



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 11:14 PM UTC

PDB ID : 1K3R / pdb_00001k3r
Title : Crystal Structure of the Methyltransferase with a Knot from Methanobacterium thermoautotrophicum
Authors : Zarembinski, T.I.; Kim, Y.; Peterson, K.; Christendat, D.; Dharamsi, A.; Arrowsmith, C.H.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2001-10-03
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

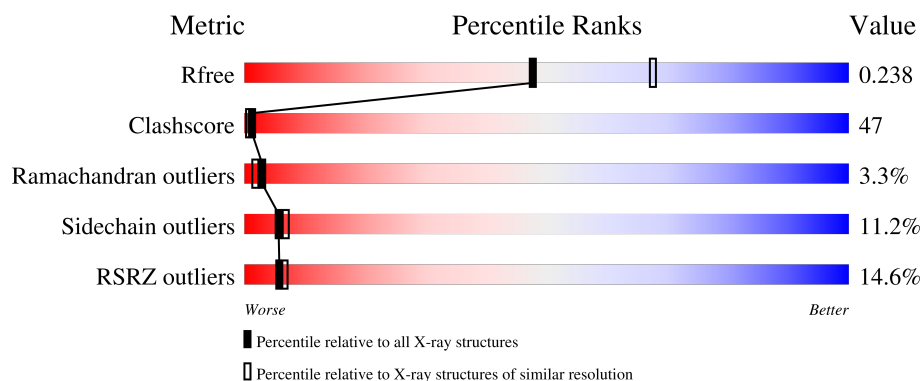
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	13% 41% 44% 12% ..
1	B	268	16% 41% 46% 11% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4278 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 conserved protein MT0001.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2071	1317	367	379	8			
1	B	264	Total	C	N	O	S	0	0	0
			2087	1327	369	383	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	LEU	ILE	conflict	UNP O26109
B	8	LEU	ILE	conflict	UNP O26109

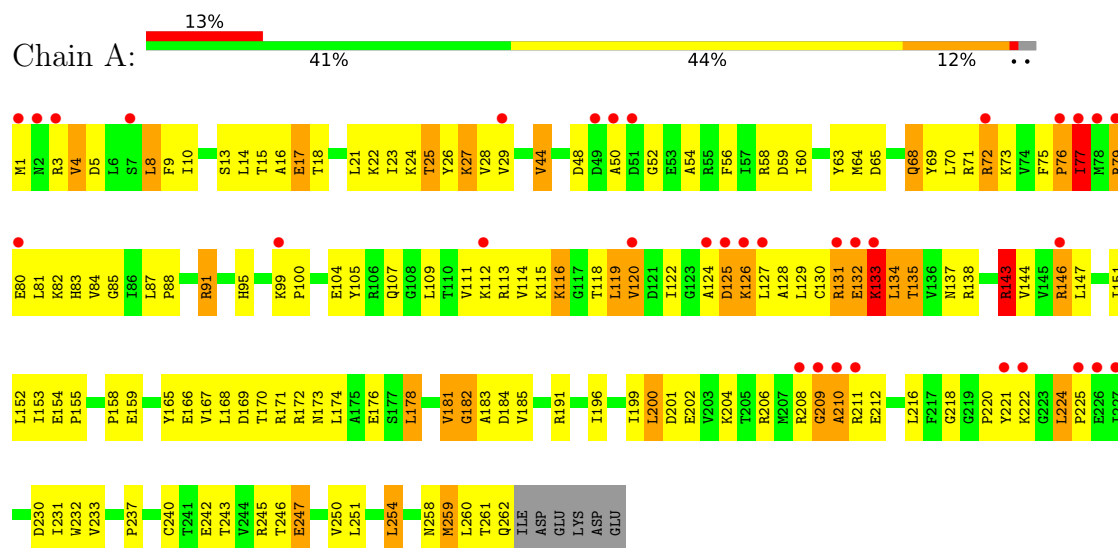
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		
2	B	49	Total	O	0	0
			49	49		

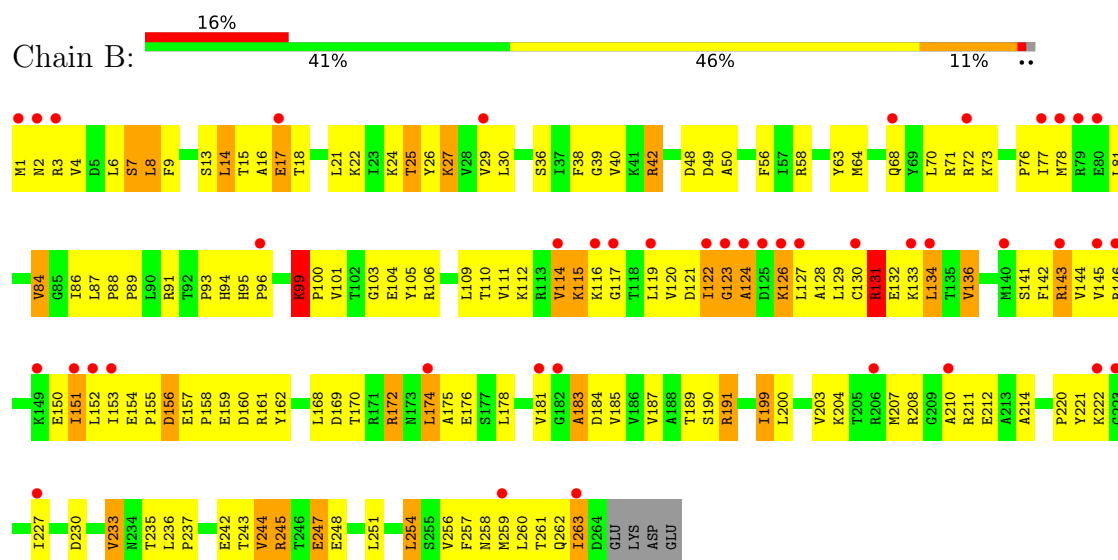
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: conserved protein MT0001



• Molecule 1: conserved protein MT0001



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.31Å 51.35Å 109.25Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	500.00 – 2.30 108.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.30) 95.4 (108.88-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.277 0.241 , 0.238	Depositor DCC
R_{free} test set	2488 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4278	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	0/2107	1.10	15/2855 (0.5%)
1	B	0.62	2/2123 (0.1%)	1.02	9/2877 (0.3%)
All	All	0.63	2/4230 (0.0%)	1.06	24/5732 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	SER	C-N	-5.83	1.25	1.33
1	B	6	LEU	C-N	-5.22	1.25	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLY	N-CA-C	-9.62	101.10	112.83
1	B	16	ALA	N-CA-C	7.58	119.55	111.28
1	A	210	ALA	N-CA-C	7.48	123.96	113.56
1	A	159	GLU	N-CA-C	-6.91	105.39	114.31
1	A	125	ASP	N-CA-C	-6.66	98.40	108.52
1	B	233	VAL	N-CA-C	6.45	116.79	107.88
1	A	133	LYS	N-CA-C	6.31	120.48	110.70
1	B	7	SER	CA-C-O	-6.30	113.89	120.70
1	B	111	VAL	N-CA-C	6.13	116.83	111.56
1	A	218	GLY	N-CA-C	-5.85	104.73	112.81
1	B	111	VAL	CB-CA-C	-5.78	105.95	111.44
1	A	52	GLY	N-CA-C	5.61	119.39	111.42
1	B	183	ALA	N-CA-C	-5.61	100.54	109.23
1	A	200	LEU	N-CA-C	5.58	117.83	111.02
1	A	107	GLN	N-CA-C	-5.45	100.83	109.76
1	B	14	LEU	N-CA-C	5.45	119.18	112.54
1	A	44	VAL	N-CA-C	5.42	115.39	107.37
1	B	244	VAL	N-CA-C	-5.42	99.71	107.78
1	A	143	ARG	N-CA-C	-5.26	100.33	108.90
1	B	42	ARG	N-CA-C	5.25	116.82	108.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ILE	CA-C-N	5.16	125.32	119.90
1	A	10	ILE	C-N-CA	5.16	125.32	119.90
1	A	16	ALA	N-CA-C	5.06	116.80	111.28
1	A	134	LEU	N-CA-C	-5.02	101.78	109.76

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	2071	0	2154	209	0
1	B	2087	0	2169	202	0
2	A	71	0	0	10	0
2	B	49	0	0	9	0
All	All	4278	0	4323	398	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 47.

All (398) 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:116:LYS:H	1:A:116:LYS:HE3	1.04	1.20
1:B:26:TYR:O	1:B:29:VAL:HG12	1.45	1.16
1:A:172:ARG:HG2	1:A:176:GLU:HB2	1.22	1.11
1:B:29:VAL:HG23	1:B:64:MET:SD	1.94	1.07
1:B:3:ARG:HH21	1:B:263:ILE:HD12	1.18	1.07
1:B:129:LEU:HD23	1:B:134:LEU:HD21	1.35	1.07
1:A:146:ARG:HA	1:A:146:ARG:HH11	1.18	1.07
1:A:29:VAL:HG11	1:A:87:LEU:HD22	1.07	1.04
1:B:29:VAL:HG21	1:B:88:PRO:HD2	1.38	1.02
1:B:120:VAL:HG21	1:B:153:ILE:HD11	1.38	1.01
1:A:127:LEU:HD22	1:A:153:ILE:HG12	1.40	1.00
1:A:29:VAL:CG1	1:A:87:LEU:HD22	1.91	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:HA	2:A:307:HOH:O	1.63	0.98
1:B:143:ARG:HB2	1:B:143:ARG:HH11	1.26	0.97
1:B:131:ARG:HB3	1:B:134:LEU:HD13	1.50	0.94
1:A:172:ARG:HB2	2:A:306:HOH:O	1.65	0.94
1:B:143:ARG:HB2	1:B:143:ARG:NH1	1.81	0.94
1:A:172:ARG:HG2	1:A:176:GLU:CB	1.98	0.93
1:B:99:LYS:HG3	1:B:100:PRO:HD2	1.51	0.91
1:A:144:VAL:HA	1:A:153:ILE:HG22	1.49	0.91
1:A:127:LEU:HD23	1:A:128:ALA:N	1.87	0.90
1:A:21:LEU:O	1:A:25:THR:HG23	1.72	0.90
1:B:76:PRO:HD2	1:B:78:MET:HE2	1.51	0.89
1:A:127:LEU:HG	1:A:151:ILE:HB	1.55	0.88
1:A:116:LYS:HE3	1:A:116:LYS:N	1.87	0.88
1:A:129:LEU:HD12	1:A:153:ILE:O	1.73	0.88
1:A:26:TYR:O	1:A:29:VAL:HG22	1.73	0.87
1:A:224:LEU:H	1:A:224:LEU:HD22	1.39	0.86
1:A:116:LYS:H	1:A:116:LYS:CE	1.88	0.84
1:A:127:LEU:HD11	1:A:153:ILE:HG23	1.60	0.84
1:A:3:ARG:HH12	1:A:210:ALA:HB1	1.41	0.84
1:B:78:MET:HE3	1:B:81:LEU:HD21	1.60	0.83
1:A:184:ASP:CG	1:A:211:ARG:HB2	2.04	0.83
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.44	0.82
1:B:127:LEU:HB3	1:B:151:ILE:HG23	1.62	0.81
1:B:8:LEU:HD21	1:B:40:VAL:HG21	1.62	0.81
1:A:72:ARG:H	1:A:72:ARG:HD3	1.46	0.81
1:B:106:ARG:HD3	1:B:122:ILE:HG13	1.63	0.81
1:B:3:ARG:HH21	1:B:263:ILE:CD1	1.94	0.80
1:B:120:VAL:CG2	1:B:153:ILE:HD11	2.10	0.80
1:A:72:ARG:HH12	1:A:73:LYS:HG3	1.47	0.79
1:B:122:ILE:HG23	1:B:123:GLY:N	1.95	0.79
1:A:221:TYR:HD1	1:A:222:LYS:H	1.31	0.78
1:A:79:ARG:HG3	1:A:82:LYS:HZ2	1.49	0.78
1:A:79:ARG:HG3	1:A:82:LYS:NZ	1.97	0.77
1:A:133:LYS:HG3	1:A:133:LYS:O	1.83	0.77
1:B:94:HIS:C	1:B:96:PRO:HD3	2.09	0.77
1:B:127:LEU:CB	1:B:151:ILE:HG23	2.15	0.77
1:A:122:ILE:CD1	1:A:127:LEU:HD12	2.15	0.77
1:A:68:GLN:H	1:A:68:GLN:CD	1.93	0.77
1:A:183:ALA:HB1	1:A:212:GLU:O	1.84	0.77
1:A:224:LEU:HD22	1:A:224:LEU:N	2.01	0.76
1:B:29:VAL:CG2	1:B:88:PRO:HD2	2.15	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HE2	1:B:124:ALA:HB2	1.66	0.76
1:A:245:ARG:HG2	1:A:245:ARG:HH11	1.51	0.76
1:B:58:ARG:HD3	1:B:169:ASP:HB2	1.67	0.76
1:A:127:LEU:HD22	1:A:153:ILE:CG1	2.15	0.75
1:B:247:GLU:OE1	2:B:309:HOH:O	2.03	0.75
1:A:127:LEU:HD23	1:A:128:ALA:H	1.50	0.74
1:A:224:LEU:H	1:A:224:LEU:CD2	2.00	0.74
1:B:145:VAL:HB	1:B:152:LEU:CD1	2.18	0.74
1:B:1:MET:HE3	1:B:258:ASN:OD1	1.88	0.74
1:B:129:LEU:HD23	1:B:134:LEU:CD2	2.17	0.73
1:B:25:THR:HG21	2:B:283:HOH:O	1.87	0.73
1:A:172:ARG:CG	1:A:176:GLU:HB2	2.12	0.73
1:B:29:VAL:HG21	1:B:88:PRO:CD	2.18	0.73
1:B:106:ARG:HB2	1:B:122:ILE:HD11	1.71	0.73
1:B:174:LEU:HD22	2:B:284:HOH:O	1.87	0.73
1:A:127:LEU:CD2	1:A:153:ILE:HG12	2.16	0.72
1:A:120:VAL:HG11	1:A:153:ILE:HD11	1.71	0.72
1:B:122:ILE:HB	1:B:127:LEU:HD21	1.71	0.72
1:B:13:SER:HB3	2:B:280:HOH:O	1.89	0.72
1:A:111:VAL:HG12	1:A:112:LYS:HG2	1.73	0.71
1:A:242:GLU:HG2	1:B:91:ARG:HB2	1.72	0.71
1:A:199:ILE:HG22	1:A:199:ILE:O	1.89	0.70
1:A:25:THR:O	1:A:29:VAL:HG13	1.90	0.70
1:A:127:LEU:CD1	1:A:153:ILE:HG23	2.21	0.70
1:B:199:ILE:O	1:B:203:VAL:HG23	1.91	0.70
1:A:174:LEU:HD23	1:A:225:PRO:HD2	1.73	0.70
1:A:129:LEU:HD11	1:A:154:GLU:HA	1.73	0.70
1:A:184:ASP:OD2	1:A:211:ARG:HB2	1.90	0.70
1:B:4:VAL:HG13	1:B:210:ALA:CB	2.21	0.70
1:A:99:LYS:NZ	1:A:124:ALA:HB1	2.07	0.69
1:B:144:VAL:HA	1:B:153:ILE:HG22	1.73	0.69
1:A:25:THR:HG21	2:A:271:HOH:O	1.93	0.69
1:B:1:MET:HB2	1:B:261:THR:OG1	1.93	0.69
1:B:21:LEU:O	1:B:25:THR:HG23	1.92	0.68
1:B:29:VAL:CG2	1:B:64:MET:SD	2.79	0.68
1:B:120:VAL:HG11	1:B:142:PHE:CZ	2.28	0.68
1:B:105:TYR:CD2	1:B:158:PRO:HD3	2.28	0.68
1:B:145:VAL:HB	1:B:152:LEU:HD12	1.76	0.68
1:B:42:ARG:HH21	1:B:181:VAL:HG22	1.59	0.68
1:A:220:PRO:HB3	1:A:243:THR:OG1	1.94	0.68
1:B:27:LYS:HB2	1:B:27:LYS:NZ	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HG2	1:A:245:ARG:NH1	2.09	0.68
1:B:27:LYS:HB2	1:B:27:LYS:HZ2	1.59	0.68
1:A:114:VAL:HB	1:A:116:LYS:NZ	2.09	0.67
1:B:172:ARG:HD2	1:B:172:ARG:N	2.09	0.67
1:A:129:LEU:CD1	1:A:154:GLU:HA	2.24	0.67
1:B:191:ARG:H	1:B:191:ARG:HD3	1.58	0.66
1:B:3:ARG:NH2	1:B:263:ILE:HD12	2.01	0.66
1:A:58:ARG:NH1	1:A:59:ASP:OD1	2.29	0.66
1:B:15:THR:HB	1:B:24:LYS:HG3	1.77	0.66
1:A:146:ARG:HA	1:A:146:ARG:NH1	2.03	0.65
1:B:29:VAL:HB	1:B:87:LEU:CD2	2.25	0.65
1:B:29:VAL:HB	1:B:87:LEU:HD22	1.78	0.65
1:B:110:THR:CG2	1:B:136:VAL:HA	2.26	0.65
1:B:17:GLU:OE1	1:B:18:THR:HG23	1.97	0.65
1:B:141:SER:OG	1:B:157:GLU:HB3	1.97	0.65
1:A:181:VAL:HA	2:A:309:HOH:O	1.96	0.64
1:A:29:VAL:HG11	1:A:87:LEU:CD2	2.04	0.64
1:B:174:LEU:HD13	2:B:284:HOH:O	1.95	0.64
1:A:72:ARG:NH1	1:A:72:ARG:HB2	2.11	0.64
1:A:146:ARG:NH1	1:A:147:LEU:H	1.96	0.64
1:B:29:VAL:HG11	1:B:88:PRO:HD2	1.79	0.64
1:A:114:VAL:HB	1:A:116:LYS:HZ2	1.62	0.64
1:B:130:CYS:SG	1:B:131:ARG:N	2.70	0.64
1:B:120:VAL:O	1:B:127:LEU:HD23	1.97	0.64
1:B:110:THR:HG22	1:B:136:VAL:HA	1.79	0.64
1:B:2:ASN:ND2	1:B:3:ARG:HD3	2.13	0.64
1:A:129:LEU:HD22	1:A:134:LEU:HD11	1.80	0.63
1:B:29:VAL:CG2	1:B:87:LEU:HD22	2.28	0.63
1:B:42:ARG:HH21	1:B:181:VAL:CG2	2.10	0.63
1:B:129:LEU:HD12	1:B:130:CYS:H	1.63	0.63
1:B:207:MET:HE2	1:B:257:PHE:HD2	1.63	0.63
1:B:143:ARG:HH11	1:B:143:ARG:CB	2.06	0.63
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.64	0.62
1:A:15:THR:HB	1:A:24:LYS:HG3	1.82	0.62
1:B:63:TYR:CZ	1:B:71:ARG:HD3	2.35	0.62
1:B:106:ARG:HD3	1:B:122:ILE:CG1	2.29	0.62
1:A:185:VAL:HA	1:A:230:ASP:OD2	1.99	0.62
1:A:120:VAL:CG1	1:A:153:ILE:HD11	2.29	0.62
1:A:17:GLU:CD	1:A:17:GLU:H	2.07	0.61
1:B:207:MET:HE2	1:B:257:PHE:CD2	2.36	0.61
1:B:129:LEU:CD2	1:B:155:PRO:HD3	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:HG2	1:B:58:ARG:HH11	1.64	0.61
1:B:127:LEU:HD23	1:B:127:LEU:H	1.64	0.61
1:A:3:ARG:HB2	1:A:3:ARG:CZ	2.30	0.61
1:A:122:ILE:HD11	1:A:127:LEU:HD12	1.83	0.61
1:A:122:ILE:HD13	1:A:127:LEU:HD12	1.83	0.60
1:A:200:LEU:HD11	1:A:260:LEU:HD21	1.84	0.60
1:A:127:LEU:HD13	1:A:153:ILE:HD13	1.84	0.60
1:A:72:ARG:H	1:A:72:ARG:HH11	1.50	0.60
1:B:127:LEU:HD12	1:B:151:ILE:HG12	1.84	0.60
1:A:72:ARG:HH11	1:A:72:ARG:N	2.00	0.60
1:B:184:ASP:OD1	1:B:211:ARG:HB3	2.02	0.59
1:A:3:ARG:HH22	1:A:210:ALA:HB2	1.67	0.59
1:A:143:ARG:HH11	1:A:143:ARG:CG	2.15	0.59
1:B:106:ARG:HE	1:B:123:GLY:CA	2.14	0.59
1:A:172:ARG:HG3	1:A:173:ASN:N	2.18	0.59
1:B:122:ILE:HG23	1:B:123:GLY:H	1.68	0.59
1:A:261:THR:O	1:A:261:THR:HG22	2.03	0.59
1:A:178:LEU:HD21	1:A:216:LEU:HD11	1.85	0.58
1:B:122:ILE:HG22	1:B:127:LEU:HD22	1.84	0.58
1:B:152:LEU:HD12	1:B:152:LEU:O	2.02	0.58
1:B:117:GLY:HA3	1:B:130:CYS:O	2.03	0.58
1:B:220:PRO:HB2	1:B:243:THR:HB	1.85	0.58
1:B:172:ARG:HB3	1:B:176:GLU:HB3	1.84	0.58
1:B:72:ARG:HH11	1:B:73:LYS:HG2	1.69	0.58
1:A:26:TYR:HB3	2:A:307:HOH:O	2.03	0.57
1:A:172:ARG:HG3	1:A:173:ASN:H	1.69	0.57
1:A:77:ILE:HG13	1:A:77:ILE:O	2.04	0.57
1:A:146:ARG:HH11	1:A:146:ARG:CA	2.07	0.57
1:A:242:GLU:HG2	1:B:91:ARG:CB	2.34	0.57
1:A:75:PHE:C	1:A:77:ILE:H	2.12	0.57
1:B:84:VAL:HG22	1:B:87:LEU:HD12	1.86	0.57
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.69	0.57
1:B:122:ILE:CG2	1:B:123:GLY:N	2.67	0.56
1:A:119:LEU:HG	1:A:126:LYS:HG2	1.87	0.56
1:B:4:VAL:HG13	1:B:210:ALA:HB3	1.87	0.56
1:A:204:LYS:O	1:A:208:ARG:HG2	2.05	0.56
1:A:68:GLN:H	1:A:68:GLN:NE2	2.03	0.56
1:A:69:TYR:CD1	1:A:70:LEU:HG	2.41	0.56
1:A:58:ARG:HD3	1:A:169:ASP:HB2	1.86	0.56
1:A:125:ASP:OD1	1:A:126:LYS:N	2.38	0.56
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HD13	1:A:127:LEU:CD1	2.36	0.56
1:A:105:TYR:CD2	1:A:158:PRO:HG3	2.41	0.56
1:A:221:TYR:CD1	1:A:222:LYS:HG2	2.41	0.56
1:B:208:ARG:C	1:B:210:ALA:H	2.13	0.56
1:B:221:TYR:HB2	1:B:222:LYS:HD2	1.88	0.56
1:A:127:LEU:HG	1:A:151:ILE:CB	2.33	0.56
1:A:84:VAL:O	1:A:87:LEU:HG	2.05	0.55
1:A:99:LYS:HZ1	1:A:124:ALA:HB1	1.70	0.55
1:B:29:VAL:CB	1:B:87:LEU:HD22	2.36	0.55
1:B:49:ASP:HB2	2:B:280:HOH:O	2.06	0.55
1:A:127:LEU:CD1	1:A:153:ILE:CG2	2.84	0.55
1:B:27:LYS:HG3	1:B:247:GLU:OE2	2.07	0.55
1:B:204:LYS:HE2	1:B:260:LEU:HD22	1.88	0.55
1:B:48:ASP:CG	1:B:49:ASP:H	2.15	0.55
1:B:127:LEU:HD11	1:B:153:ILE:HD13	1.87	0.55
1:B:190:SER:HB2	2:B:314:HOH:O	2.07	0.55
1:A:3:ARG:HH22	1:A:210:ALA:CB	2.19	0.55
1:B:245:ARG:NH1	1:B:245:ARG:HG3	2.22	0.55
1:A:129:LEU:HD23	1:A:134:LEU:HG	1.90	0.54
1:A:199:ILE:HG22	1:A:202:GLU:HB3	1.89	0.54
1:A:184:ASP:OD1	1:A:211:ARG:HB2	2.07	0.54
1:A:259:MET:HE2	1:B:256:VAL:HG13	1.90	0.54
1:B:25:THR:HG22	1:B:56:PHE:HZ	1.73	0.54
1:B:112:LYS:HD2	1:B:119:LEU:HD12	1.89	0.54
1:A:127:LEU:CG	1:A:151:ILE:HB	2.33	0.54
1:A:137:ASN:C	1:A:138:ARG:HD2	2.33	0.54
1:B:48:ASP:CG	1:B:49:ASP:N	2.66	0.54
1:A:127:LEU:HD11	1:A:153:ILE:CG2	2.36	0.54
1:A:100:PRO:HA	1:A:104:GLU:OE1	2.07	0.54
1:B:29:VAL:HG11	1:B:88:PRO:CD	2.38	0.53
1:A:130:CYS:O	1:A:132:GLU:N	2.41	0.53
1:B:27:LYS:HD3	1:B:247:GLU:OE1	2.09	0.53
1:B:122:ILE:HG13	1:B:123:GLY:H	1.72	0.53
1:A:83:HIS:C	1:A:85:GLY:N	2.65	0.53
1:A:200:LEU:HD13	1:B:259:MET:HE2	1.90	0.53
1:A:245:ARG:NH2	1:B:89:PRO:HD2	2.23	0.53
1:B:170:THR:O	1:B:170:THR:OG1	2.25	0.53
1:B:95:HIS:N	1:B:96:PRO:HD3	2.23	0.53
1:B:132:GLU:CD	1:B:132:GLU:H	2.16	0.53
1:A:99:LYS:CE	1:A:124:ALA:HB1	2.39	0.52
1:A:83:HIS:C	1:A:85:GLY:H	2.16	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HB2	1:B:151:ILE:HG23	1.89	0.52
1:B:129:LEU:HD13	1:B:153:ILE:O	2.09	0.52
1:A:3:ARG:HB2	1:A:3:ARG:NH1	2.25	0.52
1:B:129:LEU:HD13	1:B:154:GLU:HA	1.92	0.52
1:A:3:ARG:O	1:A:4:VAL:C	2.53	0.51
1:A:109:LEU:HA	1:A:138:ARG:O	2.10	0.51
1:B:144:VAL:HG22	1:B:151:ILE:HD11	1.92	0.51
1:A:131:ARG:C	2:A:301:HOH:O	2.53	0.51
1:B:129:LEU:CD1	1:B:155:PRO:HD3	2.41	0.51
1:A:258:ASN:ND2	1:B:237:PRO:HD2	2.25	0.51
1:B:2:ASN:ND2	1:B:3:ARG:CD	2.73	0.51
1:A:68:GLN:CD	1:A:68:GLN:N	2.66	0.51
1:A:196:ILE:HD12	1:A:233:VAL:HG11	1.91	0.51
1:A:230:ASP:C	1:A:231:ILE:HG13	2.36	0.51
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.21	0.51
1:B:86:ILE:C	1:B:86:ILE:HD12	2.36	0.51
1:A:129:LEU:CD2	1:A:134:LEU:HD11	2.40	0.50
1:B:222:LYS:HD2	1:B:222:LYS:N	2.26	0.50
1:B:189:THR:HA	1:B:233:VAL:O	2.12	0.50
1:A:127:LEU:HD21	1:A:152:LEU:C	2.37	0.50
1:A:221:TYR:CD1	1:A:222:LYS:N	2.72	0.50
1:B:26:TYR:CE2	1:B:30:LEU:HD21	2.47	0.50
1:A:54:ALA:HB3	1:A:171:ARG:NH1	2.27	0.50
1:B:76:PRO:CD	1:B:78:MET:HE2	2.35	0.50
1:B:181:VAL:O	1:B:181:VAL:HG13	2.12	0.50
1:A:3:ARG:NH1	1:A:210:ALA:HB1	2.19	0.50
1:A:200:LEU:HD11	1:A:260:LEU:CD2	2.40	0.50
1:A:25:THR:HG22	1:A:56:PHE:HZ	1.77	0.50
1:A:63:TYR:CZ	1:A:71:ARG:HD3	2.47	0.50
1:A:105:TYR:CG	1:A:158:PRO:HG3	2.47	0.49
1:A:99:LYS:HD2	1:A:100:PRO:HD2	1.95	0.49
1:A:129:LEU:HD11	1:A:155:PRO:CD	2.42	0.49
1:A:246:THR:O	1:A:250:VAL:HG23	2.11	0.49
1:A:72:ARG:HD3	1:A:72:ARG:N	2.21	0.49
1:A:25:THR:HG22	1:A:56:PHE:CZ	2.48	0.49
1:B:58:ARG:HG2	1:B:58:ARG:NH1	2.28	0.49
1:B:106:ARG:CB	1:B:122:ILE:HD11	2.39	0.49
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.78	0.49
1:B:122:ILE:HB	1:B:127:LEU:CD2	2.40	0.49
1:B:127:LEU:HB2	1:B:151:ILE:O	2.13	0.49
1:A:259:MET:CE	1:B:256:VAL:HG13	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:O	1:A:138:ARG:HD2	2.13	0.49
1:A:208:ARG:O	1:A:209:GLY:C	2.55	0.49
1:B:109:LEU:HD12	1:B:110:THR:N	2.28	0.49
1:B:129:LEU:HD21	1:B:155:PRO:HD3	1.95	0.49
1:A:129:LEU:CD2	1:A:155:PRO:HD3	2.43	0.48
1:B:207:MET:O	1:B:210:ALA:HB2	2.12	0.48
1:A:72:ARG:HB2	1:A:72:ARG:CZ	2.43	0.48
1:B:64:MET:O	1:B:95:HIS:HE1	1.96	0.48
1:A:131:ARG:HB2	2:A:279:HOH:O	2.13	0.48
1:A:143:ARG:CG	1:A:143:ARG:NH1	2.75	0.48
1:B:126:LYS:HD3	1:B:127:LEU:H	1.78	0.48
1:A:29:VAL:HB	1:A:64:MET:SD	2.54	0.48
1:B:29:VAL:CG1	1:B:88:PRO:HD2	2.43	0.48
1:A:129:LEU:HD21	1:A:155:PRO:HD3	1.96	0.48
1:B:235:THR:HG21	1:B:257:PHE:HE1	1.79	0.48
1:A:146:ARG:NH1	1:A:147:LEU:N	2.60	0.48
1:B:150:GLU:HG3	1:B:150:GLU:O	2.14	0.48
1:A:18:THR:HB	1:A:27:LYS:NZ	2.29	0.47
1:B:9:PHE:CE1	1:B:214:ALA:HB1	2.49	0.47
1:A:1:MET:H1	1:A:261:THR:HB	1.79	0.47
1:B:247:GLU:HG2	1:B:248:GLU:N	2.30	0.47
1:A:129:LEU:HD11	1:A:155:PRO:HD3	1.96	0.47
1:B:185:VAL:HA	1:B:230:ASP:OD1	2.14	0.47
1:A:24:LYS:HG2	1:A:56:PHE:CE2	2.48	0.47
1:A:65:ASP:O	1:A:95:HIS:HE1	1.97	0.47
1:B:127:LEU:HD23	1:B:127:LEU:N	2.27	0.47
1:A:115:LYS:N	1:A:116:LYS:HE3	2.30	0.47
1:A:118:THR:OG1	1:A:134:LEU:HB2	2.15	0.47
1:B:42:ARG:NH2	1:B:181:VAL:HG22	2.28	0.47
1:B:81:LEU:HD12	1:B:81:LEU:O	2.15	0.47
1:A:113:ARG:HH21	1:A:135:THR:HA	1.79	0.47
1:B:211:ARG:HG3	1:B:212:GLU:HG3	1.97	0.47
1:A:1:MET:N	1:A:261:THR:O	2.43	0.46
1:A:91:ARG:HH11	1:A:91:ARG:HG2	1.80	0.46
1:A:221:TYR:CE1	1:A:222:LYS:HG2	2.50	0.46
1:A:13:SER:HB3	2:A:318:HOH:O	2.14	0.46
1:A:208:ARG:C	1:A:210:ALA:N	2.69	0.46
1:B:27:LYS:NZ	1:B:27:LYS:CB	2.78	0.46
1:A:127:LEU:HD21	1:A:153:ILE:N	2.31	0.46
1:B:158:PRO:HB2	1:B:160:ASP:OD1	2.15	0.46
1:B:208:ARG:C	1:B:210:ALA:N	2.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:OE1	1:A:168:LEU:HD21	2.16	0.46
1:A:8:LEU:HD11	1:A:254:LEU:HD11	1.98	0.46
1:B:220:PRO:HB3	1:B:244:VAL:O	2.16	0.45
1:A:138:ARG:HG2	1:A:138:ARG:HH11	1.82	0.45
1:B:29:VAL:HG23	1:B:87:LEU:HD22	1.98	0.45
1:A:80:GLU:OE2	1:A:80:GLU:HA	2.16	0.45
1:A:127:LEU:HD22	1:A:153:ILE:CD1	2.45	0.45
1:A:65:ASP:HB2	1:A:165:TYR:CZ	2.52	0.45
1:A:237:PRO:HB2	1:B:262:GLN:NE2	2.32	0.45
1:A:251:LEU:HD23	1:B:251:LEU:HD23	1.99	0.45
1:B:18:THR:HG21	1:B:27:LYS:HZ1	1.82	0.45
1:A:22:LYS:HD2	1:B:22:LYS:HD2	1.98	0.45
1:B:103:GLY:HA2	1:B:143:ARG:HH22	1.81	0.45
1:B:114:VAL:HG13	1:B:116:LYS:H	1.81	0.45
1:B:183:ALA:HB1	1:B:212:GLU:O	2.17	0.45
1:A:240:CYS:HB2	1:B:36:SER:O	2.17	0.45
1:B:106:ARG:HE	1:B:123:GLY:N	2.15	0.45
1:B:106:ARG:HH21	1:B:123:GLY:CA	2.30	0.45
1:A:58:ARG:NH1	1:A:58:ARG:HG2	2.32	0.44
1:A:127:LEU:HG	1:A:151:ILE:C	2.42	0.44
1:B:106:ARG:NE	1:B:123:GLY:HA3	2.32	0.44
1:A:129:LEU:CD1	1:A:155:PRO:HD3	2.48	0.44
1:A:199:ILE:CG2	1:A:202:GLU:HB3	2.48	0.44
1:B:126:LYS:HD3	1:B:127:LEU:N	2.33	0.44
1:A:208:ARG:HH21	1:A:262:GLN:N	2.14	0.44
1:A:220:PRO:HD2	1:A:221:TYR:CE2	2.52	0.44
1:A:231:ILE:HG22	1:A:232:TRP:N	2.33	0.44
1:B:14:LEU:HD12	1:B:14:LEU:C	2.42	0.44
1:B:199:ILE:HG13	1:B:203:VAL:CG2	2.48	0.44
1:B:200:LEU:HD23	1:B:200:LEU:C	2.42	0.44
1:A:129:LEU:CD1	1:A:153:ILE:O	2.55	0.44
1:B:7:SER:HB3	1:B:42:ARG:NH1	2.32	0.44
1:B:106:ARG:NH2	1:B:123:GLY:HA3	2.33	0.44
1:A:243:THR:HG22	2:B:269:HOH:O	2.16	0.44
1:B:122:ILE:CG2	1:B:127:LEU:HD22	2.47	0.44
1:A:58:ARG:HD3	1:A:169:ASP:CB	2.48	0.43
1:A:181:VAL:O	1:A:182:GLY:C	2.61	0.43
1:B:115:LYS:H	1:B:115:LYS:HG2	1.54	0.43
1:B:4:VAL:HG13	1:B:210:ALA:HB1	2.00	0.43
1:B:39:GLY:HA2	1:B:162:TYR:CE1	2.54	0.43
1:B:245:ARG:HH11	1:B:245:ARG:CG	2.29	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HE2	1:B:124:ALA:CB	2.41	0.43
1:B:119:LEU:HD23	1:B:128:ALA:HB2	1.99	0.43
1:B:203:VAL:O	1:B:207:MET:HG2	2.17	0.43
1:A:184:ASP:OD2	1:A:184:ASP:N	2.48	0.43
1:A:199:ILE:O	1:A:199:ILE:CG2	2.61	0.43
1:B:141:SER:CB	1:B:157:GLU:HB3	2.47	0.43
1:A:9:PHE:CE2	1:A:44:VAL:HG11	2.54	0.43
1:A:170:THR:O	1:A:170:THR:OG1	2.36	0.43
1:B:121:ASP:OD1	1:B:121:ASP:C	2.61	0.43
1:A:113:ARG:NH1	1:A:113:ARG:CB	2.82	0.43
1:A:83:HIS:O	1:A:85:GLY:N	2.51	0.43
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.34	0.43
1:B:70:LEU:O	1:B:71:ARG:C	2.61	0.43
1:A:91:ARG:NH1	1:B:242:GLU:OE2	2.52	0.43
1:B:132:GLU:HG2	1:B:133:LYS:N	2.34	0.43
1:B:174:LEU:HD13	1:B:178:LEU:CD2	2.48	0.42
1:A:91:ARG:HB3	1:B:242:GLU:HB2	2.01	0.42
1:B:133:LYS:HB2	2:B:278:HOH:O	2.19	0.42
1:A:29:VAL:HG21	1:A:88:PRO:CD	2.50	0.42
1:A:58:ARG:CZ	1:A:59:ASP:OD1	2.67	0.42
1:A:69:TYR:CE1	1:A:70:LEU:HG	2.54	0.42
1:B:18:THR:HG21	1:B:27:LYS:HE2	2.01	0.42
1:B:9:PHE:HE1	1:B:214:ALA:HB1	1.83	0.42
1:B:38:PHE:HE1	1:B:251:LEU:CD1	2.32	0.42
1:B:114:VAL:HG12	1:B:117:GLY:H	1.85	0.42
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.80	0.42
1:B:143:ARG:HG2	1:B:156:ASP:HB3	2.02	0.42
1:A:76:PRO:O	1:A:77:ILE:C	2.63	0.41
1:A:127:LEU:HD13	1:A:153:ILE:CG2	2.50	0.41
1:B:58:ARG:HD3	1:B:169:ASP:CB	2.46	0.41
1:A:100:PRO:CD	1:A:124:ALA:HB2	2.50	0.41
1:B:89:PRO:HG2	1:B:91:ARG:NH1	2.35	0.41
1:B:145:VAL:HB	1:B:152:LEU:HD11	1.99	0.41
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.90	0.41
1:A:14:LEU:C	1:A:14:LEU:HD12	2.45	0.41
1:B:175:ALA:HB2	1:B:227:ILE:HD13	2.02	0.41
1:A:116:LYS:N	1:A:116:LYS:CE	2.65	0.41
1:A:127:LEU:HD21	1:A:152:LEU:CA	2.51	0.41
1:A:247:GLU:H	1:A:247:GLU:CD	2.26	0.41
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.87	0.41
1:A:5:ASP:O	1:A:212:GLU:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CE2	1:A:84:VAL:HG22	2.55	0.41
1:B:187:VAL:HG11	1:B:257:PHE:CZ	2.56	0.41
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.33	0.41
1:A:170:THR:C	1:A:172:ARG:H	2.29	0.41
1:A:48:ASP:HB3	2:A:318:HOH:O	2.21	0.40
1:A:173:ASN:HB2	2:A:319:HOH:O	2.21	0.40
1:B:93:PRO:HB3	1:B:161:ARG:HD3	2.03	0.40
1:A:28:VAL:HG11	1:A:60:ILE:HB	2.03	0.40
1:A:60:ILE:HD13	1:A:81:LEU:HD22	2.03	0.40
1:B:78:MET:HB2	1:B:81:LEU:HG	2.03	0.40
1:B:119:LEU:C	1:B:126:LYS:HE2	2.46	0.40
1:B:120:VAL:O	1:B:127:LEU:CD2	2.68	0.40
1:B:145:VAL:HG12	1:B:146:ARG:HG3	2.03	0.40
1:B:170:THR:C	1:B:172:ARG:H	2.29	0.40
1:A:127:LEU:HD13	1:A:153:ILE:HG21	2.04	0.40
1:B:68:GLN:C	1:B:70:LEU:H	2.30	0.40
1:A:127:LEU:CD2	1:A:151:ILE:O	2.69	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	260/268 (97%)	232 (89%)	20 (8%)	8 (3%)	3	2
1	B	262/268 (98%)	226 (86%)	27 (10%)	9 (3%)	3	2
All	All	522/536 (97%)	458 (88%)	47 (9%)	17 (3%)	3	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	ARG
1	A	132	GLU
1	A	131	ARG
1	A	182	GLY
1	B	50	ALA
1	B	123	GLY
1	A	50	ALA
1	B	124	ALA
1	B	134	LEU
1	B	122	ILE
1	B	131	ARG
1	B	156	ASP
1	A	76	PRO
1	A	77	ILE
1	B	99	LYS
1	B	199	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	227/233 (97%)	201 (88%)	26 (12%)	5	6
1	B	229/233 (98%)	204 (89%)	25 (11%)	6	7
All	All	456/466 (98%)	405 (89%)	51 (11%)	6	7

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	17	GLU
1	A	25	THR
1	A	27	LYS
1	A	68	GLN
1	A	72	ARG
1	A	77	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	91	ARG
1	A	116	LYS
1	A	119	LEU
1	A	120	VAL
1	A	126	LYS
1	A	133	LYS
1	A	135	THR
1	A	143	ARG
1	A	146	ARG
1	A	167	VAL
1	A	178	LEU
1	A	181	VAL
1	A	191	ARG
1	A	201	ASP
1	A	206	ARG
1	A	224	LEU
1	A	247	GLU
1	A	254	LEU
1	A	259	MET
1	B	8	LEU
1	B	17	GLU
1	B	25	THR
1	B	27	LYS
1	B	77	ILE
1	B	84	VAL
1	B	99	LYS
1	B	101	VAL
1	B	104	GLU
1	B	114	VAL
1	B	115	LYS
1	B	126	LYS
1	B	131	ARG
1	B	136	VAL
1	B	143	ARG
1	B	151	ILE
1	B	159	GLU
1	B	172	ARG
1	B	174	LEU
1	B	191	ARG
1	B	236	LEU
1	B	245	ARG
1	B	247	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	LEU
1	B	263	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	68	GLN
1	A	95	HIS
1	B	2	ASN
1	B	94	HIS
1	B	107	GLN

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 oligosaccharides 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	262/268 (97%)	0.65	34 (12%) 7 8	17, 43, 91, 119	0
1	B	264/268 (98%)	0.93	43 (16%) 4 5	21, 54, 100, 135	0
All	All	526/536 (98%)	0.79	77 (14%) 6 6	17, 47, 97, 135	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	VAL	5.5
1	A	132	GLU	5.1
1	B	1	MET	4.5
1	B	127	LEU	4.5
1	A	29	VAL	4.3
1	A	221	TYR	4.2
1	B	152	LEU	4.0
1	A	127	LEU	3.9
1	B	122	ILE	3.8
1	A	1	MET	3.8
1	A	209	GLY	3.6
1	B	125	ASP	3.5
1	A	78	MET	3.5
1	B	145	VAL	3.5
1	B	77	ILE	3.5
1	A	125	ASP	3.5
1	B	151	ILE	3.4
1	A	76	PRO	3.3
1	B	227	ILE	3.2
1	A	49	ASP	3.2
1	B	174	LEU	3.2
1	B	153	ILE	3.2
1	B	222	LYS	3.1
1	A	72	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	130	CYS	3.1
1	B	124	ALA	3.0
1	B	210	ALA	3.0
1	A	2	ASN	3.0
1	B	119	LEU	2.9
1	A	227	ILE	2.9
1	B	223	GLY	2.9
1	B	126	LYS	2.9
1	B	78	MET	2.9
1	B	80	GLU	2.8
1	A	77	ILE	2.8
1	A	210	ALA	2.7
1	A	80	GLU	2.7
1	A	222	LYS	2.7
1	B	133	LYS	2.7
1	B	17	GLU	2.7
1	B	116	LYS	2.7
1	B	146	ARG	2.7
1	A	131	ARG	2.6
1	B	96	PRO	2.6
1	B	263	ILE	2.6
1	A	208	ARG	2.6
1	B	181	VAL	2.6
1	A	226	GLU	2.6
1	B	206	ARG	2.6
1	A	50	ALA	2.6
1	A	112	LYS	2.6
1	A	133	LYS	2.5
1	B	117	GLY	2.5
1	A	99	LYS	2.5
1	B	149	LYS	2.5
1	A	3	ARG	2.5
1	B	259	MET	2.5
1	A	126	LYS	2.5
1	B	72	ARG	2.4
1	B	114	VAL	2.4
1	B	68	GLN	2.4
1	A	124	ALA	2.3
1	B	182	GLY	2.3
1	A	225	PRO	2.3
1	B	123	GLY	2.3
1	A	146	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	2.2
1	B	143	ARG	2.2
1	B	3	ARG	2.2
1	A	7	SER	2.1
1	A	120	VAL	2.1
1	B	2	ASN	2.1
1	A	211	ARG	2.1
1	A	79	ARG	2.1
1	B	79	ARG	2.1
1	B	140	MET	2.0
1	B	134	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 oligosaccharides 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.