



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:54 AM GMT

PDB ID : 2ERC
Title : CRYSTAL STRUCTURE OF ERM C' A RRNA-METHYL TRANSFERASE
Authors : Bussiere, D.E.; Muchmore, S.W.; Dealwis, C.G.; Schluckebier, G.; Abad-Zapatero, C.
Deposited on : 1998-03-13
Resolution : 3.03 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

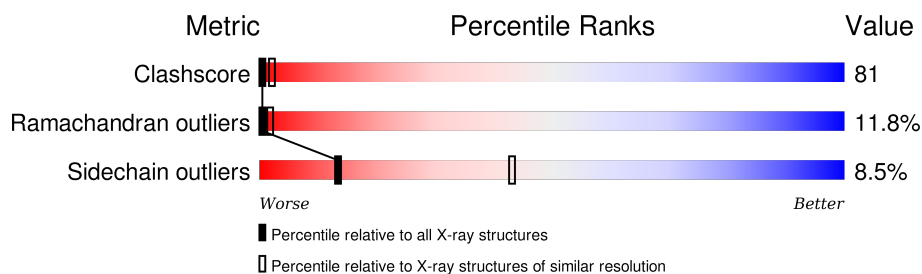
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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))
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	244	
1	B	244	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3934 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 RRNA METHYL TRANSFERASE.

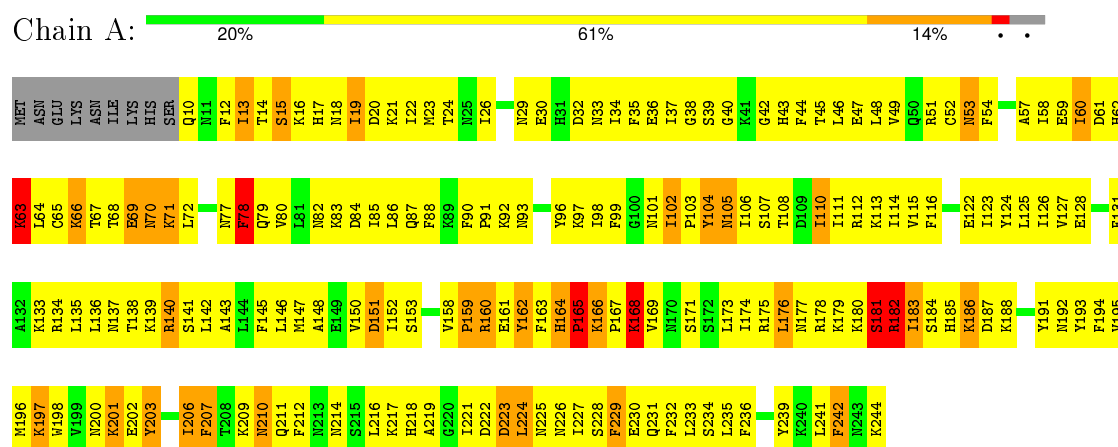
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1967	1272	339	350	6			
1	B	235	Total	C	N	O	S	0	0	0
			1967	1272	339	350	6			

3 Residue-property plots

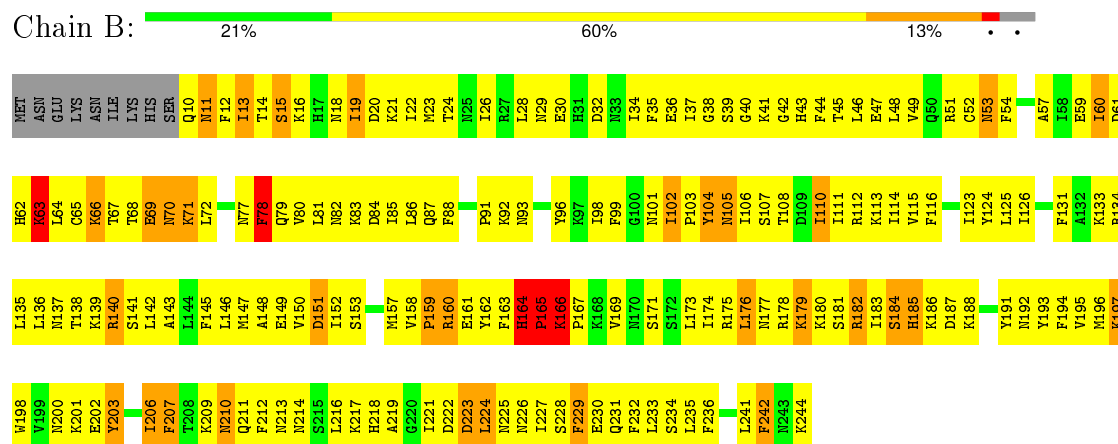
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: RRNA METHYL TRANSFERASE



• Molecule 1: RRNA METHYL TRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	146.90 Å 146.90 Å 57.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.03	Depositor
% Data completeness (in resolution range)	90.0 (8.00-3.03)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3934	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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	0.65	0/2009	0.96	3/2697 (0.1%)
1	B	0.65	0/2009	0.94	4/2697 (0.1%)
All	All	0.65	0/4018	0.95	7/5394 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LYS	N-CA-C	-8.42	88.26	111.00
1	B	182	ARG	N-CA-C	-7.74	90.10	111.00
1	B	179	LYS	N-CA-C	-5.53	96.07	111.00
1	A	181	SER	N-CA-C	5.45	125.73	111.00
1	B	166	LYS	N-CA-C	5.30	125.31	111.00
1	B	164	HIS	N-CA-C	-5.26	96.79	111.00
1	A	183	ILE	N-CA-C	-5.04	97.40	111.00

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	1967	0	2001	325	0
1	B	1967	0	2001	316	0
All	All	3934	0	4002	641	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 81.

All (641) 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:A:160:ARG:HG2	1:A:161:GLU:H	1.12	1.15
1:A:133:LYS:NZ	1:A:140:ARG:HH22	1.47	1.10
1:B:133:LYS:NZ	1:B:140:ARG:HH22	1.49	1.10
1:A:165:PRO:C	1:A:167:PRO:HD3	1.79	1.01
1:B:36:GLU:HB3	1:B:57:ALA:HA	1.42	1.01
1:A:36:GLU:HB3	1:A:57:ALA:HA	1.41	1.00
1:B:160:ARG:HG2	1:B:161:GLU:H	1.28	0.96
1:B:197:LYS:HB2	1:B:206:ILE:HD11	1.42	0.96
1:B:59:GLU:O	1:B:82:ASN:HA	1.66	0.96
1:B:66:LYS:NZ	1:B:70:ASN:HD21	1.64	0.95
1:A:197:LYS:HB2	1:A:206:ILE:HD11	1.48	0.94
1:B:107:SER:H	1:B:110:ILE:HD11	1.31	0.94
1:A:191:TYR:O	1:A:195:VAL:HG23	1.68	0.94
1:A:64:LEU:HD22	1:A:64:LEU:H	1.33	0.93
1:A:66:LYS:NZ	1:A:70:ASN:HD21	1.66	0.93
1:A:14:THR:OG1	1:A:43:HIS:HB3	1.68	0.92
1:B:39:SER:OG	1:B:59:GLU:HB2	1.68	0.91
1:A:39:SER:OG	1:A:59:GLU:HB2	1.69	0.91
1:A:59:GLU:O	1:A:82:ASN:HA	1.68	0.91
1:B:133:LYS:HZ2	1:B:140:ARG:HH22	1.14	0.91
1:B:191:TYR:O	1:B:195:VAL:HG23	1.71	0.91
1:A:63:LYS:HB2	1:A:63:LYS:HZ3	1.35	0.90
1:B:64:LEU:HD22	1:B:64:LEU:H	1.35	0.90
1:A:91:PRO:HG2	1:A:96:TYR:CE1	2.09	0.88
1:B:228:SER:O	1:B:230:GLU:N	2.06	0.88
1:B:148:ALA:O	1:B:182:ARG:HA	1.72	0.87
1:B:36:GLU:HG3	1:B:38:GLY:O	1.75	0.87
1:B:14:THR:HG21	1:B:71:LYS:HZ1	1.39	0.86
1:A:152:ILE:N	1:A:152:ILE:HD12	1.90	0.86
1:A:133:LYS:HZ2	1:A:140:ARG:HH22	1.20	0.86
1:B:14:THR:HG21	1:B:71:LYS:NZ	1.89	0.86
1:B:152:ILE:N	1:B:152:ILE:HD12	1.89	0.86
1:A:36:GLU:HG3	1:A:38:GLY:O	1.76	0.85
1:B:91:PRO:HG2	1:B:96:TYR:CE1	2.10	0.85
1:A:133:LYS:HZ3	1:A:140:ARG:HH22	1.24	0.84
1:A:164:HIS:HB3	1:A:165:PRO:CD	2.06	0.84
1:A:137:ASN:HD21	1:A:140:ARG:NH2	1.75	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:HD21	1:B:140:ARG:NH2	1.74	0.84
1:A:114:ILE:HG22	1:A:123:ILE:HD13	1.58	0.84
1:A:107:SER:H	1:A:110:ILE:HD11	1.43	0.84
1:B:34:ILE:HD11	1:B:48:LEU:HD13	1.60	0.84
1:A:164:HIS:HB3	1:A:165:PRO:HD2	1.58	0.83
1:A:160:ARG:HG2	1:A:161:GLU:N	1.94	0.83
1:B:207:PHE:HB2	1:B:211:GLN:HB2	1.60	0.83
1:A:63:LYS:HB2	1:A:63:LYS:NZ	1.94	0.82
1:A:207:PHE:HB2	1:A:211:GLN:HB2	1.59	0.82
1:B:141:SER:HB2	1:B:145:PHE:CE2	2.15	0.82
1:B:22:ILE:HD11	1:B:44:PHE:HZ	1.45	0.81
1:A:228:SER:O	1:A:230:GLU:N	2.13	0.81
1:A:49:VAL:HG13	1:A:77:ASN:HB2	1.62	0.81
1:B:45:THR:O	1:B:49:VAL:HG23	1.80	0.81
1:B:180:LYS:CG	1:B:181:SER:H	1.94	0.80
1:B:114:ILE:HG22	1:B:123:ILE:HD13	1.63	0.80
1:A:26:ILE:HD11	1:A:173:LEU:HD21	1.63	0.80
1:A:167:PRO:O	1:A:168:LYS:HG2	1.81	0.80
1:B:107:SER:H	1:B:110:ILE:CD1	1.94	0.80
1:B:107:SER:N	1:B:110:ILE:HD11	1.97	0.80
1:B:197:LYS:HB2	1:B:206:ILE:CD1	2.12	0.80
1:A:60:ILE:HG13	1:A:61:ASP:H	1.47	0.79
1:A:141:SER:HB2	1:A:145:PHE:CE2	2.18	0.79
1:B:63:LYS:HB2	1:B:63:LYS:NZ	1.96	0.79
1:A:197:LYS:HB2	1:A:206:ILE:CD1	2.12	0.78
1:A:45:THR:O	1:A:49:VAL:HG23	1.83	0.78
1:A:22:ILE:HD11	1:A:44:PHE:HZ	1.48	0.78
1:A:12:PHE:O	1:A:13:ILE:HG22	1.84	0.78
1:A:10:GLN:NE2	1:A:166:LYS:HB2	1.99	0.78
1:A:13:ILE:HD13	1:A:101:ASN:HD21	1.48	0.78
1:B:63:LYS:HZ3	1:B:63:LYS:HB2	1.48	0.77
1:A:107:SER:H	1:A:110:ILE:CD1	1.96	0.77
1:B:26:ILE:HD11	1:B:173:LEU:HD21	1.65	0.77
1:A:223:ASP:O	1:A:225:ASN:N	2.17	0.77
1:B:49:VAL:HG13	1:B:77:ASN:HB2	1.67	0.77
1:B:21:LYS:NZ	1:B:162:TYR:CE2	2.52	0.77
1:B:104:TYR:O	1:B:105:ASN:CB	2.33	0.77
1:A:148:ALA:HB1	1:A:183:ILE:HG13	1.66	0.77
1:A:60:ILE:HG13	1:A:61:ASP:N	1.98	0.76
1:B:39:SER:CB	1:B:59:GLU:HB2	2.14	0.76
1:B:223:ASP:O	1:B:225:ASN:N	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HG3	1:B:181:SER:H	1.51	0.76
1:A:60:ILE:O	1:A:82:ASN:HB2	1.86	0.76
1:A:106:ILE:HD12	1:A:110:ILE:HD12	1.67	0.75
1:A:34:ILE:HD11	1:A:48:LEU:HD13	1.68	0.75
1:A:12:PHE:CE2	1:A:164:HIS:ND1	2.55	0.75
1:B:197:LYS:CB	1:B:206:ILE:HD11	2.16	0.74
1:B:102:ILE:HG12	1:B:102:ILE:O	1.87	0.74
1:B:107:SER:OG	1:B:110:ILE:HG12	1.87	0.74
1:B:80:VAL:HG22	1:B:80:VAL:O	1.86	0.74
1:A:160:ARG:CG	1:A:161:GLU:H	1.94	0.74
1:B:60:ILE:O	1:B:82:ASN:ND2	2.20	0.74
1:B:201:LYS:HA	1:B:203:TYR:CE1	2.23	0.74
1:A:201:LYS:HA	1:A:203:TYR:CE1	2.21	0.74
1:A:104:TYR:O	1:A:105:ASN:CB	2.34	0.74
1:B:106:ILE:HA	1:B:110:ILE:CD1	2.18	0.74
1:B:108:THR:HB	1:B:112:ARG:NH1	2.03	0.74
1:B:161:GLU:OE2	1:B:165:PRO:HA	1.88	0.74
1:A:192:ASN:O	1:A:196:MET:HG2	1.88	0.73
1:B:13:ILE:HD12	1:B:163:PHE:CE1	2.24	0.73
1:A:106:ILE:HA	1:A:110:ILE:CD1	2.18	0.73
1:B:133:LYS:HZ3	1:B:140:ARG:HH22	1.34	0.73
1:A:143:ALA:O	1:A:147:MET:HG3	1.89	0.72
1:A:197:LYS:CB	1:A:206:ILE:HD11	2.19	0.72
1:A:80:VAL:HG22	1:A:80:VAL:O	1.90	0.72
1:B:22:ILE:HD11	1:B:44:PHE:CZ	2.24	0.72
1:B:21:LYS:NZ	1:B:162:TYR:HE2	1.86	0.72
1:B:160:ARG:HG2	1:B:161:GLU:N	2.04	0.71
1:A:125:LEU:O	1:A:174:ILE:HG12	1.88	0.71
1:B:133:LYS:HZ2	1:B:140:ARG:NH2	1.88	0.71
1:B:108:THR:HB	1:B:112:ARG:HH12	1.56	0.71
1:B:106:ILE:HA	1:B:110:ILE:HD11	1.70	0.71
1:B:192:ASN:O	1:B:196:MET:HG2	1.90	0.71
1:A:64:LEU:CD2	1:A:64:LEU:H	2.02	0.71
1:A:108:THR:HB	1:A:112:ARG:NH1	2.06	0.71
1:A:102:ILE:HG12	1:A:102:ILE:O	1.90	0.71
1:B:14:THR:OG1	1:B:43:HIS:HB3	1.91	0.71
1:A:161:GLU:HB3	1:A:164:HIS:O	1.89	0.71
1:B:152:ILE:HD12	1:B:152:ILE:H	1.53	0.70
1:A:70:ASN:C	1:A:72:LEU:H	1.95	0.70
1:A:104:TYR:O	1:A:105:ASN:HB2	1.92	0.70
1:A:108:THR:HB	1:A:112:ARG:HH12	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLN:HE21	1:A:166:LYS:HB2	1.55	0.70
1:A:40:GLY:HA3	1:A:43:HIS:NE2	2.06	0.70
1:B:40:GLY:HA3	1:B:43:HIS:NE2	2.07	0.70
1:A:60:ILE:O	1:A:82:ASN:ND2	2.23	0.70
1:B:64:LEU:CD2	1:B:64:LEU:H	2.04	0.70
1:B:65:CYS:SG	1:B:82:ASN:HB3	2.32	0.69
1:A:107:SER:N	1:A:110:ILE:HD11	2.06	0.69
1:A:13:ILE:HA	1:A:162:TYR:O	1.92	0.69
1:B:116:PHE:CZ	1:B:146:LEU:HD23	2.28	0.69
1:B:137:ASN:HD21	1:B:140:ARG:CZ	2.06	0.69
1:B:106:ILE:HD12	1:B:110:ILE:HD12	1.74	0.68
1:A:152:ILE:H	1:A:152:ILE:HD12	1.57	0.68
1:A:66:LYS:CE	1:A:70:ASN:HD21	2.06	0.68
1:B:180:LYS:HG3	1:B:181:SER:N	2.09	0.68
1:A:22:ILE:HD11	1:A:44:PHE:CZ	2.28	0.68
1:B:104:TYR:O	1:B:105:ASN:HB2	1.94	0.68
1:B:60:ILE:HG13	1:B:61:ASP:N	2.09	0.68
1:B:229:PHE:O	1:B:233:LEU:N	2.27	0.68
1:B:123:ILE:HG22	1:B:125:LEU:HD22	1.76	0.68
1:A:137:ASN:HD21	1:A:140:ARG:CZ	2.07	0.67
1:A:182:ARG:HD2	1:A:183:ILE:HG12	1.76	0.67
1:B:60:ILE:O	1:B:82:ASN:HB2	1.95	0.67
1:A:14:THR:HA	1:A:19:ILE:HD11	1.75	0.67
1:A:13:ILE:HD12	1:A:163:PHE:CE1	2.30	0.67
1:A:165:PRO:O	1:A:167:PRO:HD3	1.94	0.67
1:A:229:PHE:O	1:A:233:LEU:N	2.24	0.67
1:A:183:ILE:HG22	1:A:188:LYS:HD3	1.75	0.67
1:B:182:ARG:NH2	1:B:185:HIS:HA	2.09	0.67
1:B:180:LYS:CD	1:B:181:SER:H	2.07	0.67
1:B:70:ASN:C	1:B:72:LEU:H	1.96	0.67
1:A:65:CYS:SG	1:A:82:ASN:HB3	2.35	0.67
1:A:116:PHE:CZ	1:A:146:LEU:HD23	2.30	0.67
1:B:85:ILE:HG21	1:B:110:ILE:HG22	1.77	0.67
1:B:180:LYS:CG	1:B:181:SER:N	2.56	0.67
1:B:182:ARG:HG2	1:B:183:ILE:H	1.59	0.67
1:A:133:LYS:HA	1:A:136:LEU:HB2	1.75	0.66
1:A:123:ILE:HG22	1:A:125:LEU:HD22	1.76	0.66
1:B:148:ALA:HB1	1:B:183:ILE:HG12	1.77	0.66
1:B:183:ILE:O	1:B:184:SER:C	2.31	0.66
1:A:13:ILE:HB	1:A:163:PHE:CD1	2.30	0.66
1:A:182:ARG:CD	1:A:183:ILE:HG12	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:CE	1:B:70:ASN:HD21	2.09	0.66
1:B:191:TYR:HA	1:B:236:PHE:CE1	2.30	0.65
1:A:110:ILE:O	1:A:114:ILE:HG12	1.97	0.65
1:B:133:LYS:HA	1:B:136:LEU:HB2	1.78	0.65
1:A:53:ASN:O	1:A:77:ASN:ND2	2.29	0.65
1:B:66:LYS:HZ3	1:B:70:ASN:HD21	1.43	0.65
1:A:53:ASN:OD1	1:A:54:PHE:N	2.29	0.65
1:B:143:ALA:O	1:B:147:MET:HG3	1.96	0.65
1:A:133:LYS:HZ2	1:A:140:ARG:NH2	1.94	0.64
1:B:60:ILE:HG13	1:B:61:ASP:H	1.62	0.64
1:B:53:ASN:O	1:B:77:ASN:ND2	2.30	0.64
1:B:141:SER:HB2	1:B:145:PHE:HE2	1.61	0.64
1:A:106:ILE:HA	1:A:110:ILE:HD12	1.79	0.64
1:A:40:GLY:HA3	1:A:43:HIS:HE2	1.62	0.64
1:A:211:GLN:HE22	1:A:242:PHE:HB3	1.63	0.64
1:B:107:SER:H	1:B:110:ILE:CG1	2.11	0.64
1:B:223:ASP:OD2	1:B:226:ASN:ND2	2.28	0.64
1:B:139:LYS:CE	1:B:201:LYS:HD3	2.27	0.64
1:A:137:ASN:OD1	1:A:140:ARG:HB2	1.98	0.63
1:B:158:VAL:HB	1:B:171:SER:HB2	1.78	0.63
1:B:137:ASN:OD1	1:B:140:ARG:HB2	1.99	0.63
1:B:91:PRO:HG2	1:B:96:TYR:CZ	2.33	0.63
1:B:139:LYS:HE2	1:B:201:LYS:HD3	1.78	0.63
1:A:211:GLN:NE2	1:A:242:PHE:HB3	2.13	0.63
1:A:175:ARG:HH11	1:A:175:ARG:HG2	1.63	0.63
1:B:158:VAL:HG11	1:B:163:PHE:CZ	2.33	0.63
1:B:228:SER:OG	1:B:231:GLN:HG3	1.98	0.63
1:A:139:LYS:HE2	1:A:201:LYS:HD3	1.80	0.63
1:B:23:MET:CE	1:B:48:LEU:HD23	2.29	0.63
1:A:139:LYS:CE	1:A:201:LYS:HD3	2.28	0.63
1:A:107:SER:OG	1:A:110:ILE:HG12	1.98	0.63
1:A:193:TYR:O	1:A:196:MET:HB2	1.99	0.62
1:A:107:SER:H	1:A:110:ILE:CG1	2.11	0.62
1:A:23:MET:CE	1:A:48:LEU:HD23	2.30	0.62
1:B:125:LEU:O	1:B:174:ILE:HG12	1.99	0.62
1:A:212:PHE:HZ	1:A:224:LEU:HD21	1.64	0.62
1:B:53:ASN:OD1	1:B:54:PHE:N	2.33	0.62
1:A:91:PRO:HG2	1:A:96:TYR:CZ	2.35	0.62
1:A:43:HIS:ND1	1:A:44:PHE:N	2.47	0.61
1:A:60:ILE:HG22	1:A:83:LYS:O	2.00	0.61
1:B:110:ILE:O	1:B:114:ILE:HG12	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:O	1:B:166:LYS:HB3	1.98	0.61
1:B:70:ASN:O	1:B:72:LEU:N	2.33	0.61
1:B:223:ASP:O	1:B:226:ASN:N	2.27	0.61
1:B:29:ASN:O	1:B:52:CYS:HA	2.00	0.61
1:B:209:LYS:N	1:B:209:LYS:HD3	2.16	0.61
1:B:193:TYR:O	1:B:196:MET:HB2	2.01	0.61
1:B:165:PRO:HG2	1:B:166:LYS:N	2.15	0.61
1:B:30:GLU:HG3	1:B:51:ARG:O	2.01	0.61
1:B:19:ILE:HG22	1:B:47:GLU:HG2	1.83	0.61
1:B:216:LEU:HD23	1:B:221:ILE:HD12	1.83	0.61
1:A:23:MET:HE2	1:A:48:LEU:HD23	1.83	0.60
1:A:19:ILE:HG22	1:A:47:GLU:HG2	1.82	0.60
1:B:13:ILE:O	1:B:13:ILE:HG12	2.01	0.60
1:A:223:ASP:O	1:A:226:ASN:N	2.31	0.60
1:B:227:ILE:HG22	1:B:228:SER:N	2.17	0.60
1:A:106:ILE:HA	1:A:110:ILE:HD11	1.83	0.60
1:A:161:GLU:OE2	1:A:165:PRO:HA	2.01	0.60
1:A:39:SER:CB	1:A:59:GLU:HB2	2.32	0.60
1:A:142:LEU:HD11	1:A:146:LEU:HD11	1.83	0.60
1:A:164:HIS:CB	1:A:165:PRO:CD	2.77	0.60
1:A:23:MET:HE3	1:A:51:ARG:HD3	1.83	0.59
1:A:70:ASN:C	1:A:72:LEU:N	2.54	0.59
1:B:222:ASP:O	1:B:224:LEU:N	2.29	0.59
1:B:142:LEU:O	1:B:146:LEU:HG	2.03	0.59
1:B:222:ASP:C	1:B:224:LEU:H	2.05	0.59
1:A:19:ILE:HG22	1:A:19:ILE:O	2.03	0.59
1:A:142:LEU:O	1:A:146:LEU:HG	2.01	0.59
1:A:152:ILE:N	1:A:152:ILE:CD1	2.62	0.59
1:B:180:LYS:O	1:B:181:SER:OG	2.18	0.59
1:A:219:ALA:HB3	1:A:221:ILE:HG13	1.84	0.59
1:A:227:ILE:HG22	1:A:228:SER:N	2.18	0.59
1:B:39:SER:HB2	1:B:59:GLU:HB2	1.84	0.59
1:A:13:ILE:O	1:A:13:ILE:HG12	2.03	0.58
1:A:21:LYS:NZ	1:A:162:TYR:CE2	2.71	0.58
1:B:149:GLU:HB3	1:B:182:ARG:HG3	1.85	0.58
1:B:212:PHE:HZ	1:B:224:LEU:HD21	1.69	0.58
1:A:141:SER:HB2	1:A:145:PHE:HE2	1.67	0.58
1:A:85:ILE:HG23	1:A:86:LEU:N	2.17	0.58
1:A:101:ASN:C	1:A:103:PRO:HD2	2.24	0.58
1:B:184:SER:O	1:B:185:HIS:C	2.41	0.58
1:A:70:ASN:O	1:A:72:LEU:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:CG	1:B:161:GLU:H	2.03	0.58
1:A:212:PHE:CZ	1:A:224:LEU:HD21	2.39	0.58
1:B:70:ASN:C	1:B:72:LEU:N	2.57	0.58
1:A:191:TYR:HA	1:A:236:PHE:CE1	2.39	0.58
1:B:23:MET:CB	1:B:51:ARG:NH1	2.66	0.58
1:A:223:ASP:OD2	1:A:226:ASN:ND2	2.29	0.58
1:A:37:ILE:CD1	1:A:114:ILE:HD11	2.34	0.57
1:A:39:SER:HG	1:A:59:GLU:HB2	1.70	0.57
1:A:21:LYS:NZ	1:A:162:TYR:OH	2.38	0.57
1:B:15:SER:H	1:B:19:ILE:HD12	1.69	0.57
1:A:183:ILE:HG22	1:A:188:LYS:CD	2.34	0.57
1:A:14:THR:HG1	1:A:43:HIS:HB3	1.67	0.57
1:B:101:ASN:ND2	1:B:126:ILE:HD12	2.19	0.57
1:B:85:ILE:HG23	1:B:86:LEU:N	2.18	0.57
1:B:101:ASN:C	1:B:103:PRO:HD2	2.25	0.57
1:A:101:ASN:ND2	1:A:126:ILE:HD12	2.19	0.57
1:A:85:ILE:HG21	1:A:110:ILE:HG22	1.87	0.57
1:A:223:ASP:CG	1:A:226:ASN:HD22	2.08	0.56
1:A:85:ILE:CG2	1:A:86:LEU:N	2.68	0.56
1:A:15:SER:H	1:A:19:ILE:HD12	1.70	0.56
1:A:63:LYS:CB	1:A:63:LYS:NZ	2.66	0.56
1:B:223:ASP:CG	1:B:226:ASN:HD22	2.08	0.56
1:A:46:LEU:HD12	1:A:71:LYS:HG2	1.88	0.56
1:B:13:ILE:O	1:B:19:ILE:HD11	2.05	0.56
1:B:40:GLY:HA3	1:B:43:HIS:HE2	1.69	0.56
1:B:19:ILE:HG22	1:B:19:ILE:O	2.03	0.56
1:A:83:LYS:CG	1:A:84:ASP:H	2.18	0.56
1:A:60:ILE:HA	1:A:82:ASN:O	2.06	0.56
1:A:142:LEU:C	1:A:142:LEU:HD13	2.26	0.56
1:B:43:HIS:ND1	1:B:44:PHE:N	2.50	0.56
1:B:182:ARG:HH21	1:B:185:HIS:HA	1.70	0.56
1:B:46:LEU:HD12	1:B:71:LYS:HG2	1.87	0.55
1:A:212:PHE:O	1:A:216:LEU:HG	2.06	0.55
1:B:23:MET:HG3	1:B:51:ARG:NH1	2.22	0.55
1:B:102:ILE:HD13	1:B:110:ILE:HD12	1.89	0.55
1:A:114:ILE:CG2	1:A:123:ILE:HD13	2.34	0.55
1:B:211:GLN:NE2	1:B:242:PHE:HB3	2.21	0.55
1:A:161:GLU:C	1:A:163:PHE:H	2.09	0.54
1:A:209:LYS:N	1:A:209:LYS:HD3	2.22	0.54
1:A:158:VAL:HG11	1:A:163:PHE:CE2	2.42	0.54
1:A:30:GLU:HG3	1:A:51:ARG:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG11	1:B:163:PHE:CE2	2.42	0.54
1:A:64:LEU:N	1:A:64:LEU:HD22	2.12	0.54
1:B:35:PHE:HB2	1:B:98:ILE:HG12	1.89	0.54
1:A:13:ILE:HD13	1:A:101:ASN:ND2	2.20	0.54
1:A:223:ASP:O	1:A:223:ASP:OD1	2.25	0.54
1:A:35:PHE:HB2	1:A:98:ILE:HG12	1.89	0.54
1:B:23:MET:HE1	1:B:48:LEU:HD23	1.90	0.54
1:B:68:THR:O	1:B:70:ASN:N	2.40	0.54
1:B:183:ILE:HG21	1:B:191:TYR:HB2	1.90	0.54
1:A:23:MET:HG3	1:A:51:ARG:NH1	2.23	0.54
1:A:60:ILE:CG1	1:A:61:ASP:N	2.70	0.54
1:A:228:SER:OG	1:A:231:GLN:HG3	2.08	0.54
1:A:106:ILE:HG13	1:A:131:PHE:HE2	1.73	0.53
1:A:211:GLN:NE2	1:A:242:PHE:CG	2.76	0.53
1:B:106:ILE:CA	1:B:110:ILE:HD11	2.37	0.53
1:B:211:GLN:HE22	1:B:242:PHE:HB3	1.74	0.53
1:B:83:LYS:CG	1:B:84:ASP:H	2.22	0.53
1:A:29:ASN:O	1:A:52:CYS:HA	2.08	0.53
1:B:197:LYS:HA	1:B:197:LYS:HZ2	1.73	0.53
1:B:54:PHE:HE2	1:B:79:GLN:HG3	1.74	0.53
1:A:66:LYS:HZ3	1:A:70:ASN:HD21	1.51	0.53
1:B:147:MET:HB2	1:B:229:PHE:CE1	2.43	0.53
1:A:66:LYS:HZ1	1:A:70:ASN:HD21	1.55	0.53
1:B:36:GLU:HB3	1:B:57:ALA:CA	2.27	0.53
1:B:207:PHE:N	1:B:207:PHE:CD1	2.74	0.53
1:B:64:LEU:HD22	1:B:64:LEU:N	2.13	0.53
1:B:142:LEU:C	1:B:142:LEU:HD13	2.28	0.53
1:B:106:ILE:HG13	1:B:131:PHE:HE2	1.74	0.53
1:B:42:GLY:HA3	1:B:71:LYS:HD3	1.91	0.53
1:A:182:ARG:NH1	1:A:233:LEU:HD21	2.23	0.53
1:B:212:PHE:CZ	1:B:224:LEU:HD21	2.43	0.53
1:A:21:LYS:NZ	1:A:162:TYR:HE2	2.06	0.53
1:B:14:THR:CG2	1:B:71:LYS:NZ	2.70	0.53
1:A:36:GLU:HB3	1:A:57:ALA:CA	2.28	0.53
1:A:161:GLU:O	1:A:163:PHE:N	2.42	0.52
1:B:61:ASP:HB3	1:B:64:LEU:HD23	1.91	0.52
1:A:158:VAL:HB	1:A:171:SER:HB2	1.90	0.52
1:A:26:ILE:HG23	1:A:124:TYR:CE2	2.44	0.52
1:A:42:GLY:HA3	1:A:71:LYS:HD3	1.89	0.52
1:A:161:GLU:C	1:A:163:PHE:N	2.61	0.52
1:B:182:ARG:CG	1:B:183:ILE:H	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HG21	1:A:110:ILE:CG2	2.40	0.52
1:B:23:MET:HE2	1:B:48:LEU:HD23	1.91	0.52
1:A:147:MET:HB2	1:A:229:PHE:CE1	2.44	0.52
1:A:244:LYS:HD3	1:A:244:LYS:C	2.30	0.52
1:B:142:LEU:HD11	1:B:146:LEU:HD11	1.90	0.52
1:B:11:ASN:HD21	1:B:166:LYS:CB	2.22	0.52
1:A:13:ILE:CD1	1:A:101:ASN:HD21	2.21	0.52
1:A:133:LYS:NZ	1:A:140:ARG:NH2	2.33	0.52
1:B:227:ILE:HG22	1:B:228:SER:H	1.73	0.52
1:A:222:ASP:C	1:A:224:LEU:H	2.14	0.52
1:B:85:ILE:CG2	1:B:86:LEU:N	2.73	0.52
1:B:212:PHE:O	1:B:216:LEU:HG	2.10	0.52
1:B:175:ARG:HG2	1:B:175:ARG:HH11	1.74	0.52
1:B:65:CYS:O	1:B:69:GLU:HB2	2.09	0.52
1:A:23:MET:CB	1:A:51:ARG:NH1	2.74	0.51
1:B:37:ILE:CD1	1:B:114:ILE:HD11	2.39	0.51
1:A:222:ASP:O	1:A:224:LEU:N	2.37	0.51
1:B:23:MET:HB2	1:B:51:ARG:NH1	2.25	0.51
1:A:133:LYS:HZ3	1:A:140:ARG:NH2	2.00	0.51
1:A:10:GLN:C	1:A:12:PHE:H	2.13	0.51
1:A:166:LYS:N	1:A:167:PRO:HD3	2.25	0.51
1:B:164:HIS:HB3	1:B:165:PRO:HD2	1.92	0.51
1:B:244:LYS:HD3	1:B:244:LYS:C	2.30	0.51
1:A:125:LEU:HD23	1:A:174:ILE:HG13	1.93	0.51
1:B:112:ARG:O	1:B:113:LYS:C	2.49	0.51
1:B:40:GLY:HA3	1:B:43:HIS:CE1	2.46	0.51
1:B:197:LYS:HA	1:B:197:LYS:NZ	2.25	0.51
1:B:54:PHE:CE2	1:B:79:GLN:HG3	2.45	0.51
1:B:161:GLU:C	1:B:163:PHE:N	2.62	0.51
1:B:114:ILE:CG2	1:B:123:ILE:HD13	2.38	0.50
1:A:84:ASP:OD2	1:A:87:GLN:HG2	2.10	0.50
1:B:49:VAL:HG13	1:B:77:ASN:CB	2.39	0.50
1:B:223:ASP:OD1	1:B:223:ASP:O	2.30	0.50
1:A:180:LYS:O	1:A:180:LYS:HD2	2.10	0.50
1:B:23:MET:HE3	1:B:51:ARG:HD3	1.93	0.50
1:A:61:ASP:HB3	1:A:64:LEU:HD23	1.92	0.50
1:B:219:ALA:HB3	1:B:221:ILE:HG13	1.92	0.50
1:B:133:LYS:HG3	1:B:134:ARG:N	2.25	0.50
1:A:54:PHE:CE2	1:A:79:GLN:HG3	2.46	0.50
1:A:54:PHE:HE2	1:A:79:GLN:HG3	1.76	0.50
1:B:229:PHE:O	1:B:232:PHE:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD23	1:A:221:ILE:HD12	1.94	0.50
1:A:133:LYS:HG3	1:A:134:ARG:N	2.26	0.50
1:B:184:SER:HB3	1:B:186:LYS:NZ	2.26	0.50
1:B:68:THR:O	1:B:69:GLU:C	2.50	0.50
1:A:78:PHE:O	1:A:79:GLN:HB2	2.11	0.50
1:A:46:LEU:HD12	1:A:71:LYS:O	2.12	0.50
1:A:107:SER:H	1:A:110:ILE:HG13	1.76	0.50
1:B:14:THR:HG21	1:B:71:LYS:HZ3	1.74	0.50
1:B:211:GLN:NE2	1:B:242:PHE:CG	2.79	0.50
1:A:49:VAL:HG13	1:A:77:ASN:CB	2.38	0.50
1:A:68:THR:O	1:A:70:ASN:N	2.45	0.50
1:A:227:ILE:HG22	1:A:228:SER:H	1.77	0.50
1:A:184:SER:O	1:A:185:HIS:C	2.51	0.50
1:A:60:ILE:HA	1:A:82:ASN:C	2.33	0.49
1:A:210:ASN:N	1:A:210:ASN:HD22	2.09	0.49
1:B:78:PHE:O	1:B:79:GLN:HB2	2.11	0.49
1:A:197:LYS:HA	1:A:197:LYS:HZ2	1.76	0.49
1:A:216:LEU:HD23	1:A:235:LEU:HD21	1.95	0.49
1:A:90:PHE:CE2	1:A:98:ILE:HD11	2.48	0.49
1:B:18:ASN:C	1:B:20:ASP:H	2.16	0.49
1:A:197:LYS:HA	1:A:197:LYS:NZ	2.27	0.49
1:B:228:SER:C	1:B:230:GLU:N	2.66	0.49
1:B:152:ILE:CD1	1:B:152:ILE:H	2.20	0.49
1:A:102:ILE:HG23	1:A:106:ILE:HB	1.95	0.49
1:A:18:ASN:C	1:A:20:ASP:H	2.15	0.49
1:A:65:CYS:O	1:A:69:GLU:HB2	2.13	0.49
1:B:11:ASN:HD21	1:B:166:LYS:HB2	1.78	0.49
1:A:187:ASP:O	1:A:187:ASP:OD1	2.31	0.49
1:A:123:ILE:HB	1:A:176:LEU:HB2	1.93	0.49
1:B:28:LEU:HB3	1:B:52:CYS:SG	2.53	0.49
1:A:65:CYS:SG	1:A:82:ASN:CB	3.00	0.48
1:A:179:LYS:HD2	1:A:181:SER:OG	2.12	0.48
1:B:85:ILE:HG21	1:B:110:ILE:CG2	2.43	0.48
1:A:182:ARG:HD3	1:A:183:ILE:HG12	1.95	0.48
1:A:138:THR:O	1:A:139:LYS:C	2.51	0.48
1:B:46:LEU:HD12	1:B:71:LYS:O	2.14	0.48
1:A:115:VAL:O	1:A:178:ARG:NH2	2.47	0.48
1:A:134:ARG:HE	1:A:140:ARG:NH1	2.12	0.48
1:B:106:ILE:HA	1:B:110:ILE:HD12	1.92	0.48
1:B:65:CYS:SG	1:B:82:ASN:CB	2.99	0.48
1:A:207:PHE:N	1:A:207:PHE:CD1	2.73	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:THR:O	1:B:139:LYS:C	2.51	0.48
1:B:187:ASP:O	1:B:187:ASP:OD1	2.31	0.48
1:A:12:PHE:CD2	1:A:164:HIS:HB2	2.48	0.48
1:A:133:LYS:O	1:A:136:LEU:N	2.46	0.48
1:B:133:LYS:NZ	1:B:140:ARG:NH2	2.35	0.48
1:B:39:SER:HB2	1:B:59:GLU:CG	2.43	0.48
1:B:84:ASP:OD2	1:B:87:GLN:HG2	2.14	0.48
1:A:60:ILE:O	1:A:82:ASN:CB	2.61	0.48
1:A:59:GLU:O	1:A:82:ASN:CA	2.51	0.48
1:A:153:SER:OG	1:A:175:ARG:NH1	2.47	0.48
1:A:34:ILE:CD1	1:A:48:LEU:HD13	2.40	0.48
1:B:29:ASN:N	1:B:32:ASP:OD2	2.47	0.48
1:B:44:PHE:CE2	1:B:101:ASN:ND2	2.82	0.47
1:B:14:THR:CG2	1:B:71:LYS:HZ3	2.27	0.47
1:B:59:GLU:O	1:B:82:ASN:CA	2.49	0.47
1:B:54:PHE:HZ	1:B:79:GLN:HG2	1.79	0.47
1:A:57:ALA:O	1:A:58:ILE:HG13	2.13	0.47
1:A:15:SER:O	1:A:17:HIS:N	2.46	0.47
1:A:37:ILE:HD11	1:A:114:ILE:HD11	1.95	0.47
1:B:60:ILE:HG22	1:B:83:LYS:O	2.14	0.47
1:A:21:LYS:HZ1	1:A:162:TYR:HE2	1.54	0.47
1:B:103:PRO:O	1:B:104:TYR:O	2.31	0.47
1:B:158:VAL:N	1:B:159:PRO:HD3	2.30	0.47
1:B:12:PHE:CE2	1:B:41:LYS:HD3	2.50	0.47
1:A:211:GLN:CD	1:A:244:LYS:O	2.53	0.47
1:A:47:GLU:O	1:A:51:ARG:HB2	2.14	0.47
1:B:137:ASN:ND2	1:B:140:ARG:NH2	2.55	0.47
1:A:26:ILE:HG23	1:A:124:TYR:CD2	2.50	0.47
1:A:19:ILE:O	1:A:47:GLU:HG2	2.15	0.47
1:B:229:PHE:O	1:B:232:PHE:HB3	2.15	0.47
1:A:29:ASN:N	1:A:32:ASP:OD2	2.48	0.47
1:A:102:ILE:CG2	1:A:106:ILE:HD13	2.45	0.47
1:A:44:PHE:CE2	1:A:101:ASN:ND2	2.82	0.47
1:B:21:LYS:CE	1:B:162:TYR:HE2	2.27	0.47
1:B:200:ASN:C	1:B:202:GLU:H	2.18	0.47
1:A:134:ARG:HE	1:A:140:ARG:HH12	1.62	0.47
1:B:149:GLU:OE1	1:B:178:ARG:NH1	2.48	0.47
1:B:191:TYR:HA	1:B:236:PHE:HE1	1.75	0.47
1:A:128:GLU:OE2	1:A:169:VAL:HG21	2.15	0.47
1:B:62:HIS:ND1	1:B:62:HIS:C	2.68	0.47
1:A:62:HIS:C	1:A:62:HIS:ND1	2.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD11	1:A:114:ILE:CD1	2.46	0.46
1:A:142:LEU:CD1	1:A:146:LEU:HD11	2.46	0.46
1:A:80:VAL:CG2	1:A:80:VAL:O	2.61	0.46
1:B:10:GLN:O	1:B:11:ASN:C	2.54	0.46
1:B:193:TYR:CE1	1:B:197:LYS:HE2	2.50	0.46
1:A:193:TYR:CE1	1:A:197:LYS:HE2	2.50	0.46
1:B:63:LYS:CB	1:B:63:LYS:NZ	2.68	0.46
1:A:53:ASN:OD1	1:A:54:PHE:HB2	2.16	0.46
1:B:12:PHE:CZ	1:B:41:LYS:HD3	2.50	0.46
1:B:214:ASN:O	1:B:218:HIS:N	2.46	0.46
1:B:123:ILE:HB	1:B:176:LEU:HB2	1.97	0.46
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.50	0.46
1:A:193:TYR:O	1:A:196:MET:N	2.49	0.46
1:A:191:TYR:CE2	1:A:195:VAL:HG21	2.50	0.46
1:A:83:LYS:CG	1:A:84:ASP:N	2.78	0.46
1:B:14:THR:CA	1:B:43:HIS:HB3	2.46	0.46
1:B:184:SER:O	1:B:186:LYS:N	2.49	0.46
1:B:80:VAL:CG2	1:B:80:VAL:O	2.58	0.46
1:B:102:ILE:CG2	1:B:106:ILE:HD13	2.45	0.46
1:B:164:HIS:CB	1:B:165:PRO:HD2	2.46	0.46
1:A:207:PHE:HB2	1:A:211:GLN:CB	2.38	0.46
1:B:137:ASN:O	1:B:140:ARG:HB3	2.16	0.46
1:B:125:LEU:HD23	1:B:174:ILE:HG13	1.98	0.46
1:B:197:LYS:CB	1:B:206:ILE:CD1	2.86	0.46
1:A:103:PRO:O	1:A:104:TYR:CB	2.64	0.46
1:A:103:PRO:O	1:A:104:TYR:O	2.33	0.46
1:B:39:SER:HB2	1:B:59:GLU:CB	2.44	0.46
1:B:83:LYS:CG	1:B:84:ASP:N	2.79	0.45
1:B:161:GLU:OE1	1:B:161:GLU:HA	2.16	0.45
1:A:150:VAL:HG12	1:A:178:ARG:HG2	1.99	0.45
1:A:112:ARG:O	1:A:113:LYS:C	2.54	0.45
1:A:229:PHE:O	1:A:232:PHE:HB3	2.16	0.45
1:A:150:VAL:HG23	1:A:152:ILE:HD11	1.98	0.45
1:A:23:MET:HB2	1:A:51:ARG:NH1	2.32	0.45
1:A:85:ILE:O	1:A:113:LYS:HE2	2.16	0.45
1:B:102:ILE:N	1:B:103:PRO:CD	2.80	0.45
1:B:21:LYS:HZ3	1:B:162:TYR:HE2	1.44	0.45
1:B:206:ILE:HB	1:B:207:PHE:H	1.57	0.45
1:B:102:ILE:O	1:B:103:PRO:C	2.53	0.45
1:B:21:LYS:NZ	1:B:162:TYR:CZ	2.85	0.45
1:A:210:ASN:N	1:A:210:ASN:ND2	2.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:O	1:A:104:TYR:HB2	2.17	0.45
1:B:134:ARG:HE	1:B:140:ARG:NH1	2.15	0.45
1:B:60:ILE:HA	1:B:82:ASN:O	2.16	0.45
1:A:78:PHE:HB2	1:A:79:GLN:H	1.53	0.45
1:B:200:ASN:O	1:B:202:GLU:N	2.50	0.45
1:B:158:VAL:CG1	1:B:163:PHE:CE2	2.99	0.45
1:B:26:ILE:HG23	1:B:124:TYR:CE2	2.52	0.45
1:A:200:ASN:C	1:A:202:GLU:H	2.19	0.45
1:A:23:MET:HE1	1:A:48:LEU:HD23	1.99	0.45
1:A:134:ARG:HH11	1:A:134:ARG:HG2	1.82	0.45
1:B:60:ILE:CG1	1:B:61:ASP:N	2.77	0.44
1:B:54:PHE:CD1	1:B:77:ASN:HA	2.51	0.44
1:A:14:THR:O	1:A:15:SER:CB	2.65	0.44
1:B:210:ASN:OD1	1:B:244:LYS:NZ	2.43	0.44
1:A:185:HIS:O	1:A:186:LYS:C	2.55	0.44
1:A:165:PRO:C	1:A:167:PRO:CD	2.68	0.44
1:B:66:LYS:O	1:B:67:THR:C	2.56	0.44
1:A:182:ARG:HD2	1:A:182:ARG:C	2.37	0.44
1:A:97:LYS:HZ3	1:A:122:GLU:HB2	1.81	0.44
1:A:197:LYS:CB	1:A:206:ILE:CD1	2.86	0.44
1:A:180:LYS:O	1:A:181:SER:O	2.36	0.44
1:A:200:ASN:O	1:A:202:GLU:N	2.51	0.44
1:A:167:PRO:O	1:A:168:LYS:CG	2.61	0.44
1:A:135:LEU:HD22	1:A:142:LEU:HD11	2.00	0.44
1:B:15:SER:H	1:B:19:ILE:CD1	2.30	0.44
1:B:210:ASN:N	1:B:210:ASN:HD22	2.16	0.44
1:A:229:PHE:O	1:A:232:PHE:N	2.51	0.44
1:A:54:PHE:HZ	1:A:79:GLN:HG2	1.82	0.44
1:B:184:SER:HB3	1:B:186:LYS:HZ3	1.83	0.44
1:B:135:LEU:HD22	1:B:142:LEU:HD11	1.98	0.44
1:A:166:LYS:N	1:A:167:PRO:CD	2.80	0.44
1:A:102:ILE:N	1:A:103:PRO:CD	2.81	0.44
1:B:34:ILE:CD1	1:B:48:LEU:HD13	2.39	0.44
1:B:182:ARG:HG2	1:B:183:ILE:N	2.30	0.44
1:B:233:LEU:O	1:B:234:SER:C	2.55	0.44
1:B:134:ARG:HE	1:B:140:ARG:HH12	1.65	0.43
1:A:228:SER:C	1:A:230:GLU:N	2.69	0.43
1:A:166:LYS:O	1:A:166:LYS:HG3	2.19	0.43
1:A:133:LYS:C	1:A:136:LEU:H	2.22	0.43
1:B:159:PRO:O	1:B:162:TYR:CD1	2.72	0.43
1:B:66:LYS:HZ1	1:B:70:ASN:HD21	1.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:HD2	1:B:181:SER:H	1.83	0.43
1:A:102:ILE:HD13	1:A:110:ILE:HD12	2.01	0.43
1:B:10:GLN:O	1:B:11:ASN:O	2.35	0.43
1:A:68:THR:O	1:A:69:GLU:C	2.57	0.43
1:B:150:VAL:HG23	1:B:152:ILE:HD11	2.00	0.43
1:A:175:ARG:CG	1:A:175:ARG:HH11	2.31	0.43
1:B:104:TYR:O	1:B:105:ASN:HB3	2.13	0.43
1:A:236:PHE:O	1:A:239:TYR:HB3	2.19	0.43
1:B:185:HIS:O	1:B:186:LYS:C	2.56	0.43
1:B:200:ASN:HB3	1:B:202:GLU:HG3	2.00	0.43
1:B:183:ILE:HB	1:B:188:LYS:CD	2.48	0.43
1:B:78:PHE:HB2	1:B:79:GLN:H	1.64	0.43
1:A:200:ASN:HB3	1:A:202:GLU:HG3	2.01	0.43
1:B:161:GLU:C	1:B:163:PHE:H	2.18	0.43
1:A:233:LEU:O	1:A:234:SER:C	2.55	0.43
1:B:133:LYS:O	1:B:136:LEU:N	2.52	0.43
1:B:134:ARG:HH11	1:B:134:ARG:HG2	1.83	0.43
1:B:135:LEU:CD2	1:B:142:LEU:HD11	2.48	0.43
1:A:37:ILE:HD12	1:A:114:ILE:HD11	2.01	0.43
1:A:165:PRO:HG2	1:A:166:LYS:N	2.34	0.42
1:A:137:ASN:ND2	1:A:140:ARG:NH2	2.55	0.42
1:A:66:LYS:NZ	1:A:70:ASN:ND2	2.49	0.42
1:B:191:TYR:CE2	1:B:195:VAL:HG21	2.54	0.42
1:B:111:ILE:O	1:B:115:VAL:HG23	2.19	0.42
1:B:102:ILE:HG23	1:B:106:ILE:HB	2.01	0.42
1:B:165:PRO:HG2	1:B:166:LYS:H	1.83	0.42
1:A:206:ILE:HB	1:A:207:PHE:H	1.56	0.42
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.88	0.42
1:B:194:PHE:HZ	1:B:235:LEU:HB3	1.84	0.42
1:B:151:ASP:O	1:B:151:ASP:OD1	2.37	0.42
1:B:21:LYS:O	1:B:24:THR:HB	2.19	0.42
1:A:216:LEU:HD13	1:A:224:LEU:HD13	2.01	0.42
1:A:158:VAL:N	1:A:159:PRO:HD3	2.34	0.42
1:A:135:LEU:CD2	1:A:142:LEU:HD11	2.50	0.42
1:B:198:TRP:CZ2	1:B:227:ILE:HG13	2.55	0.42
1:B:54:PHE:CE1	1:B:77:ASN:HA	2.54	0.42
1:A:179:LYS:O	1:A:180:LYS:C	2.57	0.42
1:B:131:PHE:O	1:B:134:ARG:HB3	2.20	0.42
1:B:157:MET:C	1:B:159:PRO:HD3	2.40	0.42
1:B:159:PRO:O	1:B:160:ARG:C	2.58	0.42
1:A:211:GLN:NE2	1:A:244:LYS:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HG23	1:A:86:LEU:HD23	2.02	0.42
1:B:13:ILE:HD12	1:B:163:PHE:CD1	2.55	0.42
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.85	0.42
1:A:214:ASN:O	1:A:218:HIS:N	2.51	0.42
1:A:13:ILE:O	1:A:13:ILE:HG23	2.20	0.42
1:A:19:ILE:HG22	1:A:47:GLU:CG	2.49	0.42
1:B:99:PHE:HA	1:B:124:TYR:O	2.20	0.42
1:B:222:ASP:C	1:B:224:LEU:N	2.71	0.42
1:A:180:LYS:C	1:A:180:LYS:HD2	2.39	0.42
1:A:212:PHE:CZ	1:A:216:LEU:HD11	2.55	0.42
1:B:180:LYS:O	1:B:181:SER:O	2.38	0.42
1:A:214:ASN:HA	1:A:217:LYS:HB3	2.01	0.42
1:B:37:ILE:HD11	1:B:114:ILE:HD11	2.00	0.41
1:B:165:PRO:O	1:B:167:PRO:HD2	2.20	0.41
1:A:64:LEU:O	1:A:67:THR:HB	2.20	0.41
1:A:194:PHE:HZ	1:A:235:LEU:HB3	1.85	0.41
1:B:103:PRO:O	1:B:104:TYR:CB	2.67	0.41
1:B:85:ILE:HG23	1:B:86:LEU:HD23	2.02	0.41
1:A:54:PHE:CD1	1:A:77:ASN:HA	2.55	0.41
1:A:33:ASN:O	1:A:96:TYR:HB2	2.19	0.41
1:A:164:HIS:CG	1:A:165:PRO:HD3	2.55	0.41
1:A:21:LYS:O	1:A:24:THR:HB	2.20	0.41
1:B:103:PRO:O	1:B:104:TYR:HB2	2.19	0.41
1:B:106:ILE:O	1:B:106:ILE:HG23	2.19	0.41
1:B:211:GLN:CD	1:B:244:LYS:O	2.58	0.41
1:B:153:SER:OG	1:B:175:ARG:NH1	2.52	0.41
1:B:37:ILE:HD11	1:B:114:ILE:CD1	2.50	0.41
1:B:28:LEU:HD22	1:B:34:ILE:HG21	2.02	0.41
1:B:210:ASN:ND2	1:B:210:ASN:N	2.68	0.41
1:B:214:ASN:HA	1:B:217:LYS:HB3	2.02	0.41
1:A:82:ASN:CG	1:A:82:ASN:O	2.59	0.41
1:A:40:GLY:HA3	1:A:43:HIS:CE1	2.53	0.41
1:B:88:PHE:O	1:B:113:LYS:CE	2.69	0.41
1:A:57:ALA:C	1:A:58:ILE:HG13	2.40	0.41
1:B:211:GLN:C	1:B:213:ASN:N	2.73	0.41
1:A:182:ARG:CG	1:A:182:ARG:HH11	2.33	0.41
1:A:102:ILE:O	1:A:103:PRO:C	2.56	0.41
1:B:133:LYS:C	1:B:136:LEU:H	2.24	0.41
1:B:23:MET:HE1	1:B:48:LEU:CD2	2.49	0.41
1:B:82:ASN:CG	1:B:82:ASN:O	2.59	0.41
1:A:152:ILE:H	1:A:152:ILE:CD1	2.26	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD22	1:B:224:LEU:HD13	2.02	0.41
1:B:164:HIS:CB	1:B:165:PRO:CD	2.99	0.41
1:B:193:TYR:O	1:B:196:MET:N	2.53	0.41
1:B:211:GLN:NE2	1:B:244:LYS:O	2.53	0.41
1:A:66:LYS:O	1:A:67:THR:C	2.59	0.41
1:A:83:LYS:HG2	1:A:84:ASP:H	1.86	0.41
1:A:122:GLU:OE1	1:A:124:TYR:CE1	2.74	0.41
1:A:137:ASN:O	1:A:140:ARG:HB3	2.21	0.41
1:B:26:ILE:HG23	1:B:124:TYR:CD2	2.56	0.41
1:A:88:PHE:O	1:A:113:LYS:CE	2.68	0.40
1:A:133:LYS:C	1:A:135:LEU:N	2.74	0.40
1:B:66:LYS:NZ	1:B:70:ASN:ND2	2.49	0.40
1:A:49:VAL:HG21	1:A:72:LEU:HD21	2.03	0.40
1:A:99:PHE:HA	1:A:124:TYR:O	2.21	0.40
1:A:180:LYS:CD	1:A:180:LYS:C	2.88	0.40
1:B:85:ILE:O	1:B:113:LYS:HE2	2.20	0.40
1:A:198:TRP:CZ2	1:A:227:ILE:HG13	2.56	0.40
1:B:216:LEU:HD23	1:B:235:LEU:HD21	2.03	0.40
1:A:127:VAL:O	1:A:128:GLU:C	2.59	0.40
1:A:151:ASP:O	1:A:151:ASP:OD1	2.39	0.40
1:A:10:GLN:C	1:A:12:PHE:N	2.74	0.40
1:A:111:ILE:HD11	1:A:125:LEU:HD11	2.04	0.40
1:A:88:PHE:O	1:A:113:LYS:NZ	2.54	0.40
1:B:23:MET:CB	1:B:51:ARG:CZ	2.99	0.40
1:A:183:ILE:HD12	1:A:191:TYR:CD1	2.57	0.40
1:A:125:LEU:HG	1:A:174:ILE:HD11	2.03	0.40
1:B:47:GLU:O	1:B:51:ARG:HB2	2.22	0.40
1:B:211:GLN:O	1:B:213:ASN:N	2.55	0.40
1:B:182:ARG:HD2	1:B:188:LYS:NZ	2.36	0.40
1:B:54:PHE:CZ	1:B:79:GLN:HG2	2.56	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	233/244 (96%)	159 (68%)	46 (20%)	28 (12%)	0	2
1	B	233/244 (96%)	161 (69%)	45 (19%)	27 (12%)	0	2
All	All	466/488 (96%)	320 (69%)	91 (20%)	55 (12%)	0	2

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	16	LYS
1	A	160	ARG
1	A	164	HIS
1	A	165	PRO
1	A	166	LYS
1	A	181	SER
1	A	182	ARG
1	A	206	ILE
1	A	224	LEU
1	B	11	ASN
1	B	15	SER
1	B	16	LYS
1	B	164	HIS
1	B	165	PRO
1	B	166	LYS
1	B	206	ILE
1	B	224	LEU
1	A	53	ASN
1	A	69	GLU
1	A	105	ASN
1	A	168	LYS
1	A	223	ASP
1	B	53	ASN
1	B	69	GLU
1	B	71	LYS
1	B	105	ASN
1	B	160	ARG
1	B	184	SER
1	B	223	ASP
1	A	19	ILE
1	A	71	LYS
1	A	140	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	PRO
1	A	162	TYR
1	B	78	PHE
1	B	229	PHE
1	A	63	LYS
1	A	78	PHE
1	A	201	LYS
1	A	229	PHE
1	B	63	LYS
1	B	81	LEU
1	B	140	ARG
1	B	159	PRO
1	B	185	HIS
1	A	186	LYS
1	B	19	ILE
1	B	104	TYR
1	B	169	VAL
1	A	104	TYR
1	B	13	ILE
1	A	102	ILE
1	A	13	ILE
1	B	102	ILE

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	223/232 (96%)	204 (92%)	19 (8%)	13	43
1	B	223/232 (96%)	204 (92%)	19 (8%)	13	43
All	All	446/464 (96%)	408 (92%)	38 (8%)	13	43

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	63	LYS
1	A	66	LYS
1	A	70	ASN
1	A	78	PHE
1	A	92	LYS
1	A	93	ASN
1	A	110	ILE
1	A	151	ASP
1	A	165	PRO
1	A	176	LEU
1	A	177	ASN
1	A	182	ARG
1	A	197	LYS
1	A	203	TYR
1	A	207	PHE
1	A	210	ASN
1	A	241	LEU
1	A	242	PHE
1	B	60	ILE
1	B	63	LYS
1	B	66	LYS
1	B	70	ASN
1	B	78	PHE
1	B	92	LYS
1	B	93	ASN
1	B	110	ILE
1	B	151	ASP
1	B	165	PRO
1	B	176	LEU
1	B	177	ASN
1	B	179	LYS
1	B	197	LYS
1	B	203	TYR
1	B	207	PHE
1	B	210	ASN
1	B	241	LEU
1	B	242	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	70	ASN
1	A	101	ASN
1	A	137	ASN
1	A	177	ASN
1	A	192	ASN
1	A	237	ASN
1	B	11	ASN
1	B	50	GLN
1	B	70	ASN
1	B	137	ASN
1	B	164	HIS
1	B	177	ASN
1	B	192	ASN
1	B	237	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.