ALA:HA	2.26	0.47
1:J:168:LEU:HD12	1:J:171:ILE:HD11	1.96	0.47
1:E:67:ALA:C	1:E:69:HIS:N	2.68	0.47
1:F:104:MET:HE2	1:F:107:ILE:HD12	1.97	0.47
1:E:134:LEU:HD23	1:F:90:PHE:HB2	1.96	0.47
1:J:112:ILE:HB	1:J:113:PRO:CD	2.38	0.47
1:E:82:ASN:ND2	1:E:128:ASN:HD22	1.98	0.46
1:H:156:LYS:HD2	1:I:100:PRO:O	2.15	0.46
1:K:77:ILE:HD13	1:K:78:MSE:CE	2.45	0.46
1:E:15:LYS:CB	1:E:15:LYS:NZ	2.78	0.46
1:E:10:LEU:HB2	1:E:18:LYS:HZ2	1.79	0.46
1:A:7:LYS:HE3	1:A:22:SER:OG	2.16	0.46
1:D:13:TYR:HB3	1:E:69:HIS:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LYS:O	1:I:19:LEU:CD2	2.63	0.46
1:E:31:ASP:HB2	2:E:2008:HOH:O	2.15	0.46
1:E:31:ASP:OD2	1:E:34:GLN:HG3	2.14	0.46
1:H:11:PRO:HG3	1:H:171:ILE:HG21	1.95	0.46
1:L:23:SER:HA	1:L:26:ARG:HH11	1.81	0.46
1:G:17:ILE:CD1	1:H:76:ALA:HB1	2.44	0.46
1:G:141:LEU:O	1:G:144:VAL:HG22	2.15	0.46
1:D:77:ILE:HG23	1:F:17:ILE:HD11	1.97	0.46
1:E:64:SER:HB3	1:E:67:ALA:CB	2.46	0.46
1:I:3:ILE:O	1:I:7:LYS:HG3	2.15	0.46
1:A:123:ALA:O	1:A:127:ILE:HD13	2.14	0.46
1:E:137:HIS:O	1:E:141:LEU:CD2	2.63	0.46
1:E:110:PRO:HG2	1:E:112:ILE:O	2.16	0.46
1:I:23:SER:HB3	2:I:2012:HOH:O	2.14	0.46
1:A:77:ILE:HD13	1:A:80:MSE:HE2	1.98	0.46
1:I:108:ALA:O	1:I:109:ASN:CG	2.54	0.46
1:E:39:LEU:O	1:E:55:ILE:HG21	2.15	0.46
1:D:31:ASP:O	1:D:35:LEU:HB2	2.16	0.46
1:D:160:ILE:CD1	1:E:80:MSE:SE	3.13	0.46
1:J:55:ILE:N	1:J:55:ILE:HD12	2.31	0.46
1:L:26:ARG:HG2	1:L:26:ARG:HH11	1.80	0.46
1:G:170:THR:HG22	1:H:44:ALA:HB1	1.98	0.46
1:F:3:ILE:HG13	1:F:4:GLU:N	2.31	0.46
1:D:99:ARG:HH11	1:D:99:ARG:HG2	1.80	0.46
1:B:153:GLU:OE2	1:B:156:LYS:HE2	2.16	0.46
1:H:42:SER:O	1:H:46:THR:HG23	2.16	0.46
1:F:98:LEU:N	1:F:98:LEU:HD22	2.31	0.46
1:D:78:MSE:CE	1:D:125:SER:OG	2.51	0.46
1:E:156:LYS:NZ	1:E:156:LYS:CB	2.79	0.45
1:A:51:VAL:HG22	1:A:168:LEU:HD22	1.98	0.45
1:C:78:MSE:HE1	1:C:81:ASN:CB	2.46	0.45
1:E:78:MSE:HE2	1:E:125:SER:HB3	1.95	0.45
1:L:112:ILE:HD12	1:L:112:ILE:C	2.36	0.45
1:D:106:ILE:CD1	1:D:110:PRO:HA	2.46	0.45
1:B:27:SER:OG	1:B:29:VAL:HG12	2.16	0.45
1:I:138:GLU:HB3	2:I:2049:HOH:O	2.17	0.45
1:G:78:MSE:CE	1:G:121:SER:O	2.65	0.45
1:D:78:MSE:HE3	1:D:121:SER:O	2.15	0.45
1:D:9:ALA:O	1:D:171:ILE:CD1	2.64	0.45
1:B:147:ASP:HB3	1:B:149:GLU:HG2	1.99	0.45
1:E:147:ASP:CG	1:E:149:GLU:HG2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:LEU:O	1:K:122:PHE:HB3	2.16	0.45
1:I:77:ILE:HD12	1:I:107:ILE:CG1	2.47	0.45
1:J:26:ARG:HG2	1:J:26:ARG:NH1	2.30	0.45
1:I:15:LYS:O	1:I:19:LEU:HD22	2.17	0.45
1:C:26:ARG:HD3	1:C:26:ARG:HA	1.77	0.45
1:B:170:THR:HG21	2:B:2076:HOH:O	2.15	0.45
1:E:142:ARG:HG2	1:E:142:ARG:NH1	2.31	0.45
1:E:114:LYS:O	1:E:115:ALA:C	2.54	0.45
1:L:108:ALA:HB2	2:L:2038:HOH:O	2.16	0.45
1:J:19:LEU:HD13	1:J:19:LEU:C	2.37	0.45
1:E:168:LEU:O	1:E:171:ILE:HG13	2.16	0.45
1:I:37:GLY:HA3	1:I:120:TRP:CZ2	2.51	0.45
1:F:32:GLN:CA	1:F:32:GLN:NE2	2.80	0.45
1:B:174:LEU:HD21	1:C:52:LEU:HD22	1.99	0.45
1:A:88:ARG:HD2	2:A:2039:HOH:O	2.17	0.45
1:A:76:ALA:O	1:C:17:ILE:HD11	2.17	0.45
1:J:139:HIS:CD2	1:J:142:ARG:HH21	2.34	0.45
1:A:21:LEU:O	1:A:25:THR:HG22	2.17	0.45
1:H:112:ILE:HB	1:H:113:PRO:CD	2.44	0.45
1:A:17:ILE:HD12	1:B:76:ALA:HB1	1.98	0.45
1:D:88:ARG:HG2	2:D:2044:HOH:O	2.17	0.45
1:L:118:GLU:OE1	1:L:137:HIS:HD2	1.99	0.45
1:D:32:GLN:OE1	1:D:32:GLN:HA	2.17	0.45
1:J:32:GLN:HE21	1:J:62:HIS:HD2	1.64	0.45
1:C:59:ALA:O	1:C:63:LEU:HD23	2.17	0.45
1:G:37:GLY:HA3	1:G:120:TRP:CE2	2.51	0.45
1:L:149:GLU:HG2	2:L:2061:HOH:O	2.17	0.44
1:E:135:VAL:O	1:E:136:ALA:C	2.55	0.44
1:L:152:PHE:CD2	1:L:156:LYS:HD3	2.52	0.44
1:D:47:ARG:N	1:D:47:ARG:HD3	2.31	0.44
1:K:112:ILE:HD12	1:K:116:ASN:HB2	1.99	0.44
1:I:37:GLY:HA3	1:I:120:TRP:NE1	2.32	0.44
1:C:36:TRP:HB3	1:C:63:LEU:HD21	1.99	0.44
1:J:107:ILE:O	1:J:110:PRO:HD3	2.17	0.44
1:A:20:ASN:CB	1:A:160:ILE:HD12	2.38	0.44
1:D:19:LEU:CD2	1:E:103:ARG:HG3	2.48	0.44
1:I:18:LYS:HD3	2:I:2001:HOH:O	2.18	0.44
1:G:94:ARG:NH2	1:I:138:GLU:OE2	2.50	0.44
1:I:119:LEU:HA	1:I:141:LEU:HD21	1.98	0.44
1:L:116:ASN:HD22	1:L:116:ASN:N	2.15	0.44
1:C:3:ILE:CG2	1:C:4:GLU:N	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:THR:CG2	1:D:26:ARG:HE	2.31	0.44
1:E:17:ILE:HD11	1:F:76:ALA:HB1	1.99	0.44
1:D:112:ILE:HD12	1:D:112:ILE:C	2.38	0.44
1:I:59:ALA:HB1	1:I:63:LEU:HD12	1.98	0.44
1:F:3:ILE:HD12	1:F:7:LYS:NZ	2.32	0.44
1:A:19:LEU:HD13	1:A:19:LEU:C	2.38	0.44
1:K:10:LEU:HD23	1:K:168:LEU:HD13	2.00	0.44
1:G:37:GLY:HA3	1:G:120:TRP:CZ2	2.53	0.44
1:D:67:ALA:HA	1:D:112:ILE:HG21	2.00	0.44
1:C:104:MET:HE3	2:C:2059:HOH:O	2.16	0.44
1:C:98:LEU:HD13	1:C:99:ARG:HH21	1.83	0.44
1:B:5:LYS:HD2	1:B:5:LYS:HA	1.75	0.44
1:A:31:ASP:H	1:A:34:GLN:HE21	0.74	0.44
1:G:166:GLN:NE2	1:H:45:ALA:HA	2.32	0.44
1:L:112:ILE:HD12	1:L:112:ILE:O	2.18	0.44
1:L:32:GLN:HG3	1:L:36:TRP:CD1	2.53	0.44
1:E:35:LEU:HD13	1:E:39:LEU:HD22	2.00	0.44
1:I:77:ILE:HG13	1:I:78:MSE:N	2.33	0.43
1:H:37:GLY:HA3	1:H:120:TRP:CZ2	2.53	0.43
1:L:109:ASN:ND2	1:L:114:LYS:HE3	2.33	0.43
1:H:112:ILE:CB	1:H:113:PRO:HD2	2.43	0.43
1:A:166:GLN:O	1:A:170:THR:HG23	2.18	0.43
1:A:137:HIS:O	1:A:141:LEU:CD2	2.63	0.43
1:J:32:GLN:HA	1:J:32:GLN:OE1	2.18	0.43
1:L:28:SER:OG	1:L:30:LEU:O	2.34	0.43
1:K:18:LYS:HD3	2:K:2003:HOH:O	2.19	0.43
1:K:22:SER:O	1:K:26:ARG:HG3	2.19	0.43
1:F:94:ARG:CG	1:F:94:ARG:HH11	2.28	0.43
1:J:37:GLY:HA3	1:J:120:TRP:CZ2	2.53	0.43
1:A:139:HIS:CD2	1:A:142:ARG:HH21	2.37	0.43
1:G:138:GLU:HG2	1:G:151:ILE:HG21	2.00	0.43
1:C:98:LEU:CD2	1:C:98:LEU:N	2.81	0.43
1:L:32:GLN:HA	1:L:32:GLN:NE2	2.33	0.43
1:B:171:ILE:HG13	1:B:172:GLU:N	2.33	0.43
1:C:7:LYS:HG2	1:C:21:LEU:HD23	2.00	0.43
1:B:118:GLU:CB	1:B:141:LEU:CD1	2.96	0.43
1:L:119:LEU:HD11	1:L:154:ALA:HB2	2.00	0.43
1:A:77:ILE:HG23	1:A:78:MSE:HE2	2.01	0.43
1:B:22:SER:O	1:B:26:ARG:HG2	2.18	0.43
1:D:19:LEU:HD21	1:E:103:ARG:HE	1.84	0.43
1:I:15:LYS:HD2	1:I:18:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:HB3	1:D:151:ILE:HD11	2.00	0.43
1:I:28:SER:HB3	1:I:29:VAL:H	1.67	0.43
1:I:119:LEU:O	1:I:122:PHE:HB3	2.19	0.43
1:E:68:ARG:HH11	1:E:68:ARG:HG3	1.83	0.43
1:B:141:LEU:HB3	1:B:151:ILE:HD11	1.99	0.43
1:B:166:GLN:NE2	1:C:45:ALA:HA	2.30	0.43
1:J:46:THR:O	1:J:47:ARG:HB2	2.19	0.43
1:G:119:LEU:HD11	1:G:154:ALA:HB2	2.01	0.43
1:J:98:LEU:O	1:J:99:ARG:HB3	2.18	0.43
1:K:133:CYS:O	1:K:137:HIS:CD2	2.72	0.43
1:A:16:ASP:HB3	1:B:103:ARG:O	2.19	0.43
1:D:37:GLY:HA3	1:D:120:TRP:CZ2	2.53	0.43
1:F:63:LEU:HB3	1:F:68:ARG:HG3	2.01	0.43
1:J:98:LEU:HD11	1:L:148:ARG:CZ	2.47	0.43
1:B:166:GLN:NE2	1:C:47:ARG:HE	2.17	0.43
1:I:7:LYS:NZ	1:I:7:LYS:CB	2.82	0.43
1:I:48:ASN:ND2	1:I:48:ASN:C	2.72	0.43
1:C:147:ASP:OD1	1:C:149:GLU:HG2	2.18	0.43
1:E:113:PRO:O	1:E:114:LYS:C	2.57	0.43
1:J:78:MSE:HE2	1:J:82:ASN:CG	2.34	0.42
1:H:107:ILE:HA	1:H:117:PHE:CE2	2.54	0.42
1:L:30:LEU:HB3	1:L:34:GLN:HB3	2.00	0.42
1:K:15:LYS:HD2	1:K:18:LYS:HE2	2.01	0.42
1:G:59:ALA:HB1	1:G:63:LEU:HG	2.01	0.42
1:J:20:ASN:HD21	1:K:103:ARG:N	2.06	0.42
1:H:160:ILE:HD11	1:I:102:LEU:CD2	2.39	0.42
1:C:118:GLU:OE1	1:C:137:HIS:CD2	2.65	0.42
1:C:32:GLN:NE2	1:C:32:GLN:HA	2.33	0.42
1:H:116:ASN:ND2	2:H:2042:HOH:O	2.49	0.42
1:B:3:ILE:CD1	1:B:25:THR:HG21	2.43	0.42
1:K:74:ALA:HA	1:K:77:ILE:HD11	2.01	0.42
1:J:21:LEU:HD22	1:J:164:VAL:HG21	2.01	0.42
1:J:21:LEU:O	1:J:25:THR:HG22	2.19	0.42
1:I:103:ARG:HH21	1:I:105:ASN:HD22	1.61	0.42
1:I:103:ARG:NH2	1:I:105:ASN:ND2	2.64	0.42
1:F:119:LEU:HA	1:F:141:LEU:HD11	2.01	0.42
1:I:77:ILE:HD13	1:I:106:ILE:HG23	2.02	0.42
1:L:94:ARG:NH1	2:L:2035:HOH:O	2.49	0.42
1:A:47:ARG:NH2	2:A:2016:HOH:O	2.40	0.42
1:I:109:ASN:O	1:I:109:ASN:OD1	2.37	0.42
1:G:10:LEU:HA	1:G:11:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:35:LEU:C	1:L:35:LEU:CD2	2.88	0.42
1:G:78:MSE:CE	1:G:125:SER:OG	2.67	0.42
1:K:94:ARG:HD3	1:K:95:TYR:CE1	2.55	0.42
1:F:82:ASN:ND2	1:F:128:ASN:HD22	1.99	0.42
1:L:38:THR:HA	1:L:120:TRP:CD1	2.55	0.42
1:B:29:VAL:HG11	1:B:153:GLU:CD	2.39	0.42
1:K:119:LEU:HD11	1:K:154:ALA:HB2	2.02	0.42
1:H:19:LEU:O	1:H:19:LEU:HD13	2.19	0.42
1:L:82:ASN:ND2	1:L:125:SER:HA	2.35	0.42
1:J:48:ASN:HD21	1:J:50:GLN:HB3	1.85	0.42
1:K:44:ALA:HA	1:K:52:LEU:HG	2.00	0.42
1:E:24:ILE:HG13	1:E:160:ILE:HD12	2.01	0.42
1:G:82:ASN:ND2	1:G:128:ASN:HD22	2.12	0.42
1:J:48:ASN:ND2	1:J:51:VAL:HG23	2.35	0.42
1:A:77:ILE:CD1	1:A:80:MSE:HE2	2.50	0.42
1:J:19:LEU:HD13	1:J:19:LEU:O	2.20	0.42
1:C:32:GLN:NE2	1:C:32:GLN:CA	2.82	0.42
1:F:6:LEU:HD12	1:F:168:LEU:HD21	2.01	0.42
1:E:6:LEU:HD22	1:E:168:LEU:HD21	2.01	0.42
1:L:35:LEU:C	1:L:35:LEU:HD23	2.40	0.42
1:J:7:LYS:NZ	1:J:22:SER:OG	2.46	0.42
1:I:30:LEU:HD21	1:I:150:ALA:O	2.20	0.42
1:I:135:VAL:HG23	1:I:136:ALA:N	2.35	0.41
1:A:48:ASN:C	1:A:48:ASN:ND2	2.73	0.41
1:H:47:ARG:NE	2:H:2013:HOH:O	2.51	0.41
1:F:40:LEU:HD13	1:F:56:GLY:HA2	2.01	0.41
1:C:37:GLY:HA3	1:C:120:TRP:CZ2	2.55	0.41
1:G:82:ASN:HD21	1:G:125:SER:HA	1.85	0.41
1:A:72:LEU:HD22	1:C:170:THR:OG1	2.20	0.41
1:F:7:LYS:NZ	1:F:7:LYS:CB	2.81	0.41
1:J:9:ALA:O	1:J:171:ILE:CD1	2.68	0.41
1:E:142:ARG:O	1:E:145:GLY:N	2.49	0.41
1:H:48:ASN:ND2	1:H:48:ASN:C	2.72	0.41
1:H:114:LYS:HB2	1:H:114:LYS:HE2	1.89	0.41
1:L:160:ILE:O	1:L:164:VAL:HG23	2.20	0.41
1:J:47:ARG:HD3	1:J:47:ARG:N	2.35	0.41
1:B:10:LEU:HD23	1:B:168:LEU:HD13	2.03	0.41
1:K:68:ARG:HG3	1:K:68:ARG:NH1	2.36	0.41
1:D:48:ASN:ND2	1:D:51:VAL:HG23	2.34	0.41
1:K:30:LEU:HB2	2:K:2016:HOH:O	2.20	0.41
1:C:147:ASP:HB2	1:C:149:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:LEU:CD1	1:F:168:LEU:HD21	2.50	0.41
1:B:118:GLU:CB	1:B:141:LEU:HD13	2.47	0.41
1:E:156:LYS:NZ	2:E:2048:HOH:O	2.35	0.41
1:I:46:THR:HG21	1:I:161:VAL:HG12	2.02	0.41
1:E:11:PRO:HG3	1:E:13:TYR:CZ	2.55	0.41
1:G:25:THR:HG23	1:G:25:THR:O	2.20	0.41
1:K:94:ARG:HD3	1:K:95:TYR:HE1	1.86	0.41
1:K:112:ILE:CD1	1:K:116:ASN:HB2	2.50	0.41
1:B:78:MSE:HE2	1:B:121:SER:O	2.21	0.41
1:G:127:ILE:HD11	1:G:158:ALA:O	2.19	0.41
1:B:118:GLU:HB3	1:B:141:LEU:CD1	2.48	0.41
1:F:22:SER:O	1:F:25:THR:HG22	2.21	0.41
1:D:160:ILE:HD11	1:E:102:LEU:CD2	2.37	0.41
1:I:168:LEU:HD12	1:I:168:LEU:HA	1.92	0.41
1:J:42:SER:O	1:J:46:THR:HG23	2.21	0.41
1:E:94:ARG:HD2	1:E:95:TYR:CE1	2.56	0.41
1:H:82:ASN:HD22	1:H:128:ASN:ND2	2.01	0.41
1:F:82:ASN:HD22	1:F:128:ASN:ND2	2.00	0.41
1:E:6:LEU:CD2	1:E:168:LEU:HD21	2.51	0.41
1:K:148:ARG:HG2	1:K:149:GLU:OE2	2.21	0.41
1:K:127:ILE:HD11	1:K:158:ALA:O	2.21	0.41
1:K:48:ASN:ND2	1:K:48:ASN:C	2.72	0.41
1:L:6:LEU:CD1	1:L:168:LEU:HD21	2.50	0.41
1:A:17:ILE:CD1	1:B:76:ALA:HB1	2.51	0.41
1:K:148:ARG:HH22	1:L:97:ASP:CG	2.25	0.41
1:K:148:ARG:NH2	1:L:98:LEU:HD21	2.35	0.41
1:J:4:GLU:OE1	1:J:7:LYS:HD3	2.20	0.41
1:E:140:THR:O	1:E:144:VAL:HG23	2.21	0.41
1:J:107:ILE:HA	1:J:117:PHE:CE2	2.56	0.40
1:D:6:LEU:HD11	1:D:168:LEU:HD22	2.03	0.40
1:F:17:ILE:N	1:F:17:ILE:CD1	2.84	0.40
1:E:141:LEU:O	1:E:146:VAL:HG23	2.20	0.40
1:G:84:PHE:CZ	1:G:100:PRO:HB3	2.56	0.40
1:D:78:MSE:CE	1:D:121:SER:O	2.70	0.40
1:D:11:PRO:HB3	1:D:171:ILE:CG2	2.51	0.40
1:F:94:ARG:HG2	1:F:94:ARG:NH1	2.32	0.40
1:E:118:GLU:OE2	1:E:140:THR:HG21	2.21	0.40
1:F:122:PHE:CE1	1:F:134:LEU:HD11	2.56	0.40
1:G:116:ASN:HD22	1:G:116:ASN:N	2.20	0.40
1:E:170:THR:CG2	1:F:44:ALA:HB1	2.52	0.40
1:G:77:ILE:HG13	1:G:78:MSE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ASP:N	1:H:34:GLN:HE21	2.06	0.40
1:H:77:ILE:HD12	1:H:107:ILE:HG12	2.03	0.40
1:L:23:SER:HA	1:L:26:ARG:HG2	2.03	0.40
1:L:32:GLN:HG3	1:L:36:TRP:HD1	1.86	0.40
1:I:48:ASN:ND2	1:I:51:VAL:H	2.19	0.40
1:I:28:SER:O	1:I:29:VAL:HB	2.21	0.40
1:H:140:THR:O	1:H:144:VAL:HG22	2.21	0.40
1:H:152:PHE:CG	1:I:98:LEU:HD23	2.56	0.40
1:G:146:VAL:HG12	1:G:150:ALA:HB3	2.03	0.40
1:K:112:ILE:HB	1:K:113:PRO:CD	2.40	0.40
1:H:104:MET:HE3	1:H:107:ILE:CD1	2.51	0.40
1:L:109:ASN:H	1:L:114:LYS:HD3	1.86	0.40
1:A:47:ARG:NE	2:A:2016:HOH:O	2.38	0.40
1:C:140:THR:O	1:C:143:THR:HB	2.20	0.40
1:J:93:GLY:HA2	1:J:96:ASP:OD2	2.22	0.40
1:I:107:ILE:HG12	1:I:117:PHE:HE2	1.86	0.40
1:B:34:GLN:HG2	1:B:116:ASN:ND2	2.36	0.40
1:I:35:LEU:HD22	1:I:39:LEU:HD11	2.02	0.40
1:F:56:GLY:O	1:F:68:ARG:NH1	2.51	0.40
1:G:12:GLU:OE2	1:G:12:GLU:HA	2.22	0.40
1:E:38:THR:HG1	1:E:120:TRP:HD1	1.65	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	170/177 (96%)	162 (95%)	6 (4%)	2 (1%)	16	5
1	B	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	C	166/177 (94%)	157 (95%)	7 (4%)	2 (1%)	16	5
1	D	170/177 (96%)	164 (96%)	5 (3%)	1 (1%)	30	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	171/177 (97%)	157 (92%)	10 (6%)	4 (2%)	8	1
1	F	167/177 (94%)	165 (99%)	1 (1%)	1 (1%)	30	17
1	G	166/177 (94%)	155 (93%)	9 (5%)	2 (1%)	16	5
1	H	169/177 (96%)	161 (95%)	7 (4%)	1 (1%)	30	17
1	I	171/177 (97%)	160 (94%)	10 (6%)	1 (1%)	30	17
1	J	170/177 (96%)	158 (93%)	9 (5%)	3 (2%)	11	2
1	K	171/177 (97%)	163 (95%)	7 (4%)	1 (1%)	30	17
1	L	166/177 (94%)	155 (93%)	8 (5%)	3 (2%)	11	2
All	All	2028/2124 (96%)	1922 (95%)	85 (4%)	21 (1%)	19	7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	E	64	SER
1	E	115	ALA
1	G	100	PRO
1	J	109	ASN
1	C	146	VAL
1	L	108	ALA
1	C	4	GLU
1	F	4	GLU
1	J	110	PRO
1	L	110	PRO
1	D	99	ARG
1	G	99	ARG
1	I	28	SER
1	J	99	ARG
1	K	27	SER
1	E	35	LEU
1	E	114	LYS
1	L	109	ASN
1	A	31	ASP
1	H	110	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/130 (98%)	119 (93%)	9 (7%)	19	8
1	B	129/130 (99%)	123 (95%)	6 (5%)	32	20
1	C	125/130 (96%)	115 (92%)	10 (8%)	15	6
1	D	128/130 (98%)	118 (92%)	10 (8%)	16	6
1	E	129/130 (99%)	121 (94%)	8 (6%)	23	11
1	F	126/130 (97%)	116 (92%)	10 (8%)	15	6
1	G	125/130 (96%)	117 (94%)	8 (6%)	22	10
1	H	127/130 (98%)	119 (94%)	8 (6%)	22	10
1	I	129/130 (99%)	118 (92%)	11 (8%)	13	5
1	J	128/130 (98%)	123 (96%)	5 (4%)	39	27
1	K	129/130 (99%)	121 (94%)	8 (6%)	23	11
1	L	125/130 (96%)	117 (94%)	8 (6%)	22	10
All	All	1528/1560 (98%)	1427 (93%)	101 (7%)	21	10

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	26	ARG
1	A	47	ARG
1	A	48	ASN
1	A	52	LEU
1	A	77	ILE
1	A	127	ILE
1	A	141	LEU
1	A	172	GLU
1	B	5	LYS
1	B	31	ASP
1	B	141	LEU
1	B	147	ASP
1	B	149	GLU
1	B	168	LEU
1	C	32	GLN
1	C	35	LEU
1	C	52	LEU

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Mol	Chain	Res	Type
1	C	58	GLU
1	C	61	ASP
1	C	78	MSE
1	C	99	ARG
1	C	106	ILE
1	C	109	ASN
1	C	149	GLU
1	D	26	ARG
1	D	32	GLN
1	D	35	LEU
1	D	47	ARG
1	D	48	ASN
1	D	52	LEU
1	D	54	ASP
1	D	103	ARG
1	D	114	LYS
1	D	141	LEU
1	E	3	ILE
1	E	5	LYS
1	E	24	ILE
1	E	26	ARG
1	E	68	ARG
1	E	148	ARG
1	E	149	GLU
1	E	168	LEU
1	F	19	LEU
1	F	32	GLN
1	F	35	LEU
1	F	52	LEU
1	F	54	ASP
1	F	58	GLU
1	F	94	ARG
1	F	99	ARG
1	F	109	ASN
1	F	170	THR
1	G	3	ILE
1	G	19	LEU
1	G	21	LEU
1	G	34	GLN
1	G	47	ARG
1	G	48	ASN
1	G	52	LEU

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Mol	Chain	Res	Type
1	G	141	LEU
1	H	35	LEU
1	H	48	ASN
1	H	52	LEU
1	H	109	ASN
1	H	114	LYS
1	H	127	ILE
1	H	141	LEU
1	H	171	ILE
1	I	5	LYS
1	I	32	GLN
1	I	35	LEU
1	I	48	ASN
1	I	52	LEU
1	I	98	LEU
1	I	141	LEU
1	I	149	GLU
1	I	168	LEU
1	I	172	GLU
1	I	174	LEU
1	J	47	ARG
1	J	48	ASN
1	J	52	LEU
1	J	114	LYS
1	J	141	LEU
1	K	5	LYS
1	K	19	LEU
1	K	35	LEU
1	K	48	ASN
1	K	52	LEU
1	K	94	ARG
1	K	141	LEU
1	K	168	LEU
1	L	7	LYS
1	L	32	GLN
1	L	34	GLN
1	L	35	LEU
1	L	47	ARG
1	L	52	LEU
1	L	98	LEU
1	L	103	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	34	GLN
1	A	48	ASN
1	A	62	HIS
1	A	109	ASN
1	A	116	ASN
1	A	139	HIS
1	A	166	GLN
1	B	20	ASN
1	B	32	GLN
1	B	50	GLN
1	B	62	HIS
1	B	109	ASN
1	B	116	ASN
1	B	128	ASN
1	B	132	HIS
1	B	137	HIS
1	B	166	GLN
1	C	20	ASN
1	C	32	GLN
1	C	116	ASN
1	C	137	HIS
1	D	34	GLN
1	D	48	ASN
1	D	62	HIS
1	D	82	ASN
1	D	116	ASN
1	D	139	HIS
1	D	166	GLN
1	E	20	ASN
1	E	32	GLN
1	E	50	GLN
1	E	116	ASN
1	E	128	ASN
1	E	132	HIS
1	E	137	HIS
1	E	166	GLN
1	F	20	ASN
1	F	32	GLN
1	F	82	ASN
1	F	116	ASN
1	F	137	HIS

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Mol	Chain	Res	Type
1	G	34	GLN
1	G	48	ASN
1	G	82	ASN
1	G	105	ASN
1	G	116	ASN
1	G	166	GLN
1	H	34	GLN
1	H	48	ASN
1	H	81	ASN
1	H	82	ASN
1	H	116	ASN
1	H	166	GLN
1	I	34	GLN
1	I	48	ASN
1	I	69	HIS
1	I	81	ASN
1	I	82	ASN
1	I	105	ASN
1	I	109	ASN
1	I	116	ASN
1	I	166	GLN
1	J	20	ASN
1	J	34	GLN
1	J	48	ASN
1	J	62	HIS
1	J	109	ASN
1	J	116	ASN
1	J	139	HIS
1	J	166	GLN
1	K	32	GLN
1	K	48	ASN
1	K	81	ASN
1	K	82	ASN
1	K	105	ASN
1	K	116	ASN
1	K	166	GLN
1	L	20	ASN
1	L	32	GLN
1	L	34	GLN
1	L	69	HIS
1	L	82	ASN
1	L	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	170/177 (96%)	0.27	6 (3%)	48 51	9, 26, 59, 73	0
1	B	170/177 (96%)	0.42	9 (5%)	30 33	10, 30, 56, 71	0
1	C	166/177 (93%)	0.25	4 (2%)	62 66	9, 25, 50, 69	0
1	D	170/177 (96%)	0.20	6 (3%)	48 51	7, 24, 54, 67	0
1	E	170/177 (96%)	0.62	12 (7%)	19 21	10, 35, 63, 73	0
1	F	167/177 (94%)	0.15	5 (2%)	54 57	7, 24, 53, 69	0
1	G	165/177 (93%)	0.27	6 (3%)	46 50	11, 29, 55, 72	0
1	H	169/177 (95%)	0.31	11 (6%)	22 25	9, 27, 56, 75	0
1	I	171/177 (96%)	0.56	13 (7%)	17 18	11, 34, 59, 74	0
1	J	170/177 (96%)	0.38	13 (7%)	17 18	10, 31, 61, 73	0
1	K	171/177 (96%)	0.36	6 (3%)	48 51	11, 33, 59, 76	0
1	L	165/177 (93%)	0.62	12 (7%)	18 20	14, 33, 59, 77	0
All	All	2024/2124 (95%)	0.37	103 (5%)	32 35	7, 30, 59, 77	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	109	ASN	5.8
1	F	3	ILE	5.0
1	J	108	ALA	4.9
1	K	28	SER	4.9
1	B	57	ALA	4.8
1	B	3	ILE	4.7
1	E	115	ALA	4.4
1	L	146	VAL	4.3
1	K	144	VAL	4.1
1	E	141	LEU	4.1
1	E	3	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	L	144	VAL	3.8
1	E	59	ALA	3.7
1	I	108	ALA	3.7
1	J	60	THR	3.7
1	J	175	SER	3.6
1	E	143	THR	3.4
1	B	144	VAL	3.4
1	L	26	ARG	3.3
1	H	175	SER	3.2
1	D	174	LEU	3.2
1	J	25	THR	3.1
1	I	59	ALA	3.1
1	J	109	ASN	3.1
1	H	174	LEU	3.1
1	H	60	THR	3.1
1	D	175	SER	3.1
1	L	98	LEU	3.1
1	F	171	ILE	2.9
1	C	99	ARG	2.9
1	E	144	VAL	2.8
1	I	29	VAL	2.8
1	E	26	ARG	2.8
1	K	56	GLY	2.8
1	E	60	THR	2.8
1	I	61	ASP	2.8
1	H	171	ILE	2.7
1	H	108	ALA	2.7
1	I	60	THR	2.7
1	F	65	ALA	2.7
1	H	173	ALA	2.7
1	H	109	ASN	2.7
1	B	113	PRO	2.7
1	E	145	GLY	2.7
1	E	5	LYS	2.6
1	K	143	THR	2.6
1	J	63	LEU	2.6
1	H	172	GLU	2.6
1	C	98	LEU	2.6
1	C	113	PRO	2.5
1	K	150	ALA	2.5
1	C	3	ILE	2.5
1	L	6	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	171	ILE	2.5
1	L	28	SER	2.4
1	L	108	ALA	2.4
1	I	66	ALA	2.4
1	I	27	SER	2.4
1	L	65	ALA	2.4
1	A	61	ASP	2.4
1	A	60	THR	2.4
1	G	109	ASN	2.3
1	J	173	ALA	2.3
1	B	145	GLY	2.3
1	D	60	THR	2.3
1	I	65	ALA	2.3
1	A	12	GLU	2.3
1	D	173	ALA	2.3
1	L	30	LEU	2.3
1	H	26	ARG	2.3
1	D	171	ILE	2.3
1	H	63	LEU	2.2
1	H	25	THR	2.2
1	F	112	ILE	2.2
1	I	3	ILE	2.2
1	J	26	ARG	2.2
1	B	69	HIS	2.2
1	B	141	LEU	2.2
1	B	64	SER	2.2
1	E	30	LEU	2.2
1	A	98	LEU	2.2
1	I	64	SER	2.1
1	A	57	ALA	2.1
1	I	69	HIS	2.1
1	J	66	ALA	2.1
1	K	5	LYS	2.1
1	J	4	GLU	2.1
1	G	28	SER	2.1
1	D	93	GLY	2.1
1	G	142	ARG	2.1
1	L	5	LYS	2.1
1	E	6	LEU	2.1
1	L	97	ASP	2.1
1	G	3	ILE	2.1
1	A	65	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	98	LEU	2.1
1	G	146	VAL	2.1
1	I	56	GLY	2.1
1	B	147	ASP	2.1
1	G	114	LYS	2.0
1	J	61	ASP	2.1
1	F	26	ARG	2.0
1	I	141	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.