



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:58 AM GMT

PDB ID : 2YW7
Title : Crystal structure of C-terminal deletion mutant of Mycobacterium smegmatis Dps
Authors : Roy, S.; Saraswathi, R.; Gupta, S.; Sekar, K.; Chatterji, D.; Vijayan, M.
Deposited on : 2007-04-19
Resolution : 3.30 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

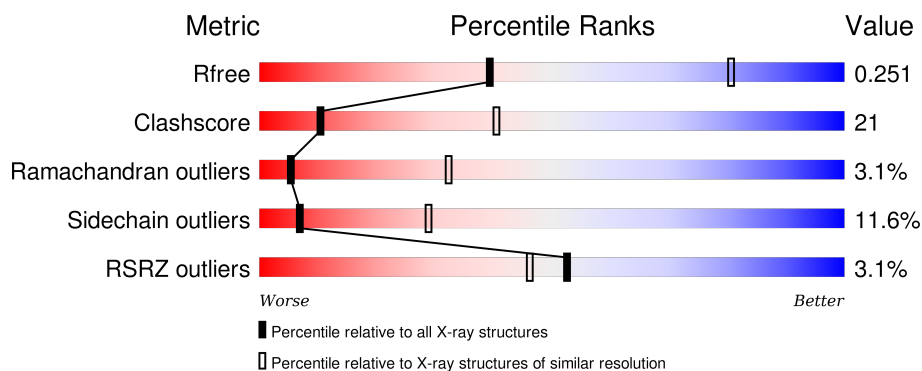
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	183	<div> <div>2%</div> <div>45% 30% 5% 20%</div> </div>
1	B	183	<div> <div>2%</div> <div>40% 31% 8% 21%</div> </div>
1	C	183	<div> <div>2%</div> <div>43% 33% 5% 20%</div> </div>
1	D	183	<div> <div>4%</div> <div>41% 34% • • 21%</div> </div>
1	E	183	<div> <div>2%</div> <div>39% 34% 6% 21%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	183	<div><div><div></div><div></div><div></div><div></div></div><div>%44%29%7%20%</div></div>
1	G	183	<div><div><div></div><div></div><div></div><div></div></div><div>%47%29%•21%</div></div>
1	H	183	<div><div><div></div><div></div><div></div><div></div></div><div>4%33%42%••20%</div></div>
1	I	183	<div><div><div></div><div></div><div></div><div></div></div><div>4%41%32%6%21%</div></div>
1	J	183	<div><div><div></div><div></div><div></div><div></div></div><div>5%48%27%5%20%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11597 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.

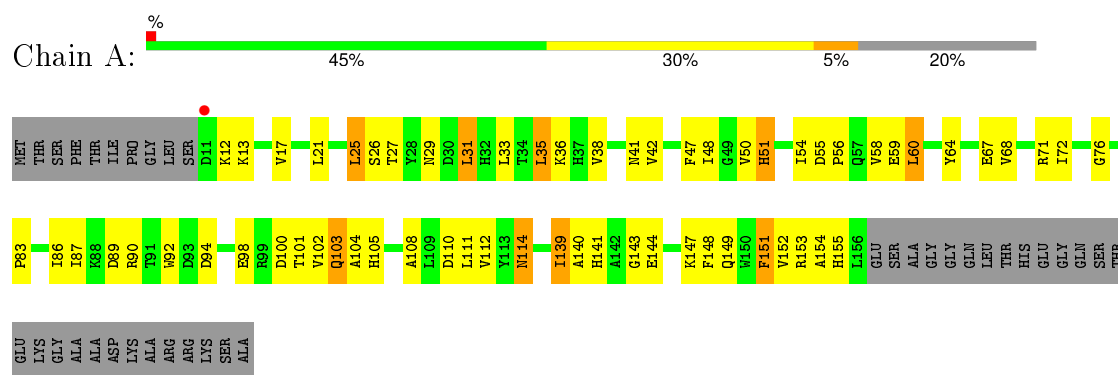
- Molecule 1 is a protein called Starvation-induced DNA protecting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1164	739	201	223	1			
1	B	145	Total	C	N	O	S	0	0	0
			1156	733	200	222	1			
1	C	147	Total	C	N	O	S	0	0	0
			1173	744	202	226	1			
1	D	145	Total	C	N	O	S	0	0	0
			1155	733	200	221	1			
1	E	145	Total	C	N	O	S	0	0	0
			1156	733	200	222	1			
1	F	146	Total	C	N	O	S	0	0	0
			1160	737	201	221	1			
1	G	144	Total	C	N	O	S	0	0	0
			1147	729	198	219	1			
1	H	146	Total	C	N	O	S	0	0	0
			1165	740	201	223	1			
1	I	145	Total	C	N	O	S	0	0	0
			1156	735	200	220	1			
1	J	146	Total	C	N	O	S	0	0	0
			1165	740	201	223	1			

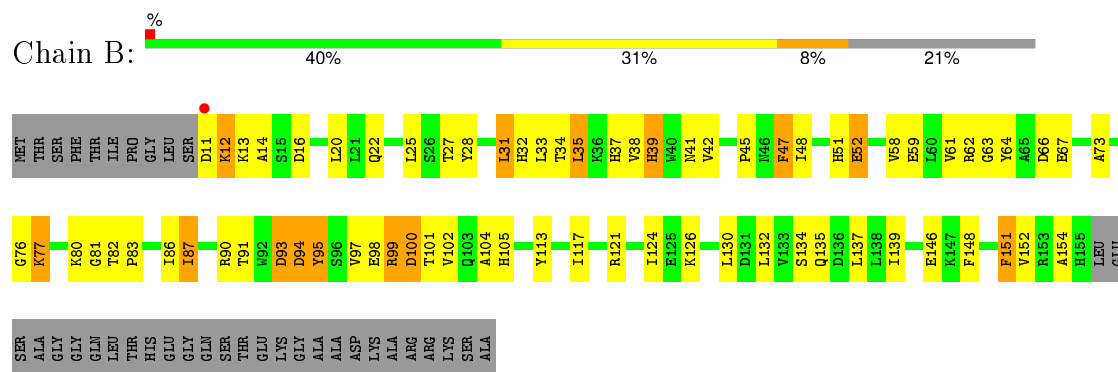
3 Residue-property plots [i](#)

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.

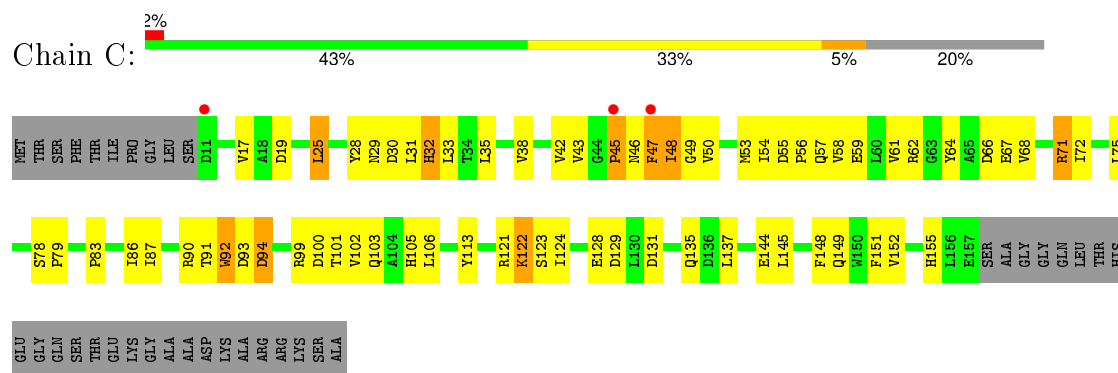
• Molecule 1: Starvation-induced DNA protecting protein



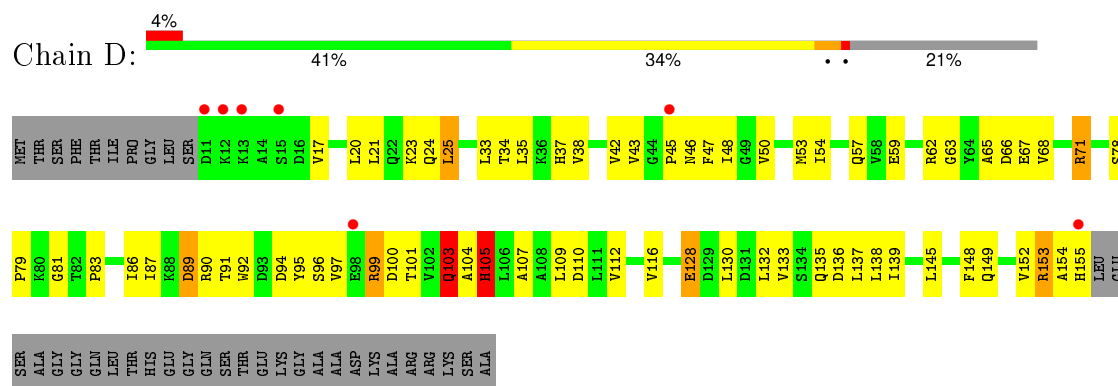
• Molecule 1: Starvation-induced DNA protecting protein



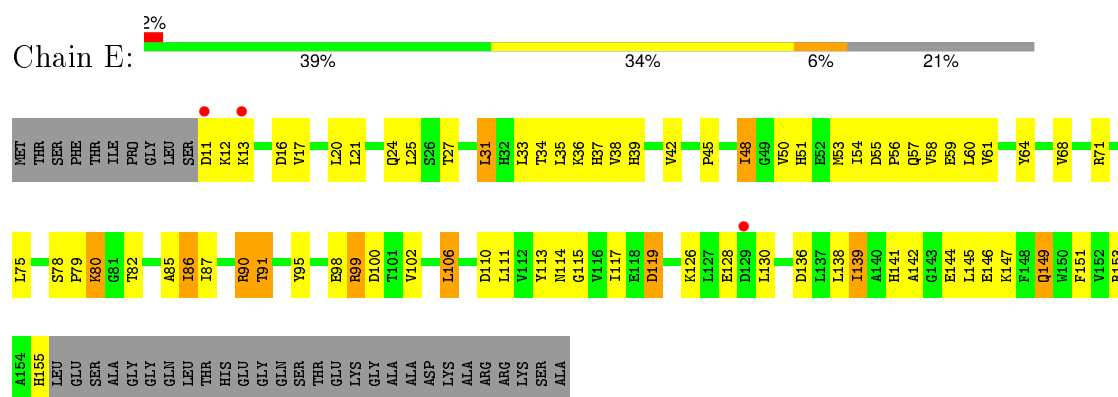
• Molecule 1: Starvation-induced DNA protecting protein



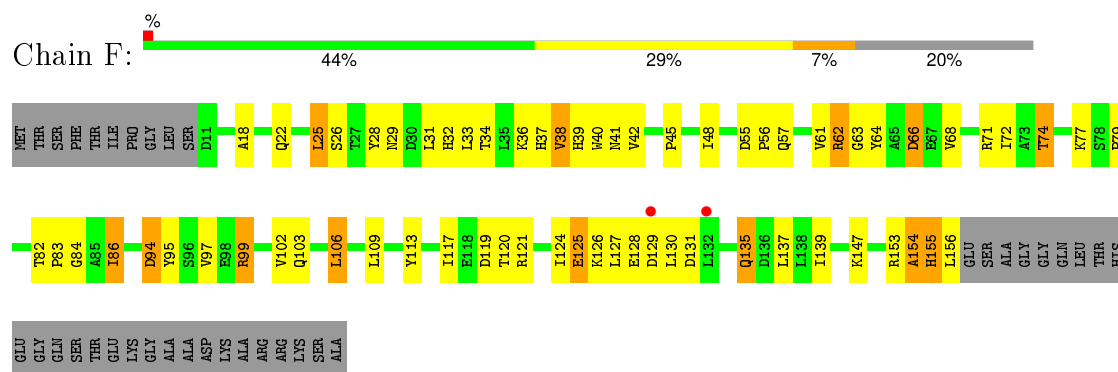
- Molecule 1: Starvation-induced DNA protecting protein



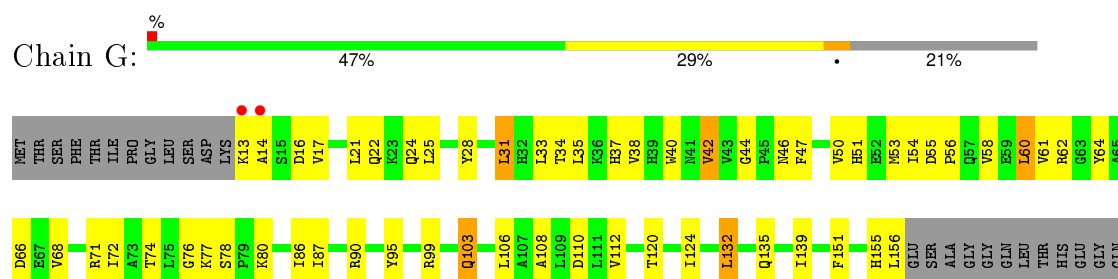
- Molecule 1: Starvation-induced DNA protecting protein



- Molecule 1: Starvation-induced DNA protecting protein

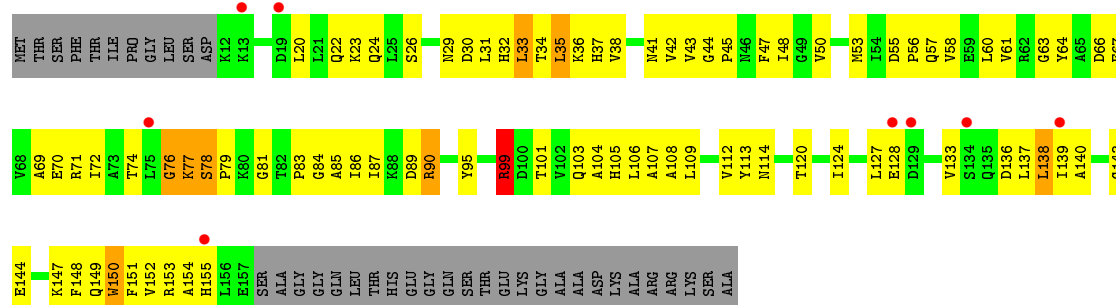


- Molecule 1: Starvation-induced DNA protecting protein

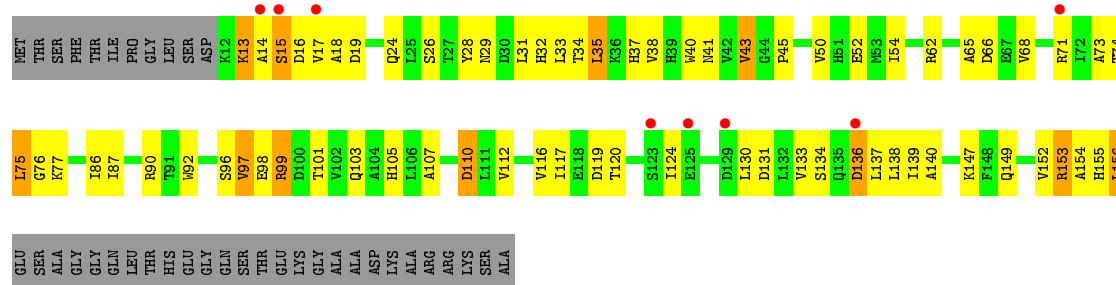


SER
THR
GLU
LYS
GLY
ALA
ALA
ASP
LYS
ARG
ARG
LYS
SER
ALA

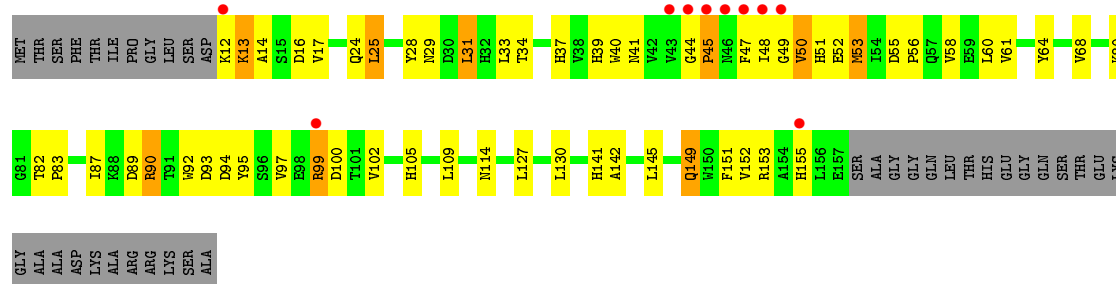
• Molecule 1: Starvation-induced DNA protecting protein



• Molecule 1: Starvation-induced DNA protecting protein



• Molecule 1: Starvation-induced DNA protecting protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.52Å 83.94Å 111.91Å 90.00° 105.89° 90.00°	Depositor
Resolution (Å)	28.54 – 3.30 29.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.54-3.30) 99.2 (29.39-3.30)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.259 0.216 , 0.251	Depositor DCC
R_{free} test set	1318 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25935 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11597	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/1187	0.57	0/1612
1	B	0.33	0/1179	0.58	0/1601
1	C	0.33	0/1196	0.56	0/1624
1	D	0.34	0/1178	0.54	0/1600
1	E	0.34	0/1179	0.56	0/1601
1	F	0.35	0/1183	0.52	0/1607
1	G	0.34	0/1170	0.56	0/1590
1	H	0.35	0/1188	0.55	0/1613
1	I	0.34	0/1179	0.54	0/1601
1	J	0.35	0/1188	0.57	0/1613
All	All	0.34	0/11827	0.56	0/16062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1164	0	1153	61	0
1	B	1156	0	1142	58	0
1	C	1173	0	1159	49	0
1	D	1155	0	1139	52	0
1	E	1156	0	1142	65	0
1	F	1160	0	1149	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1147	0	1136	47	0
1	H	1165	0	1155	80	0
1	I	1156	0	1149	46	0
1	J	1165	0	1155	40	0
All	All	11597	0	11479	496	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 21.

All (496) 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:C:79:PRO:HD2	1:F:41:ASN:HD21	1.14	1.08
1:D:153:ARG:HB3	1:D:155:HIS:CE1	1.95	1.01
1:I:13:LYS:HE3	1:I:13:LYS:H	1.26	0.98
1:H:147:LYS:HA	1:H:150:TRP:HE3	1.34	0.93
1:H:147:LYS:HA	1:H:150:TRP:CE3	2.04	0.93
1:H:77:LYS:HD3	1:H:78:SER:H	1.34	0.92
1:H:79:PRO:HD2	1:J:41:ASN:HD21	1.37	0.90
1:C:35:LEU:HD21	1:C:57:GLN:HG3	1.53	0.90
1:A:83:PRO:HG3	1:E:86:ILE:HD11	1.55	0.88
1:B:87:ILE:HA	1:B:90:ARG:HD2	1.53	0.88
1:E:151:PHE:HE1	1:H:48:ILE:HD11	1.37	0.88
1:D:62:ARG:HD2	1:I:62:ARG:HH12	1.38	0.87
1:A:114:ASN:ND2	1:A:149:GLN:HE22	1.72	0.87
1:A:114:ASN:HD21	1:A:149:GLN:HE22	1.23	0.87
1:D:42:VAL:HG21	1:D:50:VAL:HG11	1.56	0.86
1:G:87:ILE:HA	1:G:90:ARG:HD2	1.57	0.85
1:C:25:LEU:HD22	1:C:29:ASN:HD21	1.40	0.85
1:I:16:ASP:HA	1:I:19:ASP:HB2	1.57	0.85
1:C:79:PRO:HD2	1:F:41:ASN:ND2	1.92	0.84
1:A:114:ASN:HD21	1:A:149:GLN:NE2	1.77	0.83
1:E:42:VAL:HG11	1:E:50:VAL:HG21	1.60	0.83
1:E:117:ILE:HD11	1:E:149:GLN:HG3	1.60	0.83
1:E:117:ILE:CD1	1:E:149:GLN:HG3	2.10	0.81
1:E:151:PHE:CE1	1:H:48:ILE:HD11	2.17	0.80
1:F:31:LEU:HD12	1:F:61:VAL:HG11	1.64	0.80
1:H:107:ALA:HB2	1:H:155:HIS:CE1	2.17	0.80
1:J:152:VAL:HA	1:J:155:HIS:ND1	1.98	0.79
1:C:25:LEU:HD22	1:C:29:ASN:ND2	1.98	0.77
1:B:22:GLN:HE21	1:B:80:LYS:H	1.30	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:PRO:HD2	1:I:41:ASN:HD21	1.48	0.76
1:B:113:TYR:O	1:B:117:ILE:HG13	1.84	0.76
1:I:153:ARG:HD2	1:I:153:ARG:H	1.51	0.76
1:H:42:VAL:HG11	1:H:50:VAL:HG11	1.66	0.76
1:F:72:ILE:HB	1:F:79:PRO:HG3	1.69	0.74
1:H:81:GLY:HA3	1:J:40:TRP:HZ3	1.51	0.74
1:A:114:ASN:HD22	1:A:114:ASN:N	1.85	0.74
1:C:42:VAL:HG12	1:C:47:PHE:HB2	1.71	0.73
1:H:23:LYS:HG2	1:H:89:ASP:HB2	1.68	0.73
1:F:25:LEU:HD22	1:F:29:ASN:HD21	1.52	0.73
1:H:43:VAL:HG11	1:H:99:ARG:HH11	1.54	0.72
1:E:21:LEU:HD22	1:E:68:VAL:HG23	1.71	0.72
1:A:83:PRO:CG	1:E:86:ILE:HD11	2.19	0.71
1:B:76:GLY:O	1:B:77:LYS:HB3	1.89	0.71
1:G:14:ALA:HA	1:G:17:VAL:HB	1.71	0.71
1:I:124:ILE:HG12	1:I:138:LEU:HB2	1.72	0.71
1:A:114:ASN:ND2	1:A:149:GLN:NE2	2.37	0.71
1:C:33:LEU:HD11	1:F:33:LEU:HD11	1.72	0.70
1:E:27:THR:O	1:E:31:LEU:HB2	1.91	0.70
1:J:37:HIS:HD2	1:J:95:TYR:HD2	1.38	0.70
1:H:53:MET:HE2	1:H:148:PHE:CE1	2.27	0.70
1:H:107:ALA:HB2	1:H:155:HIS:HE1	1.55	0.70
1:A:38:VAL:O	1:A:42:VAL:HG23	1.92	0.69
1:J:141:HIS:O	1:J:145:LEU:HG	1.92	0.69
1:B:35:LEU:HB3	1:B:58:VAL:HG22	1.76	0.68
1:I:155:HIS:CG	1:I:156:LEU:H	2.10	0.67
1:I:112:VAL:O	1:I:116:VAL:HG23	1.95	0.67
1:B:39:HIS:CE1	1:B:51:HIS:ND1	2.63	0.66
1:A:102:VAL:C	1:A:104:ALA:H	1.98	0.66
1:G:87:ILE:HA	1:G:90:ARG:CD	2.26	0.66
1:A:151:PHE:CD1	1:A:155:HIS:HE1	2.13	0.66
1:B:41:ASN:O	1:B:99:ARG:HA	1.95	0.66
1:A:114:ASN:HD22	1:A:114:ASN:H	1.42	0.66
1:H:24:GLN:HG2	1:H:138:LEU:HD21	1.78	0.66
1:F:28:TYR:CE2	1:F:64:TYR:HB3	2.31	0.66
1:A:76:GLY:HA2	1:E:99:ARG:NH2	2.11	0.65
1:A:31:LEU:HD22	1:A:35:LEU:HD22	1.79	0.65
1:C:45:PRO:HG2	1:C:103:GLN:OE1	1.97	0.64
1:D:99:ARG:NH2	1:I:73:ALA:O	2.31	0.64
1:J:34:THR:O	1:J:37:HIS:HB3	1.96	0.64
1:B:31:LEU:HD12	1:B:61:VAL:HG11	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:SER:HA	1:I:29:ASN:HD22	1.62	0.64
1:B:13:LYS:HG3	1:B:14:ALA:N	2.12	0.64
1:A:48:ILE:O	1:A:51:HIS:HB2	1.97	0.64
1:D:33:LEU:HD11	1:I:33:LEU:HD11	1.78	0.64
1:D:38:VAL:O	1:D:42:VAL:HG23	1.98	0.63
1:C:35:LEU:HD21	1:C:57:GLN:CG	2.26	0.63
1:B:117:ILE:HD13	1:B:146:GLU:HG2	1.81	0.63
1:H:77:LYS:NZ	1:H:77:LYS:HA	2.14	0.63
1:H:153:ARG:C	1:H:155:HIS:H	2.01	0.63
1:H:78:SER:OG	1:J:99:ARG:HG2	1.99	0.63
1:D:101:THR:O	1:D:105:HIS:HB2	1.99	0.62
1:E:31:LEU:HD22	1:E:35:LEU:HD22	1.79	0.62
1:H:20:LEU:HD12	1:H:127:LEU:HD21	1.81	0.62
1:G:155:HIS:O	1:G:156:LEU:HG	1.98	0.62
1:G:155:HIS:ND1	1:G:155:HIS:O	2.33	0.62
1:C:55:ASP:HB2	1:C:56:PRO:HD3	1.81	0.62
1:J:44:GLY:O	1:J:47:PHE:CE1	2.53	0.62
1:D:35:LEU:HG	1:D:54:ILE:HG23	1.80	0.62
1:J:24:GLN:HG3	1:J:28:TYR:CE1	2.35	0.62
1:D:135:GLN:C	1:D:137:LEU:H	2.03	0.62
1:I:17:VAL:HG22	1:I:130:LEU:HD23	1.80	0.62
1:E:13:LYS:O	1:E:17:VAL:HG23	1.99	0.61
1:I:86:ILE:O	1:I:90:ARG:HB2	2.00	0.61
1:G:28:TYR:CE1	1:G:64:TYR:HB3	2.35	0.61
1:B:76:GLY:O	1:B:77:LYS:CB	2.49	0.60
1:D:128:GLU:HA	1:D:135:GLN:HE22	1.65	0.60
1:D:128:GLU:HA	1:D:135:GLN:NE2	2.16	0.60
1:E:24:GLN:HG2	1:E:138:LEU:HD21	1.83	0.60
1:F:25:LEU:HD22	1:F:29:ASN:ND2	2.15	0.60
1:G:50:VAL:O	1:G:54:ILE:HG12	2.01	0.60
1:J:17:VAL:HG13	1:J:127:LEU:HD21	1.83	0.60
1:G:54:ILE:HG22	1:G:58:VAL:HG23	1.84	0.59
1:E:35:LEU:HD21	1:E:57:GLN:HG3	1.82	0.59
1:A:50:VAL:HG12	1:A:54:ILE:CD1	2.33	0.59
1:B:38:VAL:O	1:B:42:VAL:HG23	2.02	0.59
1:A:25:LEU:HD22	1:A:29:ASN:HD21	1.67	0.59
1:H:32:HIS:HA	1:H:35:LEU:HD22	1.84	0.59
1:A:25:LEU:HD22	1:A:29:ASN:ND2	2.17	0.59
1:B:13:LYS:O	1:B:16:ASP:N	2.35	0.59
1:I:65:ALA:HA	1:I:68:VAL:HG12	1.84	0.59
1:C:46:ASN:HD22	1:C:49:GLY:HA3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ILE:HA	1:E:90:ARG:HD2	1.85	0.58
1:H:38:VAL:HG23	1:H:105:HIS:CG	2.38	0.58
1:G:132:LEU:HD12	1:G:132:LEU:H	1.69	0.58
1:J:60:LEU:HD22	1:J:64:TYR:OH	2.03	0.58
1:J:152:VAL:HA	1:J:155:HIS:CE1	2.38	0.58
1:A:48:ILE:H	1:A:48:ILE:HD12	1.69	0.57
1:J:50:VAL:HG21	1:J:102:VAL:HG12	1.86	0.57
1:E:110:ASP:OD2	1:E:149:GLN:NE2	2.37	0.57
1:J:55:ASP:HB2	1:J:56:PRO:HD3	1.86	0.57
1:A:149:GLN:HG2	1:A:153:ARG:HE	1.69	0.57
1:I:50:VAL:HG12	1:I:54:ILE:HD11	1.85	0.57
1:D:149:GLN:O	1:D:153:ARG:HG3	2.05	0.57
1:H:149:GLN:NE2	1:H:153:ARG:HH21	2.02	0.57
1:C:53:MET:HE1	1:C:152:VAL:HA	1.85	0.57
1:I:43:VAL:HG21	1:I:99:ARG:HG3	1.86	0.57
1:F:155:HIS:ND1	1:F:155:HIS:N	2.52	0.57
1:F:102:VAL:HG12	1:F:106:LEU:HD22	1.87	0.57
1:H:64:TYR:OH	1:H:144:GLU:HG3	2.04	0.57
1:E:34:THR:O	1:E:38:VAL:HG23	2.05	0.56
1:H:37:HIS:HE1	1:J:80:LYS:HA	1.69	0.56
1:H:63:GLY:O	1:H:67:GLU:HG3	2.04	0.56
1:A:50:VAL:HG12	1:A:54:ILE:HD12	1.87	0.56
1:D:90:ARG:HD3	1:D:92:TRP:O	2.05	0.56
1:F:124:ILE:HD13	1:F:139:ILE:HB	1.87	0.56
1:H:148:PHE:O	1:H:152:VAL:HG23	2.05	0.56
1:G:68:VAL:O	1:G:72:ILE:HG13	2.05	0.55
1:B:42:VAL:HG12	1:B:47:PHE:HB2	1.87	0.55
1:H:155:HIS:O	1:H:155:HIS:CD2	2.59	0.55
1:B:93:ASP:O	1:B:94:ASP:HB2	2.05	0.55
1:A:139:ILE:HD11	1:B:132:LEU:HG	1.88	0.55
1:I:18:ALA:HB2	1:I:75:LEU:CD1	2.36	0.55
1:G:135:GLN:O	1:G:139:ILE:HG13	2.05	0.55
1:F:125:GLU:HG3	1:F:126:LYS:N	2.20	0.55
1:I:120:THR:O	1:I:124:ILE:HG13	2.06	0.55
1:C:124:ILE:HG23	1:C:135:GLN:HG3	1.89	0.55
1:G:108:ALA:O	1:G:112:VAL:HG23	2.07	0.55
1:C:72:ILE:HB	1:C:79:PRO:HG3	1.89	0.55
1:F:82:THR:O	1:F:86:ILE:HG12	2.07	0.55
1:I:155:HIS:CG	1:I:156:LEU:N	2.74	0.54
1:J:31:LEU:HB3	1:J:61:VAL:HG11	1.89	0.54
1:E:57:GLN:O	1:E:61:VAL:HG23	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:VAL:O	1:E:42:VAL:HG23	2.08	0.54
1:D:83:PRO:HA	1:D:86:ILE:HG12	1.90	0.54
1:E:16:ASP:O	1:E:20:LEU:HG	2.08	0.54
1:I:139:ILE:HG23	1:I:140:ALA:H	1.73	0.54
1:J:92:TRP:HD1	1:J:93:ASP:O	1.90	0.54
1:H:33:LEU:HD11	1:J:33:LEU:HD11	1.88	0.54
1:H:155:HIS:O	1:H:155:HIS:CG	2.61	0.53
1:A:41:ASN:HD21	1:E:79:PRO:HD2	1.74	0.53
1:H:71:ARG:NH1	1:H:133:VAL:HG12	2.24	0.53
1:J:39:HIS:CE1	1:J:51:HIS:HD2	2.25	0.53
1:J:25:LEU:HD22	1:J:29:ASN:ND2	2.23	0.53
1:F:120:THR:O	1:F:124:ILE:HG22	2.08	0.53
1:E:113:TYR:HB3	1:E:149:GLN:HG2	1.89	0.53
1:D:90:ARG:HG2	1:D:92:TRP:H	1.74	0.53
1:G:35:LEU:HG	1:G:54:ILE:HG23	1.90	0.53
1:H:87:ILE:HG21	1:J:87:ILE:HD13	1.91	0.52
1:E:42:VAL:HG11	1:E:50:VAL:CG2	2.36	0.52
1:J:13:LYS:HE2	1:J:130:LEU:HB3	1.90	0.52
1:A:154:ALA:O	1:G:44:GLY:N	2.38	0.52
1:D:100:ASP:OD1	1:D:101:THR:N	2.38	0.52
1:C:42:VAL:HG12	1:C:47:PHE:CB	2.39	0.52
1:I:76:GLY:O	1:I:77:LYS:HG3	2.08	0.52
1:F:32:HIS:CG	1:F:62:ARG:HD2	2.44	0.52
1:E:80:LYS:HB3	1:E:85:ALA:HB1	1.90	0.52
1:J:48:ILE:HG22	1:J:52:GLU:HG3	1.92	0.52
1:B:80:LYS:HA	1:G:37:HIS:HE1	1.75	0.52
1:C:30:ASP:OD1	1:F:83:PRO:HG2	2.10	0.52
1:E:80:LYS:HB3	1:E:85:ALA:CB	2.39	0.52
1:A:42:VAL:HG22	1:A:105:HIS:CG	2.45	0.52
1:I:24:GLN:HG3	1:I:28:TYR:CE1	2.45	0.52
1:A:55:ASP:HB2	1:A:56:PRO:HD3	1.90	0.52
1:G:60:LEU:HD22	1:G:64:TYR:CE1	2.44	0.52
1:E:35:LEU:HB3	1:E:58:VAL:HG22	1.91	0.52
1:E:136:ASP:O	1:E:139:ILE:HG22	2.10	0.52
1:H:43:VAL:HG11	1:H:99:ARG:NH1	2.24	0.51
1:C:124:ILE:O	1:C:135:GLN:NE2	2.41	0.51
1:I:155:HIS:ND1	1:I:156:LEU:N	2.47	0.51
1:H:84:GLY:C	1:H:86:ILE:H	2.13	0.51
1:B:63:GLY:O	1:B:66:ASP:HB2	2.11	0.51
1:F:55:ASP:HB2	1:F:56:PRO:HD3	1.92	0.51
1:H:26:SER:OG	1:H:86:ILE:HG12	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ASP:HB2	1:E:56:PRO:HD3	1.92	0.51
1:E:153:ARG:C	1:E:155:HIS:N	2.63	0.51
1:G:24:GLN:HA	1:G:24:GLN:NE2	2.26	0.51
1:H:108:ALA:O	1:H:112:VAL:HG23	2.11	0.51
1:B:95:TYR:CE2	1:B:97:VAL:HB	2.45	0.51
1:G:86:ILE:O	1:G:90:ARG:HB3	2.10	0.51
1:B:13:LYS:CG	1:B:14:ALA:N	2.74	0.51
1:H:105:HIS:O	1:H:109:LEU:HB2	2.11	0.51
1:H:137:LEU:C	1:H:137:LEU:HD23	2.31	0.51
1:J:64:TYR:CD1	1:J:141:HIS:CD2	2.99	0.51
1:A:33:LEU:HD11	1:E:33:LEU:HD11	1.93	0.51
1:H:78:SER:OG	1:J:99:ARG:CG	2.59	0.50
1:A:35:LEU:O	1:A:38:VAL:HG22	2.10	0.50
1:A:151:PHE:CE1	1:A:155:HIS:HE1	2.29	0.50
1:A:51:HIS:O	1:A:55:ASP:OD2	2.28	0.50
1:E:38:VAL:HG12	1:E:42:VAL:CG2	2.41	0.50
1:B:121:ARG:HH12	1:D:132:LEU:H	1.58	0.50
1:J:44:GLY:O	1:J:47:PHE:CZ	2.64	0.50
1:C:50:VAL:HG12	1:C:54:ILE:HD13	1.92	0.50
1:E:53:MET:HE1	1:E:106:LEU:HD11	1.92	0.50
1:C:33:LEU:HD12	1:F:83:PRO:HG3	1.92	0.50
1:C:28:TYR:CE1	1:C:64:TYR:HB3	2.47	0.50
1:H:106:LEU:HD23	1:H:155:HIS:HA	1.93	0.50
1:B:31:LEU:HD13	1:B:35:LEU:HD23	1.93	0.50
1:F:63:GLY:O	1:F:66:ASP:HB2	2.12	0.50
1:D:152:VAL:O	1:D:154:ALA:N	2.45	0.50
1:I:92:TRP:HE3	1:I:92:TRP:H	1.58	0.50
1:E:153:ARG:C	1:E:155:HIS:H	2.14	0.50
1:B:135:GLN:O	1:B:139:ILE:HG13	2.11	0.50
1:I:13:LYS:N	1:I:13:LYS:HE3	2.10	0.49
1:I:32:HIS:HA	1:I:35:LEU:HD22	1.94	0.49
1:D:135:GLN:O	1:D:139:ILE:HG12	2.13	0.49
1:H:35:LEU:HB3	1:H:58:VAL:HG22	1.94	0.49
1:G:77:LYS:HG3	1:G:78:SER:H	1.77	0.49
1:J:55:ASP:CB	1:J:56:PRO:HD3	2.42	0.49
1:F:34:THR:O	1:F:37:HIS:HB3	2.12	0.49
1:F:38:VAL:HG21	1:F:109:LEU:HD11	1.95	0.49
1:G:34:THR:HG23	1:G:95:TYR:HB2	1.94	0.49
1:B:33:LEU:HD21	1:G:33:LEU:HD21	1.94	0.49
1:B:82:THR:HB	1:B:83:PRO:CD	2.43	0.49
1:C:29:ASN:HA	1:C:32:HIS:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:ALA:O	1:I:77:LYS:NZ	2.46	0.49
1:C:113:TYR:CB	1:C:149:GLN:HG3	2.42	0.49
1:A:13:LYS:O	1:A:17:VAL:HG23	2.12	0.49
1:A:102:VAL:O	1:A:104:ALA:N	2.44	0.49
1:C:122:LYS:O	1:C:122:LYS:CG	2.61	0.49
1:I:133:VAL:O	1:I:137:LEU:HB2	2.13	0.49
1:E:36:LYS:HG2	1:E:58:VAL:HG11	1.95	0.49
1:F:131:ASP:O	1:F:135:GLN:HB3	2.12	0.49
1:B:31:LEU:CD1	1:B:61:VAL:HG11	2.42	0.48
1:B:134:SER:O	1:B:137:LEU:HB3	2.13	0.48
1:A:87:ILE:CD1	1:E:87:ILE:HG12	2.43	0.48
1:D:95:TYR:CE2	1:D:97:VAL:HB	2.49	0.48
1:C:32:HIS:HB3	1:C:61:VAL:HG12	1.95	0.48
1:H:37:HIS:CE1	1:J:80:LYS:HA	2.47	0.48
1:C:92:TRP:HE3	1:C:92:TRP:H	1.60	0.48
1:F:18:ALA:O	1:F:22:GLN:N	2.37	0.48
1:A:110:ASP:OD2	1:A:149:GLN:NE2	2.41	0.48
1:I:18:ALA:HB2	1:I:75:LEU:HD11	1.95	0.48
1:C:90:ARG:NH2	1:F:83:PRO:HB2	2.27	0.48
1:F:153:ARG:O	1:F:154:ALA:HB2	2.13	0.48
1:B:39:HIS:NE2	1:B:51:HIS:ND1	2.62	0.48
1:I:117:ILE:HD12	1:I:149:GLN:OE1	2.12	0.48
1:E:34:THR:O	1:E:37:HIS:HB3	2.14	0.48
1:C:94:ASP:OD1	1:F:84:GLY:HA3	2.14	0.48
1:I:13:LYS:O	1:I:17:VAL:HG23	2.14	0.48
1:A:143:GLY:O	1:A:147:LYS:HB2	2.14	0.48
1:C:38:VAL:HG13	1:C:105:HIS:ND1	2.29	0.48
1:F:45:PRO:HA	1:J:155:HIS:O	2.14	0.47
1:A:155:HIS:CE1	1:G:47:PHE:CE2	3.02	0.47
1:I:32:HIS:CD2	1:I:62:ARG:HG2	2.49	0.47
1:E:64:TYR:O	1:E:68:VAL:HG12	2.13	0.47
1:D:35:LEU:HD21	1:D:57:GLN:HG3	1.96	0.47
1:I:34:THR:O	1:I:38:VAL:HG13	2.14	0.47
1:H:31:LEU:HD12	1:H:61:VAL:HG11	1.96	0.47
1:F:32:HIS:ND1	1:F:62:ARG:HD2	2.29	0.47
1:C:64:TYR:OH	1:C:144:GLU:HB2	2.13	0.47
1:E:126:LYS:O	1:E:130:LEU:HD13	2.13	0.47
1:E:102:VAL:O	1:E:106:LEU:HB2	2.14	0.47
1:D:24:GLN:HG2	1:D:138:LEU:HD21	1.96	0.47
1:G:31:LEU:HD13	1:G:61:VAL:HG21	1.96	0.47
1:A:148:PHE:O	1:A:152:VAL:HG23	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:HA	1:G:37:HIS:CE1	2.50	0.47
1:H:70:GLU:C	1:H:72:ILE:H	2.18	0.47
1:H:53:MET:HE3	1:H:151:PHE:CD1	2.49	0.47
1:B:32:HIS:HA	1:B:35:LEU:HB2	1.96	0.47
1:B:31:LEU:HD12	1:B:61:VAL:CG1	2.45	0.47
1:G:38:VAL:O	1:G:42:VAL:HG22	2.15	0.47
1:D:59:GLU:HA	1:D:62:ARG:HG2	1.97	0.47
1:E:50:VAL:HG12	1:E:54:ILE:HD12	1.95	0.47
1:C:148:PHE:O	1:C:152:VAL:HG23	2.15	0.47
1:J:87:ILE:HA	1:J:90:ARG:HD2	1.96	0.47
1:E:155:HIS:CE1	1:H:44:GLY:HA2	2.50	0.47
1:E:48:ILE:O	1:E:51:HIS:HB2	2.14	0.47
1:E:117:ILE:HD12	1:E:149:GLN:HG3	1.94	0.47
1:E:78:SER:HA	1:E:79:PRO:HD3	1.81	0.47
1:C:48:ILE:H	1:C:48:ILE:HD12	1.80	0.47
1:D:62:ARG:HG3	1:D:63:GLY:N	2.30	0.47
1:A:102:VAL:C	1:A:104:ALA:N	2.67	0.47
1:B:33:LEU:HD21	1:G:33:LEU:HD11	1.97	0.47
1:H:34:THR:O	1:H:38:VAL:HG12	2.16	0.46
1:B:77:LYS:HA	1:G:99:ARG:NH2	2.31	0.46
1:H:35:LEU:HD23	1:H:58:VAL:HA	1.98	0.46
1:J:50:VAL:HG21	1:J:102:VAL:CG1	2.44	0.46
1:A:101:THR:O	1:A:104:ALA:HB3	2.16	0.46
1:B:11:ASP:HB3	1:B:12:LYS:H	1.57	0.46
1:C:38:VAL:O	1:C:42:VAL:HG23	2.16	0.46
1:H:113:TYR:CZ	1:H:148:PHE:CD2	3.04	0.46
1:B:47:PHE:HA	1:B:102:VAL:CG2	2.46	0.46
1:H:57:GLN:HE21	1:H:61:VAL:HG23	1.80	0.46
1:H:71:ARG:HH12	1:H:133:VAL:HG12	1.80	0.46
1:H:77:LYS:HZ3	1:H:77:LYS:HA	1.80	0.46
1:B:100:ASP:HB3	1:B:104:ALA:HB3	1.98	0.46
1:G:22:GLN:NE2	1:G:80:LYS:HB2	2.31	0.46
1:F:127:LEU:O	1:F:130:LEU:N	2.44	0.46
1:H:38:VAL:HG23	1:H:105:HIS:ND1	2.31	0.46
1:G:21:LEU:CD1	1:G:71:ARG:HG3	2.46	0.46
1:F:117:ILE:O	1:F:121:ARG:HG2	2.16	0.46
1:D:53:MET:HE3	1:D:148:PHE:CZ	2.51	0.46
1:C:35:LEU:HB3	1:C:58:VAL:HG22	1.98	0.46
1:E:111:LEU:O	1:E:114:ASN:HB2	2.16	0.46
1:G:74:THR:C	1:G:76:GLY:H	2.19	0.46
1:H:86:ILE:O	1:H:90:ARG:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:ARG:O	1:I:74:THR:HG22	2.16	0.45
1:I:131:ASP:HB3	1:I:134:SER:OG	2.16	0.45
1:J:13:LYS:HG3	1:J:14:ALA:N	2.30	0.45
1:C:113:TYR:HB2	1:C:149:GLN:HG3	1.96	0.45
1:E:71:ARG:NH2	1:E:75:LEU:HD21	2.31	0.45
1:B:22:GLN:NE2	1:B:80:LYS:H	2.07	0.45
1:B:81:GLY:HA3	1:G:40:TRP:HZ3	1.81	0.45
1:B:148:PHE:O	1:B:151:PHE:HB3	2.16	0.45
1:B:152:VAL:C	1:B:154:ALA:H	2.20	0.45
1:D:46:ASN:O	1:D:48:ILE:N	2.48	0.45
1:A:67:GLU:OE2	1:A:141:HIS:NE2	2.39	0.45
1:A:114:ASN:ND2	1:A:114:ASN:N	2.58	0.45
1:G:103:GLN:CD	1:G:103:GLN:H	2.19	0.45
1:I:18:ALA:HB2	1:I:75:LEU:HD12	1.98	0.45
1:B:28:TYR:CE1	1:B:64:TYR:HB3	2.52	0.45
1:D:107:ALA:O	1:D:110:ASP:HB3	2.17	0.45
1:D:66:ASP:O	1:D:67:GLU:C	2.55	0.45
1:G:34:THR:O	1:G:37:HIS:HB3	2.17	0.45
1:C:47:PHE:CD1	1:C:47:PHE:C	2.90	0.45
1:A:151:PHE:CE1	1:A:155:HIS:CE1	3.05	0.45
1:I:97:VAL:HB	1:I:105:HIS:CE1	2.52	0.45
1:B:62:ARG:HD3	1:G:62:ARG:NH1	2.32	0.45
1:H:77:LYS:HD3	1:H:78:SER:N	2.17	0.44
1:A:76:GLY:HA2	1:E:99:ARG:HH22	1.82	0.44
1:C:53:MET:CE	1:C:152:VAL:HA	2.45	0.44
1:F:127:LEU:O	1:F:129:ASP:N	2.50	0.44
1:A:35:LEU:HB3	1:A:58:VAL:HG22	2.00	0.44
1:H:143:GLY:O	1:H:147:LYS:HG3	2.17	0.44
1:J:41:ASN:O	1:J:105:HIS:NE2	2.50	0.44
1:H:101:THR:HG23	1:H:104:ALA:H	1.82	0.44
1:I:50:VAL:HG12	1:I:54:ILE:CD1	2.48	0.44
1:C:106:LEU:HD22	1:C:152:VAL:HG13	1.99	0.44
1:A:94:ASP:OD2	1:E:82:THR:HB	2.17	0.44
1:C:83:PRO:HA	1:C:86:ILE:HG12	2.00	0.44
1:A:110:ASP:O	1:A:114:ASN:ND2	2.51	0.44
1:D:38:VAL:HG13	1:D:105:HIS:ND1	2.32	0.44
1:F:86:ILE:HG12	1:F:86:ILE:H	1.57	0.44
1:F:40:TRP:C	1:F:41:ASN:HD22	2.21	0.44
1:H:101:THR:OG1	1:H:103:GLN:OE1	2.35	0.44
1:H:120:THR:HG23	1:H:138:LEU:CD1	2.48	0.44
1:H:22:GLN:C	1:H:24:GLN:H	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:LYS:HG3	1:E:13:LYS:H	1.82	0.44
1:H:57:GLN:HE21	1:H:61:VAL:CG2	2.31	0.44
1:B:67:GLU:HB3	1:B:137:LEU:HD11	1.98	0.44
1:D:112:VAL:O	1:D:116:VAL:HG23	2.18	0.44
1:E:34:THR:HG23	1:E:95:TYR:HB2	1.99	0.44
1:I:153:ARG:HD2	1:I:153:ARG:N	2.23	0.44
1:C:67:GLU:HB3	1:C:137:LEU:HD11	2.00	0.44
1:H:32:HIS:O	1:H:35:LEU:HB2	2.18	0.44
1:C:53:MET:CE	1:C:151:PHE:HD1	2.31	0.44
1:H:140:ALA:O	1:H:144:GLU:HG2	2.16	0.44
1:B:124:ILE:HG22	1:D:132:LEU:HD12	1.99	0.44
1:G:31:LEU:HB3	1:G:61:VAL:HG11	2.00	0.44
1:D:87:ILE:HD13	1:I:87:ILE:HD13	2.00	0.44
1:E:144:GLU:O	1:E:147:LYS:HB3	2.17	0.44
1:E:113:TYR:HB3	1:E:149:GLN:CG	2.48	0.44
1:B:98:GLU:O	1:B:105:HIS:CE1	2.70	0.44
1:E:42:VAL:HG21	1:E:50:VAL:HG11	2.00	0.44
1:B:35:LEU:HD13	1:B:35:LEU:HA	1.79	0.44
1:A:87:ILE:HD11	1:E:87:ILE:HG12	2.00	0.43
1:F:28:TYR:HE2	1:F:64:TYR:HB3	1.79	0.43
1:A:68:VAL:O	1:A:71:ARG:HB3	2.18	0.43
1:D:90:ARG:HG2	1:D:91:THR:N	2.32	0.43
1:B:27:THR:O	1:B:31:LEU:HB2	2.18	0.43
1:C:46:ASN:O	1:C:50:VAL:HG23	2.17	0.43
1:D:54:ILE:O	1:D:57:GLN:HB3	2.18	0.43
1:H:74:THR:C	1:H:76:GLY:H	2.22	0.43
1:E:142:ALA:O	1:E:146:GLU:HG3	2.18	0.43
1:F:68:VAL:O	1:F:72:ILE:HG13	2.18	0.43
1:F:71:ARG:HA	1:F:74:THR:HB	2.00	0.43
1:I:26:SER:HA	1:I:29:ASN:ND2	2.33	0.43
1:F:135:GLN:C	1:F:137:LEU:H	2.22	0.43
1:F:42:VAL:O	1:F:42:VAL:HG13	2.18	0.43
1:I:107:ALA:O	1:I:110:ASP:HB3	2.19	0.43
1:D:135:GLN:C	1:D:137:LEU:N	2.71	0.43
1:D:90:ARG:NH2	1:D:94:ASP:OD2	2.52	0.43
1:A:64:TYR:OH	1:A:144:GLU:HB2	2.19	0.43
1:E:86:ILE:O	1:E:90:ARG:HB3	2.19	0.43
1:E:117:ILE:HG21	1:E:146:GLU:HG2	2.00	0.43
1:J:55:ASP:O	1:J:58:VAL:HB	2.19	0.43
1:D:78:SER:CB	1:I:98:GLU:HB3	2.48	0.43
1:A:26:SER:HB3	1:A:86:ILE:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:SER:HA	1:I:77:LYS:HE2	2.00	0.43
1:F:57:GLN:NE2	1:F:113:TYR:OH	2.48	0.43
1:H:113:TYR:CZ	1:H:148:PHE:HD2	2.36	0.42
1:A:151:PHE:O	1:A:155:HIS:ND1	2.52	0.42
1:A:139:ILE:HG22	1:A:140:ALA:N	2.33	0.42
1:C:62:ARG:HD3	1:F:62:ARG:NH2	2.33	0.42
1:C:46:ASN:HD21	1:C:155:HIS:HE1	1.66	0.42
1:A:90:ARG:HG3	1:A:92:TRP:CE2	2.54	0.42
1:G:42:VAL:HB	1:G:47:PHE:HB2	2.02	0.42
1:B:13:LYS:HD3	1:B:130:LEU:HD23	2.02	0.42
1:I:34:THR:O	1:I:37:HIS:HB3	2.19	0.42
1:E:98:GLU:O	1:E:100:ASP:N	2.52	0.42
1:D:17:VAL:O	1:D:20:LEU:HB3	2.18	0.42
1:D:103:GLN:CD	1:D:103:GLN:H	2.23	0.42
1:H:29:ASN:HA	1:H:32:HIS:CD2	2.54	0.42
1:A:141:HIS:H	1:A:141:HIS:CD2	2.37	0.42
1:D:153:ARG:HB3	1:D:155:HIS:HE1	1.71	0.42
1:G:13:LYS:O	1:G:17:VAL:HG23	2.19	0.42
1:B:12:LYS:HB2	1:B:12:LYS:HE2	1.83	0.42
1:J:53:MET:SD	1:J:155:HIS:CE1	3.13	0.42
1:E:126:LYS:O	1:E:130:LEU:CD1	2.67	0.42
1:H:55:ASP:N	1:H:56:PRO:HD2	2.35	0.42
1:H:71:ARG:HA	1:H:74:THR:OG1	2.20	0.42
1:H:147:LYS:HA	1:H:150:TRP:CZ3	2.51	0.42
1:D:42:VAL:HG11	1:D:50:VAL:HG21	2.02	0.42
1:F:31:LEU:HD12	1:F:61:VAL:CG1	2.40	0.42
1:H:57:GLN:NE2	1:H:61:VAL:HG23	2.35	0.42
1:H:43:VAL:O	1:H:101:THR:HA	2.19	0.42
1:B:39:HIS:CD2	1:B:51:HIS:HA	2.54	0.42
1:B:13:LYS:O	1:B:14:ALA:C	2.57	0.42
1:E:12:LYS:O	1:E:16:ASP:OD1	2.38	0.42
1:D:23:LYS:HG2	1:D:89:ASP:HB2	2.01	0.42
1:E:60:LEU:HG	1:E:64:TYR:CE2	2.55	0.41
1:A:155:HIS:CE1	1:G:47:PHE:HE2	2.38	0.41
1:J:25:LEU:O	1:J:28:TYR:HB2	2.19	0.41
1:H:32:HIS:HB3	1:H:61:VAL:HG12	2.01	0.41
1:F:135:GLN:C	1:F:137:LEU:N	2.73	0.41
1:B:20:LEU:HD21	1:B:126:LYS:NZ	2.35	0.41
1:D:38:VAL:HG21	1:D:109:LEU:HD13	2.02	0.41
1:G:64:TYR:O	1:G:68:VAL:HG12	2.20	0.41
1:C:17:VAL:HG21	1:C:131:ASP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ALA:O	1:D:105:HIS:HB2	2.19	0.41
1:H:103:GLN:H	1:H:103:GLN:CD	2.24	0.41
1:A:25:LEU:HG	1:A:68:VAL:HG12	2.01	0.41
1:G:132:LEU:HA	1:G:135:GLN:HB3	2.02	0.41
1:H:95:TYR:HD1	1:H:112:VAL:HG21	1.84	0.41
1:B:11:ASP:O	1:B:12:LYS:HB2	2.20	0.41
1:G:120:THR:O	1:G:124:ILE:HG13	2.20	0.41
1:H:30:ASP:OD2	1:J:83:PRO:HG2	2.20	0.41
1:H:83:PRO:O	1:H:86:ILE:HB	2.20	0.41
1:G:24:GLN:HE21	1:G:24:GLN:HA	1.83	0.41
1:F:26:SER:OG	1:F:86:ILE:HA	2.20	0.41
1:A:111:LEU:O	1:A:112:VAL:C	2.59	0.41
1:D:21:LEU:HD22	1:D:68:VAL:HG23	2.01	0.41
1:C:121:ARG:C	1:C:123:SER:H	2.22	0.41
1:H:147:LYS:HG2	1:H:150:TRP:HZ3	1.86	0.41
1:H:41:ASN:HB3	1:H:99:ARG:HA	2.03	0.41
1:E:36:LYS:O	1:E:39:HIS:HB3	2.21	0.41
1:G:47:PHE:CE1	1:G:51:HIS:CE1	3.08	0.41
1:F:117:ILE:HG22	1:F:121:ARG:HG2	2.01	0.41
1:B:73:ALA:HA	1:G:99:ARG:NH2	2.35	0.41
1:G:24:GLN:HE21	1:G:24:GLN:CA	2.32	0.41
1:B:82:THR:O	1:B:86:ILE:HG13	2.20	0.41
1:A:108:ALA:O	1:A:112:VAL:HG23	2.20	0.41
1:D:25:LEU:HD23	1:D:65:ALA:O	2.21	0.41
1:H:77:LYS:HZ2	1:H:77:LYS:HA	1.82	0.41
1:H:124:ILE:HG13	1:H:138:LEU:HD12	2.03	0.41
1:G:50:VAL:HA	1:G:53:MET:HG2	2.02	0.41
1:E:115:GLY:O	1:E:119:ASP:HB2	2.21	0.41
1:C:78:SER:OG	1:F:99:ARG:HB2	2.21	0.41
1:D:71:ARG:HH21	1:D:133:VAL:HB	1.86	0.41
1:C:100:ASP:OD1	1:C:101:THR:N	2.54	0.41
1:F:36:LYS:O	1:F:39:HIS:HB3	2.20	0.41
1:E:141:HIS:H	1:E:141:HIS:CD2	2.39	0.41
1:F:102:VAL:O	1:F:106:LEU:HB2	2.20	0.41
1:H:41:ASN:O	1:H:43:VAL:HG13	2.21	0.40
1:D:35:LEU:HD21	1:D:57:GLN:CG	2.50	0.40
1:A:60:LEU:HD22	1:A:64:TYR:CZ	2.56	0.40
1:B:34:THR:O	1:B:37:HIS:HB3	2.21	0.40
1:D:81:GLY:HA3	1:I:40:TRP:HZ3	1.86	0.40
1:D:38:VAL:HG22	1:D:95:TYR:CE2	2.56	0.40
1:J:37:HIS:O	1:J:40:TRP:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:VAL:HG21	1:C:102:VAL:HG22	2.02	0.40
1:A:27:THR:HA	1:A:92:TRP:CH2	2.56	0.40
1:F:103:GLN:HE21	1:F:156:LEU:HD11	1.86	0.40
1:B:48:ILE:O	1:B:52:GLU:HB2	2.21	0.40
1:C:71:ARG:NH2	1:C:75:LEU:HD21	2.36	0.40
1:E:141:HIS:O	1:E:142:ALA:C	2.60	0.40
1:G:55:ASP:HB2	1:G:56:PRO:CD	2.51	0.40
1:J:149:GLN:NE2	1:J:153:ARG:HE	2.19	0.40
1:D:34:THR:O	1:D:37:HIS:HB3	2.21	0.40
1:H:69:ALA:O	1:H:79:PRO:HG3	2.21	0.40
1:B:35:LEU:HB3	1:B:58:VAL:CG2	2.49	0.40
1:A:50:VAL:HG12	1:A:54:ILE:HD11	2.04	0.40
1:A:21:LEU:HB2	1:A:72:ILE:HG12	2.02	0.40
1:F:95:TYR:CE2	1:F:97:VAL:HB	2.56	0.40
1:F:28:TYR:CD1	1:F:28:TYR:N	2.89	0.40
1:J:44:GLY:HA3	1:J:45:PRO:HD2	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	144/183 (79%)	127 (88%)	16 (11%)	1 (1%)	26	66
1	B	143/183 (78%)	118 (82%)	20 (14%)	5 (4%)	4	29
1	C	145/183 (79%)	121 (83%)	22 (15%)	2 (1%)	14	50
1	D	143/183 (78%)	120 (84%)	15 (10%)	8 (6%)	2	16
1	E	143/183 (78%)	121 (85%)	17 (12%)	5 (4%)	4	29
1	F	144/183 (79%)	120 (83%)	21 (15%)	3 (2%)	9	42
1	G	142/183 (78%)	124 (87%)	18 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	144/183 (79%)	114 (79%)	24 (17%)	6 (4%)	3	23
1	I	143/183 (78%)	110 (77%)	24 (17%)	9 (6%)	2	13
1	J	144/183 (79%)	113 (78%)	25 (17%)	6 (4%)	3	23
All	All	1435/1830 (78%)	1188 (83%)	202 (14%)	45 (3%)	5	32

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	LYS
1	D	47	PHE
1	D	105	HIS
1	E	45	PRO
1	E	91	THR
1	E	99	ARG
1	F	128	GLU
1	F	154	ALA
1	H	128	GLU
1	I	153	ARG
1	J	45	PRO
1	J	94	ASP
1	B	93	ASP
1	B	94	ASP
1	C	45	PRO
1	D	45	PRO
1	D	153	ARG
1	F	94	ASP
1	H	76	GLY
1	I	99	ARG
1	I	136	ASP
1	I	152	VAL
1	J	142	ALA
1	A	103	GLN
1	D	130	LEU
1	D	136	ASP
1	E	128	GLU
1	I	101	THR
1	B	45	PRO
1	B	95	TYR
1	D	103	GLN
1	E	90	ARG
1	H	85	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	99	ARG
1	H	154	ALA
1	I	110	ASP
1	J	97	VAL
1	C	122	LYS
1	D	128	GLU
1	I	154	ALA
1	J	100	ASP
1	I	96	SER
1	H	45	PRO
1	I	45	PRO
1	J	49	GLY

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	126/153 (82%)	110 (87%)	16 (13%)	5	24
1	B	125/153 (82%)	111 (89%)	14 (11%)	7	30
1	C	127/153 (83%)	107 (84%)	20 (16%)	3	15
1	D	124/153 (81%)	115 (93%)	9 (7%)	17	53
1	E	125/153 (82%)	112 (90%)	13 (10%)	9	34
1	F	125/153 (82%)	109 (87%)	16 (13%)	5	23
1	G	124/153 (81%)	112 (90%)	12 (10%)	10	38
1	H	126/153 (82%)	111 (88%)	15 (12%)	6	27
1	I	125/153 (82%)	111 (89%)	14 (11%)	7	30
1	J	126/153 (82%)	110 (87%)	16 (13%)	5	24
All	All	1253/1530 (82%)	1108 (88%)	145 (12%)	7	29

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	25	LEU
1	A	31	LEU
1	A	35	LEU
1	A	36	LYS
1	A	47	PHE
1	A	51	HIS
1	A	59	GLU
1	A	60	LEU
1	A	89	ASP
1	A	98	GLU
1	A	100	ASP
1	A	103	GLN
1	A	114	ASN
1	A	139	ILE
1	A	151	PHE
1	B	12	LYS
1	B	25	LEU
1	B	31	LEU
1	B	35	LEU
1	B	39	HIS
1	B	47	PHE
1	B	52	GLU
1	B	59	GLU
1	B	87	ILE
1	B	91	THR
1	B	99	ARG
1	B	100	ASP
1	B	101	THR
1	B	151	PHE
1	C	19	ASP
1	C	25	LEU
1	C	31	LEU
1	C	32	HIS
1	C	43	VAL
1	C	47	PHE
1	C	48	ILE
1	C	59	GLU
1	C	66	ASP
1	C	68	VAL
1	C	71	ARG
1	C	87	ILE
1	C	91	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	92	TRP
1	C	93	ASP
1	C	94	ASP
1	C	99	ARG
1	C	128	GLU
1	C	129	ASP
1	C	145	LEU
1	D	25	LEU
1	D	43	VAL
1	D	71	ARG
1	D	89	ASP
1	D	96	SER
1	D	99	ARG
1	D	103	GLN
1	D	105	HIS
1	D	145	LEU
1	E	11	ASP
1	E	25	LEU
1	E	31	LEU
1	E	48	ILE
1	E	59	GLU
1	E	80	LYS
1	E	86	ILE
1	E	91	THR
1	E	106	LEU
1	E	119	ASP
1	E	139	ILE
1	E	145	LEU
1	E	149	GLN
1	F	25	LEU
1	F	38	VAL
1	F	48	ILE
1	F	62	ARG
1	F	66	ASP
1	F	74	THR
1	F	77	LYS
1	F	86	ILE
1	F	94	ASP
1	F	99	ARG
1	F	106	LEU
1	F	119	ASP
1	F	125	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	135	GLN
1	F	147	LYS
1	F	155	HIS
1	G	16	ASP
1	G	25	LEU
1	G	31	LEU
1	G	42	VAL
1	G	46	ASN
1	G	60	LEU
1	G	66	ASP
1	G	103	GLN
1	G	106	LEU
1	G	110	ASP
1	G	132	LEU
1	G	151	PHE
1	H	33	LEU
1	H	35	LEU
1	H	36	LYS
1	H	47	PHE
1	H	60	LEU
1	H	66	ASP
1	H	77	LYS
1	H	78	SER
1	H	90	ARG
1	H	99	ARG
1	H	114	ASN
1	H	136	ASP
1	H	138	LEU
1	H	139	ILE
1	H	150	TRP
1	I	13	LYS
1	I	15	SER
1	I	31	LEU
1	I	35	LEU
1	I	43	VAL
1	I	52	GLU
1	I	66	ASP
1	I	75	LEU
1	I	97	VAL
1	I	103	GLN
1	I	119	ASP
1	I	136	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	147	LYS
1	I	156	LEU
1	J	12	LYS
1	J	13	LYS
1	J	16	ASP
1	J	25	LEU
1	J	31	LEU
1	J	50	VAL
1	J	53	MET
1	J	68	VAL
1	J	82	THR
1	J	89	ASP
1	J	90	ARG
1	J	99	ARG
1	J	109	LEU
1	J	114	ASN
1	J	149	GLN
1	J	151	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	29	ASN
1	A	41	ASN
1	A	46	ASN
1	A	57	GLN
1	A	103	GLN
1	A	114	ASN
1	A	135	GLN
1	A	155	HIS
1	B	22	GLN
1	B	41	ASN
1	B	135	GLN
1	C	24	GLN
1	C	29	ASN
1	C	41	ASN
1	C	46	ASN
1	C	114	ASN
1	C	149	GLN
1	D	41	ASN
1	D	103	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	ASN
1	D	149	GLN
1	D	155	HIS
1	E	24	GLN
1	E	29	ASN
1	E	41	ASN
1	E	57	GLN
1	E	149	GLN
1	E	155	HIS
1	F	24	GLN
1	F	29	ASN
1	F	41	ASN
1	F	103	GLN
1	F	114	ASN
1	F	135	GLN
1	F	149	GLN
1	G	24	GLN
1	G	41	ASN
1	H	24	GLN
1	H	41	ASN
1	H	46	ASN
1	H	57	GLN
1	H	114	ASN
1	H	149	GLN
1	H	155	HIS
1	I	24	GLN
1	I	29	ASN
1	I	41	ASN
1	I	103	GLN
1	I	114	ASN
1	I	135	GLN
1	J	24	GLN
1	J	37	HIS
1	J	41	ASN
1	J	51	HIS
1	J	114	ASN
1	J	141	HIS
1	J	149	GLN

5.3.3 RNA ⓘ

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	146/183 (79%)	-0.63	1 (0%) 89 86	8, 17, 34, 94	0
1	B	145/183 (79%)	-0.42	1 (0%) 89 86	11, 24, 75, 96	0
1	C	147/183 (80%)	-0.21	3 (2%) 68 62	13, 32, 86, 126	0
1	D	145/183 (79%)	-0.13	7 (4%) 34 28	21, 39, 102, 138	0
1	E	145/183 (79%)	-0.50	3 (2%) 67 60	9, 21, 56, 100	0
1	F	146/183 (79%)	-0.23	2 (1%) 78 73	13, 36, 67, 84	0
1	G	144/183 (78%)	-0.35	2 (1%) 78 73	10, 24, 54, 96	0
1	H	146/183 (79%)	0.22	8 (5%) 29 23	17, 69, 119, 154	0
1	I	145/183 (79%)	0.23	8 (5%) 29 23	33, 73, 115, 136	0
1	J	146/183 (79%)	0.04	10 (6%) 20 17	19, 48, 109, 158	0
All	All	1455/1830 (79%)	-0.20	45 (3%) 52 46	8, 34, 101, 158	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	11	ASP	5.3
1	G	14	ALA	4.9
1	C	11	ASP	4.7
1	J	12	LYS	4.1
1	I	129	ASP	3.6
1	A	11	ASP	3.3
1	J	45	PRO	3.2
1	I	17	VAL	3.1
1	J	49	GLY	3.0
1	D	13	LYS	2.9
1	J	99	ARG	2.9
1	J	44	GLY	2.7
1	C	47	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	46	ASN	2.6
1	H	13	LYS	2.5
1	J	47	PHE	2.5
1	E	11	ASP	2.5
1	H	128	GLU	2.5
1	I	123	SER	2.5
1	F	132	LEU	2.4
1	J	48	ILE	2.4
1	J	155	HIS	2.3
1	E	13	LYS	2.3
1	C	45	PRO	2.3
1	J	43	VAL	2.3
1	F	129	ASP	2.3
1	G	13	LYS	2.3
1	H	134	SER	2.3
1	B	11	ASP	2.3
1	D	155	HIS	2.3
1	D	12	LYS	2.3
1	E	129	ASP	2.2
1	I	125	GLU	2.2
1	H	75	LEU	2.2
1	H	129	ASP	2.2
1	I	14	ALA	2.1
1	D	45	PRO	2.1
1	D	98	GLU	2.1
1	I	136	ASP	2.1
1	I	71	ARG	2.1
1	D	15	SER	2.1
1	H	19	ASP	2.1
1	H	155	HIS	2.1
1	I	15	SER	2.0
1	H	139	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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.