Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:59 PM EDT

PDB ID	:	1GZ0
Title	:	23S RIBOSOMAL RNA G2251 2'O-METHYLTRANSFERASE RLMB
Authors	:	Michel, G.; Cygler, M.
Deposited on	:	2002-05-03
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

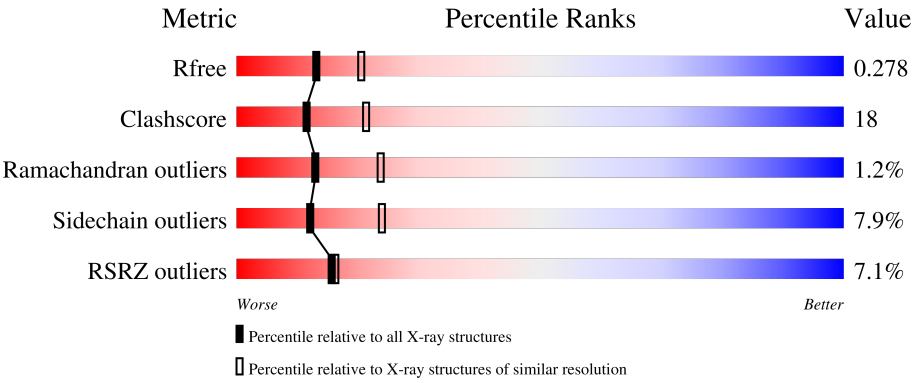
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	253	8% 62% 30%
1	B	253	7% 60% 31% 5%
1	C	253	5% 63% 28%
1	D	253	6% 62% 32%
1	E	253	% 45% 18% 34%

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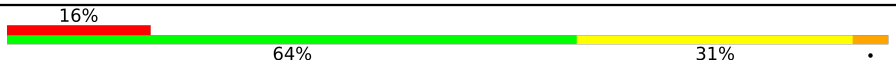
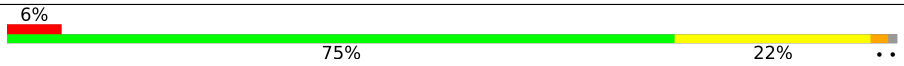
Mol	Chain	Length	Quality of chain
1	F	253	
1	G	253	
1	H	253	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13953 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 HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	Se	4	0	0
			1851	1153	339	348	4	7			
1	B	244	Total	C	N	O	S	Se	0	0	0
			1869	1164	343	350	4	8			
1	C	242	Total	C	N	O	S	Se	0	0	0
			1851	1153	339	348	4	7			
1	D	244	Total	C	N	O	S	Se	0	0	0
			1869	1164	343	350	4	8			
1	E	166	Total	C	N	O	S	Se	0	0	0
			1248	770	228	240	4	6			
1	F	253	Total	C	N	O	S	Se	0	0	0
			1928	1199	355	362	4	8			
1	G	166	Total	C	N	O	S	Se	0	0	0
			1248	770	228	240	4	6			
1	H	250	Total	C	N	O	S	Se	0	0	0
			1912	1191	352	357	4	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	19	Total	O	0	0
			19	19		
2	C	14	Total	O	0	0
			14	14		
2	D	24	Total	O	0	0
			24	24		
2	E	28	Total	O	0	0
			28	28		
2	F	38	Total	O	0	0
			38	38		

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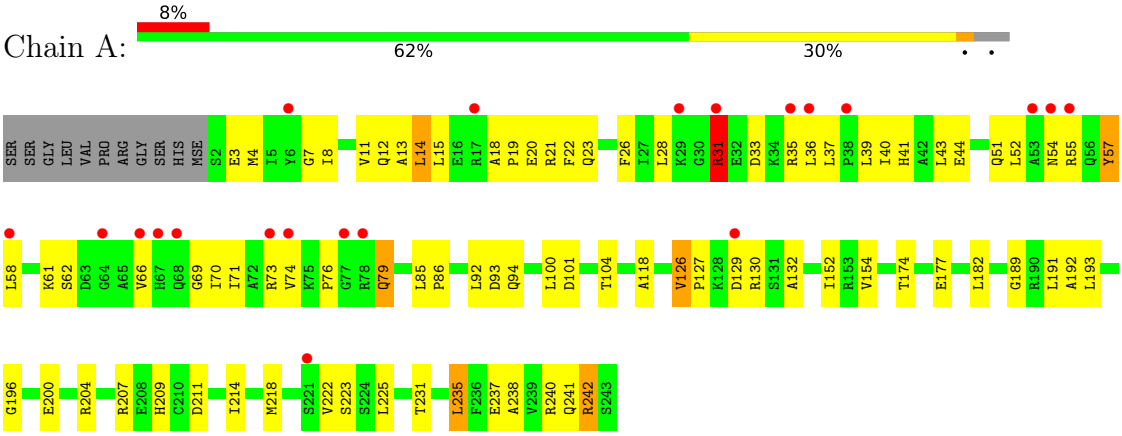
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	9	Total O 9 9	0	0
2	H	31	Total O 31 31	0	0

3 Residue-property plots (i)

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.

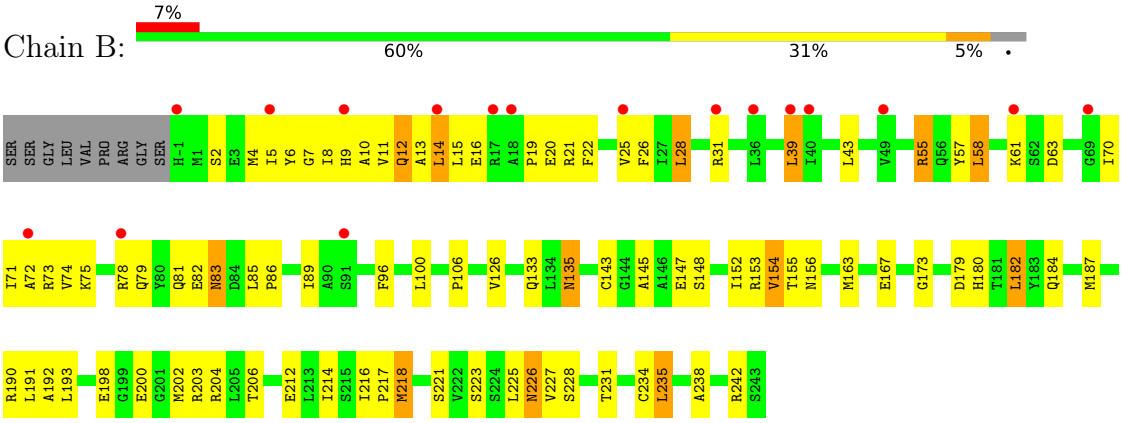
• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

Chain A:



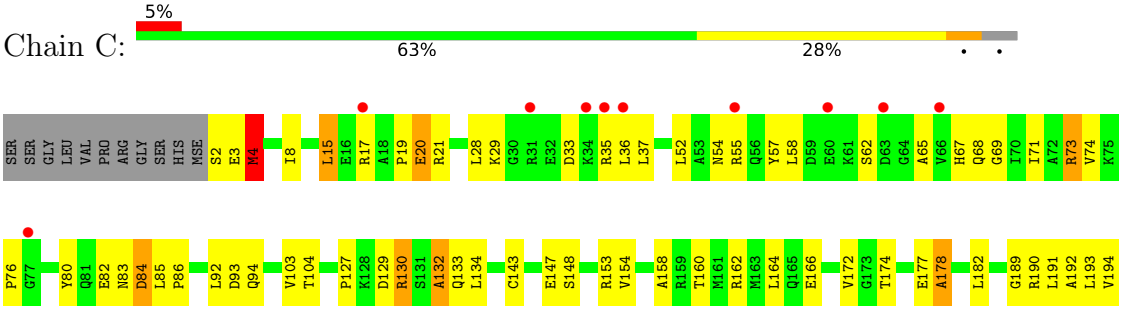
• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

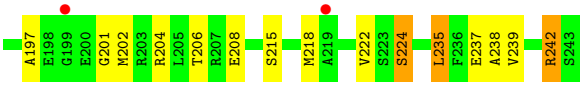
Chain B:



• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

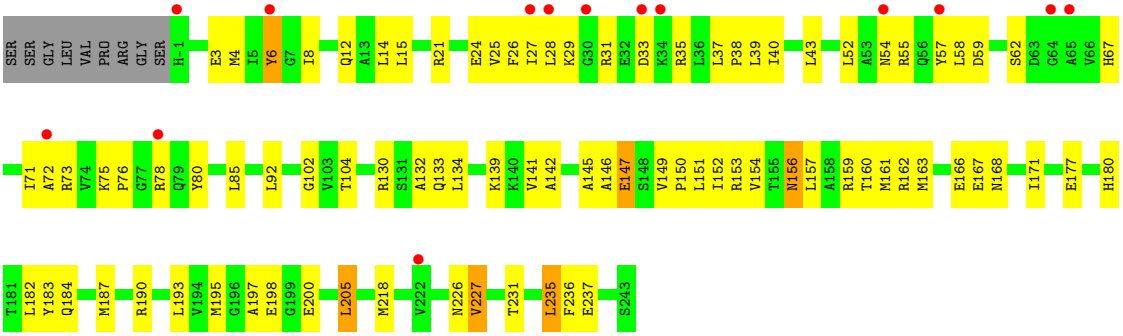
Chain C:





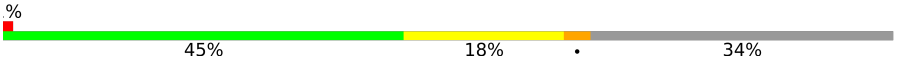
• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

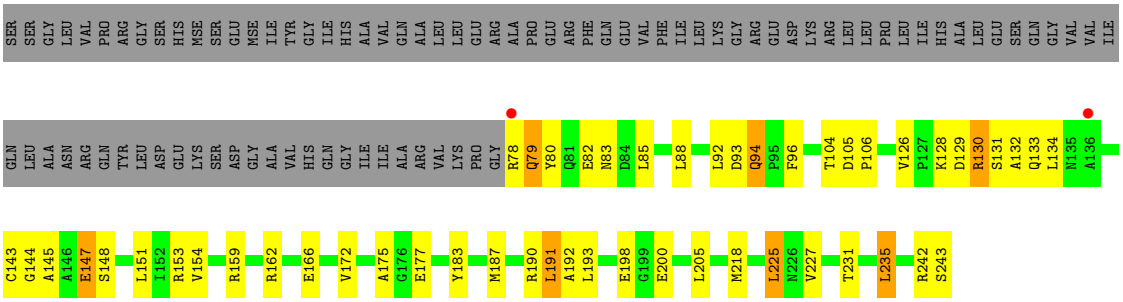
Chain D:



• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

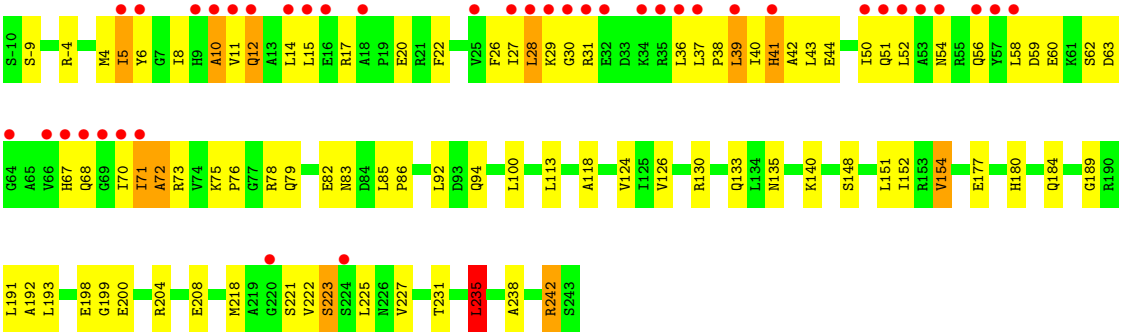
Chain E:





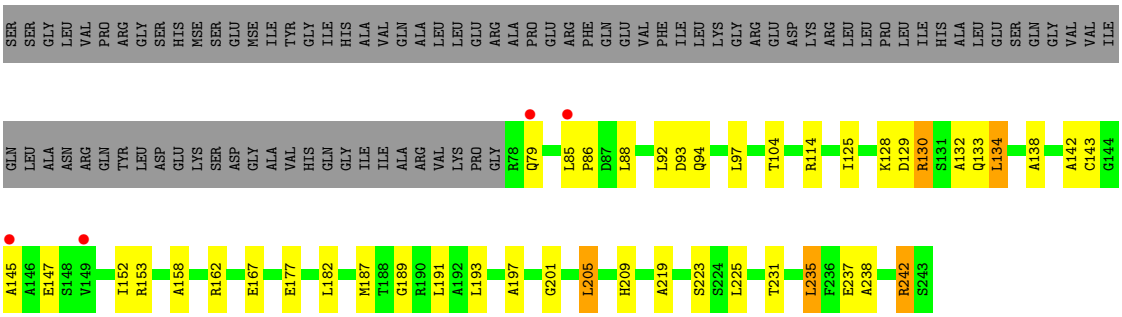
• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

Chain F:



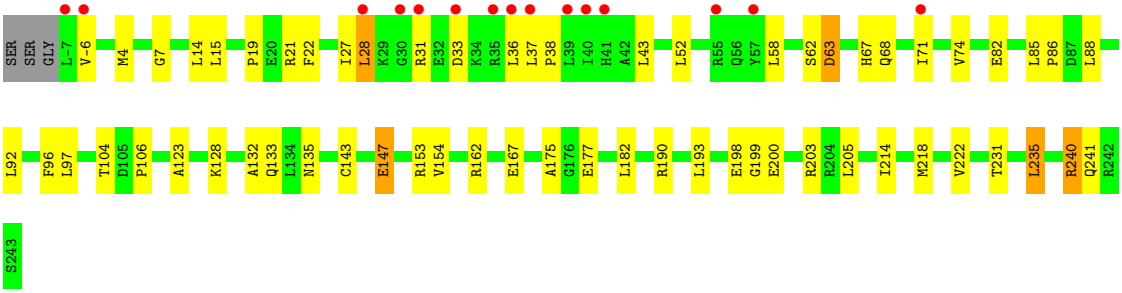
• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

Chain G:



• Molecule 1: HYPOTHETICAL TRNA/RRNA METHYLTRANSFERASE YJFH

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.48Å 132.29Å 90.71Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	46.86 – 2.50 46.85 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.86-2.50) 98.9 (46.85-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.231 , 0.279 0.230 , 0.278	Depositor DCC
R_{free} test set	3587 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13953	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	0/1869	0.66	0/2514
1	B	0.42	0/1887	0.67	0/2536
1	C	0.44	1/1869 (0.1%)	0.69	0/2514
1	D	0.43	0/1887	0.69	0/2536
1	E	0.47	0/1257	0.77	2/1691 (0.1%)
1	F	0.44	0/1947	0.72	1/2617 (0.0%)
1	G	0.46	0/1257	0.75	1/1691 (0.1%)
1	H	0.44	0/1931	0.69	0/2596
All	All	0.44	1/13904 (0.0%)	0.70	4/18695 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	MSE	CG-SE	-5.02	1.78	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	130	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	E	190	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	G	130	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	F	235	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	183	TYR	Sidechain

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	1851	0	1887	82	0
1	B	1869	0	1906	90	0
1	C	1851	0	1887	66	0
1	D	1869	0	1906	66	0
1	E	1248	0	1264	32	0
1	F	1928	0	1967	92	0
1	G	1248	0	1264	34	0
1	H	1912	0	1954	42	0
2	A	14	0	0	0	0
2	B	19	0	0	1	0
2	C	14	0	0	0	0
2	D	24	0	0	0	0
2	E	28	0	0	1	0
2	F	38	0	0	0	0
2	G	9	0	0	0	0
2	H	31	0	0	0	0
All	All	13953	0	14035	489	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 18.

All (489) 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:79:GLN:HE21	1:A:79:GLN:HA	1.24	1.00
1:D:85:LEU:HD11	1:D:152:ILE:HG21	1.47	0.97
1:F:26:PHE:HB2	1:F:71:ILE:HG13	1.49	0.94
1:C:8:ILE:HD11	1:C:36:LEU:HD23	1.50	0.93
1:F:12:GLN:HA	1:F:12:GLN:HE21	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG3	1:A:76:PRO:HG3	1.47	0.93
1:B:25:VAL:HG21	1:B:43:LEU:HD13	1.49	0.92
1:A:52:LEU:HD23	1:A:52:LEU:H	1.36	0.90
1:B:15:LEU:HD21	1:B:43:LEU:HD23	1.52	0.89
1:C:172:VAL:HG23	1:C:191:LEU:HD11	1.56	0.88
1:A:118:ALA:HA	1:F:223:SER:HB3	1.53	0.88
1:F:58:LEU:HD22	1:F:71:ILE:HD11	1.56	0.87
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.41	0.84
1:A:28:LEU:HD13	1:A:69:GLY:HA2	1.57	0.84
1:G:187:MSE:HE2	1:G:191:LEU:HD21	1.57	0.84
1:B:9:HIS:CE1	1:G:223:SER:HB3	2.12	0.84
1:C:4:MSE:HE3	1:C:73:ARG:HG3	1.60	0.83
1:B:20:GLU:CD	1:B:20:GLU:H	1.82	0.82
1:F:5:ILE:HG22	1:F:72:ALA:HB3	1.61	0.81
1:A:28:LEU:HD12	1:A:58:LEU:HD12	1.63	0.81
1:G:182:LEU:HG	1:G:237:GLU:HG2	1.63	0.81
1:B:28:LEU:HD22	1:B:31:ARG:HB2	1.64	0.79
1:A:79:GLN:HE21	1:A:79:GLN:CA	1.95	0.79
1:E:187:MSE:HE2	1:E:191:LEU:HD21	1.65	0.79
1:B:4:MSE:HG3	1:B:72:ALA:O	1.81	0.79
1:G:88:LEU:O	1:G:92:LEU:HD13	1.83	0.79
1:D:85:LEU:CD1	1:D:152:ILE:HG21	2.12	0.79
1:A:28:LEU:HB2	1:A:31:ARG:HD2	1.64	0.78
1:C:29:LYS:HB2	1:C:52:LEU:HB3	1.66	0.78
1:E:200:GLU:HG3	2:E:2016:HOH:O	1.82	0.77
1:F:29:LYS:O	1:F:31:ARG:HG3	1.84	0.76
1:B:85:LEU:HD11	1:B:152:ILE:HD13	1.67	0.76
1:A:129:ASP:OD1	1:D:168:ASN:HB3	1.86	0.75
1:F:82:GLU:HG3	1:F:154:VAL:HG22	1.68	0.75
1:B:58:LEU:HD22	1:B:71:ILE:CD1	2.16	0.75
1:B:85:LEU:HD13	1:B:152:ILE:HG21	1.70	0.74
1:H:21:ARG:HH12	1:H:147:GLU:HG3	1.50	0.74
1:A:3:GLU:OE1	1:A:76:PRO:HA	1.89	0.73
1:C:58:LEU:HD22	1:C:71:ILE:HG13	1.70	0.73
1:B:180:HIS:HB2	1:B:184:GLN:HB2	1.69	0.73
1:H:33:ASP:HB3	1:H:36:LEU:HB2	1.71	0.73
1:C:17:ARG:HG3	1:C:148:SER:CB	2.19	0.73
1:F:238:ALA:O	1:F:242:ARG:HG2	1.89	0.72
1:D:133:GLN:HA	1:D:153:ARG:NH2	2.04	0.72
1:A:23:GLN:HB3	1:A:73:ARG:HH21	1.55	0.72
1:C:218:MSE:CE	1:C:224:SER:HA	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:HD13	1:B:14:LEU:HD12	1.70	0.72
1:F:94:GLN:NE2	1:F:189:GLY:HA2	2.04	0.72
1:A:126:VAL:HG22	1:A:127:PRO:HD2	1.72	0.71
1:F:40:ILE:O	1:F:44:GLU:HG3	1.90	0.71
1:A:15:LEU:O	1:A:19:PRO:HG3	1.91	0.71
1:A:193:LEU:HD23	1:A:235:LEU:HD13	1.73	0.71
1:B:135:ASN:H	1:B:135:ASN:HD22	1.39	0.71
1:H:21:ARG:NH1	1:H:147:GLU:HG3	2.06	0.71
1:G:187:MSE:HE1	1:G:193:LEU:HD13	1.74	0.70
1:A:31:ARG:O	1:A:31:ARG:HD3	1.91	0.70
1:B:81:GLN:HE21	1:B:81:GLN:HA	1.56	0.70
1:B:238:ALA:O	1:B:242:ARG:HG3	1.92	0.69
1:F:27:ILE:HD13	1:F:40:ILE:HD13	1.75	0.69
1:C:218:MSE:HE3	1:C:224:SER:HA	1.74	0.69
1:H:85:LEU:HB3	1:H:86:PRO:HD3	1.73	0.69
1:F:222:VAL:HG23	1:F:223:SER:H	1.58	0.69
1:F:78:ARG:HG2	1:F:78:ARG:HH11	1.59	0.68
1:C:172:VAL:CG2	1:C:191:LEU:HD11	2.24	0.68
1:C:62:SER:HB3	1:C:71:ILE:HD13	1.75	0.68
1:A:118:ALA:HA	1:F:223:SER:CB	2.25	0.67
1:D:85:LEU:HD11	1:D:152:ILE:HD13	1.76	0.67
1:B:85:LEU:CD1	1:B:152:ILE:HD13	2.24	0.67
1:E:187:MSE:HE1	1:E:193:LEU:HD13	1.76	0.67
1:C:17:ARG:HG3	1:C:148:SER:HB3	1.76	0.67
1:H:182:LEU:HD23	1:H:182:LEU:H	1.60	0.67
1:F:85:LEU:HD13	1:F:152:ILE:HD13	1.75	0.66
1:B:135:ASN:HD22	1:B:135:ASN:N	1.91	0.66
1:E:198:GLU:HB2	1:E:227:VAL:HG23	1.77	0.66
1:A:40:ILE:O	1:A:44:GLU:HG3	1.95	0.65
1:B:182:LEU:HB2	1:B:214:ILE:HD12	1.77	0.65
1:F:12:GLN:HA	1:F:12:GLN:NE2	2.09	0.65
1:C:197:ALA:O	1:C:201:GLY:HA2	1.96	0.65
1:F:29:LYS:HA	1:F:52:LEU:HB3	1.78	0.65
1:B:9:HIS:NE2	1:G:223:SER:HB3	2.11	0.65
1:A:238:ALA:O	1:A:242:ARG:HG3	1.97	0.65
1:C:204:ARG:O	1:C:208:GLU:HG3	1.97	0.65
1:F:40:ILE:HG23	1:F:50:ILE:HD13	1.79	0.65
1:A:28:LEU:HD13	1:A:69:GLY:CA	2.28	0.64
1:B:14:LEU:CD1	1:B:74:VAL:HG21	2.27	0.64
1:D:28:LEU:HD23	1:D:58:LEU:HD12	1.79	0.64
1:E:159:ARG:HA	1:E:162:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:MSE:HE1	1:A:225:LEU:HD22	1.78	0.64
1:B:2:SER:HB3	1:B:73:ARG:HG2	1.80	0.64
1:D:133:GLN:HA	1:D:153:ARG:HH22	1.62	0.64
1:E:218:MSE:HE1	1:E:225:LEU:HD22	1.80	0.64
1:D:134:LEU:HB3	1:D:139:LYS:NZ	2.14	0.63
1:F:56:GLN:O	1:F:60:GLU:HG3	1.99	0.63
1:A:14:LEU:HB3	1:A:22:PHE:HE1	1.64	0.63
1:C:85:LEU:HB3	1:C:86:PRO:HD3	1.80	0.63
1:F:27:ILE:HG13	1:F:52:LEU:HD23	1.81	0.63
1:D:4:MSE:HE2	1:D:71:ILE:HG22	1.81	0.63
1:D:21:ARG:HD2	1:D:75:LYS:O	1.99	0.63
1:A:28:LEU:CB	1:A:31:ARG:HD2	2.28	0.62
1:H:88:LEU:O	1:H:92:LEU:HD22	1.99	0.62
1:D:8:ILE:HD13	1:D:35:ARG:HG2	1.81	0.62
1:H:240:ARG:HH11	1:H:240:ARG:HB3	1.64	0.62
1:C:28:LEU:HD12	1:C:28:LEU:O	1.99	0.62
1:F:82:GLU:HG3	1:F:154:VAL:CG2	2.29	0.62
1:F:58:LEU:HA	1:F:71:ILE:HD11	1.80	0.62
1:F:75:LYS:HB3	1:F:76:PRO:HD2	1.82	0.62
1:D:6:TYR:HD2	1:D:71:ILE:HG12	1.65	0.61
1:E:128:LYS:HG3	1:E:154:VAL:O	2.00	0.61
1:B:14:LEU:HD11	1:B:74:VAL:HG21	1.83	0.61
1:B:133:GLN:HA	1:B:153:ARG:NH2	2.16	0.61
1:C:193:LEU:HD23	1:C:235:LEU:HD13	1.83	0.61
1:D:85:LEU:CD1	1:D:152:ILE:HD13	2.31	0.61
1:H:88:LEU:HD21	1:H:123:ALA:HB2	1.83	0.60
1:A:14:LEU:HD21	1:A:74:VAL:HG11	1.82	0.60
1:C:2:SER:HA	1:C:76:PRO:HD3	1.82	0.60
1:B:218:MSE:HG2	1:B:223:SER:HB2	1.82	0.60
1:E:193:LEU:HD23	1:E:235:LEU:HD13	1.82	0.60
1:A:126:VAL:HG22	1:A:127:PRO:CD	2.31	0.60
1:H:27:ILE:HG13	1:H:52:LEU:HG	1.83	0.60
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.12	0.60
1:B:15:LEU:HD21	1:B:43:LEU:CD2	2.29	0.59
1:B:218:MSE:HG2	1:B:223:SER:CB	2.31	0.59
2:B:2004:HOH:O	1:G:219:ALA:HB2	2.01	0.59
1:A:28:LEU:CD1	1:A:69:GLY:HA2	2.30	0.59
1:F:59:ASP:HA	1:F:62:SER:OG	2.02	0.59
1:D:25:VAL:HG21	1:D:43:LEU:HD13	1.84	0.59
1:F:36:LEU:O	1:F:40:ILE:HG13	2.03	0.59
1:A:11:VAL:HG11	1:A:70:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ASP:O	1:C:37:LEU:HD13	2.03	0.59
1:F:29:LYS:HA	1:F:52:LEU:HD13	1.85	0.59
1:B:28:LEU:H	1:B:28:LEU:HD12	1.68	0.58
1:B:135:ASN:H	1:B:135:ASN:ND2	2.01	0.58
1:G:142:ALA:HB1	1:G:145:ALA:HB3	1.86	0.58
1:B:28:LEU:HD12	1:B:28:LEU:N	2.17	0.58
1:H:193:LEU:HD23	1:H:235:LEU:HD13	1.84	0.58
1:D:157:LEU:O	1:D:161:MSE:HG3	2.04	0.58
1:F:58:LEU:HD22	1:F:71:ILE:CD1	2.31	0.58
1:D:4:MSE:HE3	1:D:72:ALA:C	2.24	0.58
1:D:62:SER:HB2	1:D:71:ILE:HD11	1.85	0.58
1:F:26:PHE:HB2	1:F:71:ILE:CG1	2.29	0.57
1:F:130:ARG:NH2	1:F:200:GLU:HG3	2.19	0.57
1:A:85:LEU:N	1:A:86:PRO:HD2	2.19	0.57
1:A:4:MSE:CE	1:A:73:ARG:HG3	2.35	0.57
1:D:58:LEU:HD23	1:D:71:ILE:HD12	1.86	0.57
1:D:180:HIS:HB2	1:D:184:GLN:OE1	2.03	0.57
1:B:11:VAL:HG21	1:B:70:ILE:HD13	1.87	0.57
1:B:82:GLU:OE2	1:B:154:VAL:HG22	2.05	0.57
1:C:21:ARG:O	1:C:74:VAL:HG13	2.04	0.57
1:G:85:LEU:N	1:G:86:PRO:HD2	2.20	0.57
1:H:62:SER:O	1:H:63:ASP:HB3	2.05	0.57
1:H:203:ARG:HG2	1:H:203:ARG:HH11	1.69	0.57
1:G:129:ASP:O	1:G:130:ARG:HB2	2.05	0.56
1:G:205:LEU:HD23	1:G:209:HIS:CE1	2.40	0.56
1:H:28:LEU:HD22	1:H:31:ARG:HB2	1.86	0.56
1:A:37:LEU:HD12	1:A:40:ILE:HD12	1.88	0.56
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.70	0.56
1:C:15:LEU:O	1:C:19:PRO:HG3	2.06	0.56
1:F:12:GLN:HE21	1:F:12:GLN:CA	2.09	0.56
1:E:133:GLN:HA	1:E:153:ARG:NH2	2.19	0.56
1:D:130:ARG:HG3	1:D:130:ARG:HH11	1.71	0.56
1:E:80:TYR:CE2	1:E:88:LEU:HD13	2.41	0.56
1:B:231:THR:HG22	1:B:235:LEU:HD22	1.88	0.56
1:G:128:LYS:HG2	1:G:153:ARG:HB3	1.89	0.56
1:H:133:GLN:HA	1:H:153:ARG:NH2	2.19	0.56
1:B:231:THR:O	1:B:235:LEU:HB2	2.05	0.55
1:F:28:LEU:HD22	1:F:31:ARG:HB2	1.88	0.55
1:A:33:ASP:C	1:A:35:ARG:H	2.09	0.55
1:G:205:LEU:HD23	1:G:209:HIS:HE1	1.71	0.55
1:A:85:LEU:HD13	1:A:152:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:CD2	1:A:235:LEU:HD13	2.35	0.55
1:H:231:THR:HG22	1:H:235:LEU:HD22	1.87	0.55
1:A:52:LEU:H	1:A:52:LEU:CD2	2.15	0.55
1:F:-4:ARG:HH11	1:F:-4:ARG:HG2	1.72	0.55
1:A:4:MSE:HE1	1:A:73:ARG:HG3	1.88	0.55
1:A:100:LEU:O	1:A:127:PRO:HD3	2.06	0.55
1:H:15:LEU:HA	1:H:22:PHE:HE2	1.71	0.55
1:A:204:ARG:HA	1:A:207:ARG:NH1	2.21	0.55
1:B:81:GLN:HA	1:B:81:GLN:NE2	2.21	0.55
1:B:191:LEU:HD12	1:B:192:ALA:H	1.71	0.55
1:F:100:LEU:HB2	1:F:126:VAL:HG12	1.88	0.55
1:A:13:ALA:HA	1:F:222:VAL:CG1	2.37	0.55
1:A:85:LEU:HD13	1:A:152:ILE:CD1	2.37	0.55
1:H:37:LEU:HB2	1:H:38:PRO:HD3	1.89	0.55
1:D:78:ARG:HH11	1:D:78:ARG:HG2	1.72	0.55
1:D:236:PHE:HB3	1:E:183:TYR:OH	2.07	0.55
1:D:104:THR:O	1:D:132:ALA:HB2	2.08	0.54
1:A:7:GLY:O	1:A:11:VAL:HG23	2.07	0.54
1:B:12:GLN:C	1:B:14:LEU:H	2.11	0.54
1:C:3:GLU:OE2	1:C:76:PRO:HA	2.07	0.54
1:H:82:GLU:HG3	1:H:154:VAL:HG22	1.89	0.54
1:C:194:VAL:HG12	1:C:202:MSE:HE2	1.90	0.54
1:B:4:MSE:HE2	1:B:73:ARG:HG3	1.90	0.54
1:C:21:ARG:HB3	1:C:74:VAL:CG1	2.38	0.54
1:C:127:PRO:HG3	1:C:130:ARG:NH1	2.23	0.54
1:B:82:GLU:CD	1:B:154:VAL:HG22	2.28	0.53
1:C:147:GLU:HA	1:C:147:GLU:OE1	2.07	0.53
1:F:218:MSE:HB3	1:F:223:SER:HB2	1.90	0.53
1:B:180:HIS:HE2	1:B:212:GLU:HG3	1.74	0.53
1:C:133:GLN:HA	1:C:153:ARG:NH2	2.24	0.53
1:F:15:LEU:HD12	1:F:43:LEU:HG	1.90	0.53
1:H:128:LYS:HG2	1:H:153:ARG:HB3	1.89	0.53
1:A:21:ARG:HB3	1:A:74:VAL:CG1	2.38	0.53
1:A:79:GLN:CA	1:A:79:GLN:NE2	2.69	0.53
1:C:84:ASP:N	1:C:84:ASP:OD1	2.41	0.53
1:F:17:ARG:HG2	1:F:17:ARG:HH11	1.73	0.53
1:F:58:LEU:CD2	1:F:71:ILE:HD11	2.35	0.53
1:A:28:LEU:CD1	1:A:58:LEU:HD12	2.36	0.53
1:D:28:LEU:HD23	1:D:58:LEU:CD1	2.39	0.53
1:A:28:LEU:HD21	1:A:55:ARG:HH21	1.74	0.53
1:E:126:VAL:HG13	1:E:131:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:GLU:HG2	1:F:50:ILE:HD12	1.91	0.52
1:A:58:LEU:HD22	1:A:71:ILE:HD12	1.89	0.52
1:F:78:ARG:HG2	1:F:78:ARG:NH1	2.24	0.52
1:G:197:ALA:O	1:G:201:GLY:HA2	2.10	0.52
1:B:58:LEU:HD22	1:B:71:ILE:HD11	1.90	0.52
1:B:83:ASN:O	1:B:86:PRO:HD2	2.10	0.52
1:C:8:ILE:HD11	1:C:36:LEU:CD2	2.32	0.52
1:D:141:VAL:HG12	1:D:141:VAL:O	2.08	0.52
1:F:29:LYS:CA	1:F:52:LEU:HB3	2.39	0.52
1:G:187:MSE:O	1:G:242:ARG:HD2	2.09	0.52
1:A:240:ARG:NH1	1:A:241:GLN:HG3	2.24	0.52
1:C:54:ASN:HD21	1:C:57:TYR:HB2	1.74	0.52
1:F:113:LEU:HD23	1:F:124:VAL:HG21	1.91	0.52
1:G:242:ARG:HG2	1:G:242:ARG:NH1	2.24	0.52
1:H:240:ARG:HH12	1:H:241:GLN:HG3	1.74	0.52
1:G:177:GLU:CD	1:G:177:GLU:H	2.13	0.52
1:G:231:THR:HG22	1:G:235:LEU:HD22	1.92	0.52
1:C:3:GLU:HG3	1:C:76:PRO:HG3	1.92	0.52
1:E:94:GLN:HE21	1:E:94:GLN:CA	2.23	0.52
1:B:21:ARG:HA	1:B:75:LYS:HG2	1.92	0.51
1:G:231:THR:O	1:G:235:LEU:HB2	2.10	0.51
1:C:52:LEU:HD12	1:C:52:LEU:N	2.25	0.51
1:C:133:GLN:HA	1:C:153:ARG:HH22	1.75	0.51
1:F:6:TYR:HE2	1:F:62:SER:HA	1.75	0.51
1:F:58:LEU:HA	1:F:71:ILE:CD1	2.41	0.51
1:B:12:GLN:O	1:B:16:GLU:HG2	2.11	0.51
1:H:4:MSE:HE3	1:H:71:ILE:HG22	1.91	0.51
1:H:52:LEU:HD12	1:H:52:LEU:N	2.26	0.51
1:A:118:ALA:CA	1:F:223:SER:HB3	2.35	0.51
1:A:11:VAL:HG11	1:A:70:ILE:CD1	2.41	0.51
1:E:231:THR:HG22	1:E:235:LEU:HD22	1.93	0.51
1:C:17:ARG:HG3	1:C:148:SER:HB2	1.90	0.51
1:C:235:LEU:O	1:C:238:ALA:HB3	2.11	0.51
1:F:83:ASN:O	1:F:86:PRO:HD2	2.11	0.51
1:A:40:ILE:HA	1:A:43:LEU:HD12	1.93	0.51
1:A:174:THR:HA	1:A:214:ILE:O	2.11	0.51
1:F:37:LEU:N	1:F:38:PRO:HD2	2.26	0.50
1:D:27:ILE:HG21	1:D:40:ILE:HD11	1.94	0.50
1:B:21:ARG:HD2	1:B:75:LYS:HG3	1.93	0.50
1:B:106:PRO:HB3	1:B:135:ASN:HD21	1.76	0.50
1:D:182:LEU:HG	1:D:237:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:GLU:CG	1:F:154:VAL:HG22	2.40	0.50
1:A:3:GLU:CG	1:A:76:PRO:HG3	2.32	0.50
1:D:193:LEU:HD23	1:D:235:LEU:HD13	1.91	0.50
1:F:40:ILE:O	1:F:40:ILE:HG22	2.11	0.50
1:F:26:PHE:HD2	1:F:71:ILE:HB	1.77	0.50
1:F:28:LEU:HD13	1:F:31:ARG:HB2	1.93	0.50
1:A:21:ARG:O	1:A:74:VAL:HG13	2.12	0.50
1:F:12:GLN:HE22	1:F:15:LEU:HD13	1.76	0.50
1:B:216:ILE:HD11	1:B:234:CYS:SG	2.51	0.50
1:D:146:ALA:HB3	1:D:147:GLU:OE2	2.11	0.50
1:F:39:LEU:C	1:F:41:HIS:H	2.15	0.50
1:H:7:GLY:HA2	1:H:67:HIS:O	2.11	0.50
1:B:145:ALA:HA	1:B:148:SER:OG	2.12	0.49
1:B:21:ARG:HB3	1:B:74:VAL:HG12	1.93	0.49
1:E:94:GLN:HE21	1:E:94:GLN:HA	1.77	0.49
1:G:104:THR:O	1:G:132:ALA:HB2	2.13	0.49
1:C:178:ALA:HB3	1:C:215:SER:HB3	1.95	0.49
1:B:193:LEU:HD23	1:B:235:LEU:HD13	1.94	0.49
1:D:130:ARG:HH11	1:D:130:ARG:CG	2.25	0.49
1:A:37:LEU:C	1:A:39:LEU:H	2.16	0.49
1:D:102:GLY:O	1:D:197:ALA:HB2	2.13	0.49
1:E:191:LEU:HB3	1:E:242:ARG:NH2	2.28	0.49
1:C:160:THR:O	1:C:164:LEU:HG	2.12	0.49
1:C:218:MSE:HE1	1:C:224:SER:HA	1.93	0.49
1:F:67:HIS:O	1:F:68:GLN:HB2	2.11	0.49
1:H:218:MSE:HE2	1:H:218:MSE:HA	1.94	0.49
1:B:57:TYR:CZ	1:B:61:LYS:HD2	2.48	0.49
1:C:104:THR:O	1:C:132:ALA:HB2	2.13	0.49
1:F:8:ILE:O	1:F:12:GLN:HB3	2.13	0.49
1:F:30:GLY:H	1:F:52:LEU:HD13	1.77	0.49
1:A:21:ARG:HB3	1:A:74:VAL:HG13	1.94	0.48
1:A:79:GLN:HA	1:A:79:GLN:NE2	2.08	0.48
1:B:26:PHE:HB2	1:B:71:ILE:CG1	2.42	0.48
1:E:145:ALA:HA	1:E:148:SER:HB3	1.95	0.48
1:H:104:THR:C	1:H:132:ALA:HB2	2.33	0.48
1:A:211:ASP:OD1	1:B:203:ARG:HB2	2.14	0.48
1:E:78:ARG:HG2	1:E:79:GLN:N	2.29	0.48
1:G:238:ALA:O	1:G:242:ARG:HB2	2.13	0.48
1:B:6:TYR:O	1:B:10:ALA:HB3	2.14	0.48
1:B:21:ARG:HB3	1:B:74:VAL:CG1	2.43	0.48
1:F:70:ILE:HG13	1:F:70:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HG21	1:B:43:LEU:CD1	2.33	0.48
1:F:204:ARG:O	1:F:208:GLU:HG3	2.13	0.48
1:G:85:LEU:HD13	1:G:152:ILE:HD13	1.95	0.48
1:C:28:LEU:HD23	1:C:69:GLY:HA2	1.96	0.47
1:D:134:LEU:HB3	1:D:139:LYS:HZ2	1.78	0.47
1:H:67:HIS:O	1:H:68:GLN:HB2	2.14	0.47
1:A:18:ALA:HB3	1:A:21:ARG:HD3	1.95	0.47
1:H:15:LEU:HD13	1:H:43:LEU:HD23	1.95	0.47
1:G:242:ARG:HG2	1:G:242:ARG:HH11	1.80	0.47
1:A:8:ILE:O	1:A:12:GLN:HG3	2.15	0.47
1:C:20:GLU:H	1:C:20:GLU:HG3	1.33	0.47
1:D:37:LEU:N	1:D:38:PRO:HD2	2.29	0.47
1:D:134:LEU:HG	1:D:151:LEU:CD2	2.44	0.47
1:F:27:ILE:CD1	1:F:40:ILE:HD13	2.43	0.47
1:G:193:LEU:HD23	1:G:235:LEU:HD13	1.95	0.47
1:C:62:SER:HB2	1:C:65:ALA:HB3	1.96	0.47
1:A:31:ARG:NH1	1:A:36:LEU:HD11	2.29	0.47
1:B:198:GLU:HB2	1:B:227:VAL:HG23	1.97	0.47
1:C:182:LEU:HG	1:C:237:GLU:HG2	1.97	0.47
1:D:12:GLN:HB2	1:D:39:LEU:HD21	1.95	0.47
1:F:15:LEU:HD21	1:F:42:ALA:HB1	1.96	0.47
1:F:231:THR:O	1:F:235:LEU:HB2	2.14	0.47
1:A:13:ALA:HA	1:F:222:VAL:HG11	1.96	0.47
1:B:4:MSE:HE2	1:B:73:ARG:CG	2.45	0.47
1:B:78:ARG:HG2	1:B:78:ARG:NH1	2.30	0.47
1:C:202:MSE:HG2	1:C:206:THR:HB	1.97	0.47
1:C:158:ALA:O	1:C:162:ARG:HG3	2.16	0.46
1:G:158:ALA:HB1	1:G:162:ARG:HH21	1.80	0.46
1:B:19:PRO:HA	1:B:22:PHE:CD1	2.50	0.46
1:B:100:LEU:HB2	1:B:126:VAL:HG12	1.97	0.46
1:D:14:LEU:HD21	1:D:21:ARG:HB2	1.97	0.46
1:A:101:ASP:O	1:A:196:GLY:HA2	2.16	0.46
1:F:26:PHE:HA	1:F:51:GLN:O	2.16	0.46
1:A:191:LEU:HG	1:A:192:ALA:N	2.29	0.46
1:B:198:GLU:HB2	1:B:227:VAL:CG2	2.44	0.46
1:B:11:VAL:HG12	1:B:39:LEU:HD11	1.98	0.46
1:B:173:GLY:HA3	1:B:202:MSE:HE1	1.98	0.46
1:C:8:ILE:CD1	1:C:36:LEU:HD23	2.33	0.46
1:F:28:LEU:HB2	1:F:31:ARG:HD2	1.97	0.46
1:F:71:ILE:HG22	1:F:72:ALA:H	1.81	0.46
1:H:22:PHE:HA	1:H:74:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:CD1	1:B:152:ILE:HG21	2.41	0.46
1:B:226:ASN:OD1	1:B:228:SER:HB2	2.16	0.46
1:D:78:ARG:HH11	1:D:78:ARG:CG	2.28	0.46
1:H:15:LEU:HD12	1:H:19:PRO:HB3	1.98	0.46
1:D:6:TYR:CD2	1:D:71:ILE:HG12	2.48	0.45
1:E:134:LEU:HD12	1:E:151:LEU:HD23	1.98	0.45
1:C:33:ASP:C	1:C:37:LEU:HD13	2.36	0.45
1:D:27:ILE:HG13	1:D:52:LEU:HD23	1.98	0.45
1:F:17:ARG:HG2	1:F:17:ARG:NH1	2.31	0.45
1:F:177:GLU:H	1:F:177:GLU:HG3	1.52	0.45
1:A:14:LEU:HB3	1:A:22:PHE:CE1	2.49	0.45
1:B:19:PRO:HA	1:B:22:PHE:HD1	1.81	0.45
1:C:193:LEU:CD2	1:C:235:LEU:HD13	2.46	0.45
1:A:13:ALA:HA	1:F:222:VAL:HG12	1.99	0.45
1:A:26:PHE:CD1	1:A:51:GLN:HB3	2.52	0.45
1:C:33:ASP:OD1	1:C:35:ARG:HB3	2.17	0.45
1:D:54:ASN:O	1:D:57:TYR:HB3	2.16	0.45
1:B:2:SER:CB	1:B:73:ARG:HG2	2.45	0.45
1:F:27:ILE:O	1:F:52:LEU:HA	2.17	0.45
1:F:28:LEU:HD22	1:F:31:ARG:CB	2.46	0.45
1:A:57:TYR:HD1	1:A:57:TYR:O	2.00	0.45
1:D:193:LEU:CD2	1:D:235:LEU:HD13	2.45	0.45
1:E:191:LEU:HG	1:E:192:ALA:N	2.32	0.45
1:F:15:LEU:HD23	1:F:15:LEU:C	2.37	0.45
1:H:96:PHE:C	1:H:97:LEU:HD23	2.37	0.45
1:H:14:LEU:CD2	1:H:74:VAL:HG11	2.47	0.45
1:H:28:LEU:N	1:H:28:LEU:HD12	2.32	0.45
1:C:104:THR:C	1:C:132:ALA:HB2	2.38	0.44
1:D:195:MSE:HE2	1:D:231:THR:HA	1.99	0.44
1:A:94:GLN:NE2	1:A:189:GLY:HA2	2.32	0.44
1:F:12:GLN:NE2	1:F:12:GLN:CA	2.76	0.44
1:B:5:ILE:CD1	1:B:14:LEU:HD12	2.44	0.44
1:F:14:LEU:HA	1:F:17:ARG:HB2	1.98	0.44
1:B:191:LEU:HD12	1:B:192:ALA:N	2.32	0.44
1:F:28:LEU:HD13	1:F:31:ARG:O	2.16	0.44
1:H:82:GLU:HG3	1:H:154:VAL:CG2	2.46	0.44
1:G:104:THR:C	1:G:132:ALA:HB2	2.38	0.44
1:A:223:SER:HB3	1:F:118:ALA:HA	2.00	0.44
1:B:218:MSE:HG2	1:B:223:SER:HB3	1.98	0.44
1:D:161:MSE:CE	1:D:171:ILE:HG21	2.48	0.44
1:D:168:ASN:O	1:D:190:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:VAL:HG22	1:C:222:VAL:O	2.18	0.43
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.79	0.43
1:F:191:LEU:HG	1:F:192:ALA:N	2.33	0.43
1:F:200:GLU:H	1:F:200:GLU:HG2	1.58	0.43
1:D:218:MSE:HA	1:D:218:MSE:HE2	2.01	0.43
1:F:-4:ARG:HG2	1:F:-4:ARG:NH1	2.33	0.43
1:F:8:ILE:HG12	1:F:70:ILE:HD13	1.99	0.43
1:A:39:LEU:HD22	1:A:43:LEU:HD11	2.00	0.43
1:E:129:ASP:C	1:E:131:SER:H	2.21	0.43
1:G:94:GLN:NE2	1:G:189:GLY:HA2	2.34	0.43
1:G:147:GLU:OE1	1:G:147:GLU:N	2.52	0.43
1:B:7:GLY:O	1:B:11:VAL:HG23	2.18	0.43
1:D:102:GLY:HA2	1:D:130:ARG:HG2	2.00	0.43
1:D:167:GLU:O	1:D:190:ARG:NH1	2.51	0.43
1:E:82:GLU:O	1:E:85:LEU:HB2	2.19	0.43
1:F:198:GLU:HG3	1:F:227:VAL:HG22	2.00	0.43
1:A:209:HIS:HA	1:B:204:ARG:HD2	2.01	0.43
1:E:104:THR:C	1:E:132:ALA:HB2	2.39	0.43
1:E:144:GLY:O	1:E:147:GLU:HG2	2.18	0.43
1:D:14:LEU:HD23	1:D:14:LEU:O	2.19	0.43
1:D:78:ARG:HD3	1:D:80:TYR:CZ	2.53	0.43
1:F:180:HIS:HB2	1:F:184:GLN:OE1	2.19	0.43
1:C:204:ARG:HD3	1:C:208:GLU:OE2	2.19	0.43
1:D:28:LEU:HD12	1:D:31:ARG:HD3	2.01	0.43
1:H:182:LEU:HD23	1:H:182:LEU:N	2.32	0.43
1:H:182:LEU:HB3	1:H:214:ILE:HD12	2.00	0.43
1:A:37:LEU:HA	1:A:40:ILE:HD12	2.00	0.43
1:C:83:ASN:O	1:C:86:PRO:HD2	2.19	0.43
1:G:235:LEU:HD12	1:G:235:LEU:HA	1.86	0.43
1:D:231:THR:HG22	1:D:235:LEU:HD22	2.01	0.43
1:F:6:TYR:CE2	1:F:62:SER:HA	2.54	0.43
1:F:140:LYS:HE3	1:F:140:LYS:HB2	1.85	0.43
1:H:58:LEU:HB3	1:H:67:HIS:NE2	2.34	0.43
1:H:193:LEU:CD2	1:H:235:LEU:HD13	2.47	0.43
1:C:174:THR:H	1:C:202:MSE:HE1	1.84	0.42
1:D:4:MSE:HE3	1:D:73:ARG:N	2.33	0.42
1:B:21:ARG:HD2	1:B:75:LYS:CG	2.48	0.42
1:B:26:PHE:CD1	1:B:26:PHE:N	2.86	0.42
1:D:149:VAL:HA	1:D:150:PRO:HD3	1.87	0.42
1:E:93:ASP:OD1	1:E:93:ASP:N	2.52	0.42
1:A:23:GLN:HB3	1:A:73:ARG:NH2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:O	1:B:89:ILE:HG13	2.18	0.42
1:B:133:GLN:HA	1:B:153:ARG:HH22	1.82	0.42
1:D:130:ARG:CG	1:D:130:ARG:NH1	2.81	0.42
1:E:231:THR:O	1:E:235:LEU:HB2	2.19	0.42
1:A:200:GLU:H	1:A:200:GLU:HG2	1.53	0.42
1:B:167:GLU:O	1:B:190:ARG:NH1	2.52	0.42
1:B:198:GLU:CD	1:G:114:ARG:HH22	2.21	0.42
1:C:80:TYR:HA	1:C:84:ASP:OD2	2.19	0.42
1:D:29:LYS:C	1:D:31:ARG:H	2.22	0.42
1:D:200:GLU:H	1:D:200:GLU:HG2	1.64	0.42
1:C:177:GLU:O	1:C:178:ALA:O	2.37	0.42
1:C:191:LEU:HG	1:C:192:ALA:N	2.34	0.42
1:D:198:GLU:HB2	1:D:227:VAL:HG22	2.02	0.42
1:F:8:ILE:C	1:F:10:ALA:H	2.22	0.42
1:G:134:LEU:HD23	1:G:138:ALA:HB3	2.02	0.42
1:A:182:LEU:HG	1:A:237:GLU:HG2	2.00	0.42
1:A:231:THR:HG22	1:A:235:LEU:HD22	2.01	0.42
1:B:85:LEU:HB3	1:B:163:MSE:CE	2.49	0.42
1:E:175:ALA:HB1	1:E:177:GLU:OE2	2.19	0.42
1:H:106:PRO:HG3	1:H:135:ASN:HD21	1.83	0.42
1:A:8:ILE:HD11	1:A:36:LEU:CD2	2.50	0.42
1:A:33:ASP:C	1:A:35:ARG:N	2.72	0.42
1:B:217:PRO:O	1:B:218:MSE:HE3	2.19	0.42
1:D:59:ASP:CG	1:D:67:HIS:HE2	2.23	0.42
1:E:104:THR:O	1:E:132:ALA:HB2	2.20	0.42
1:B:85:LEU:N	1:B:86:PRO:HD2	2.34	0.42
1:D:160:THR:O	1:D:163:MSE:HB3	2.20	0.42
1:F:71:ILE:O	1:F:72:ALA:HB2	2.20	0.42
1:B:31:ARG:NH1	1:B:55:ARG:HE	2.18	0.42
1:B:58:LEU:HD22	1:B:71:ILE:CG1	2.50	0.42
1:B:202:MSE:SE	1:B:206:THR:HG22	2.70	0.42
1:F:54:ASN:O	1:F:58:LEU:HG	2.19	0.42
1:C:67:HIS:O	1:C:68:GLN:HB2	2.20	0.42
1:E:172:VAL:CG2	1:E:191:LEU:HD11	2.50	0.41
1:F:133:GLN:O	1:F:135:ASN:N	2.49	0.41
1:B:58:LEU:HD22	1:B:71:ILE:HG12	2.02	0.41
1:F:39:LEU:C	1:F:41:HIS:N	2.73	0.41
1:C:238:ALA:O	1:C:242:ARG:HG3	2.20	0.41
1:A:4:MSE:HE2	1:A:73:ARG:HG3	2.03	0.41
1:H:15:LEU:CA	1:H:22:PHE:HE2	2.32	0.41
1:B:82:GLU:CG	1:B:154:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLU:HG2	1:D:26:PHE:CE1	2.56	0.41
1:E:105:ASP:HA	1:E:106:PRO:HD3	1.89	0.41
1:F:11:VAL:HB	1:F:70:ILE:HD12	2.03	0.41
1:F:14:LEU:HD23	1:F:22:PHE:CE2	2.56	0.41
1:A:41:HIS:HA	1:A:44:GLU:OE1	2.21	0.41
1:C:33:ASP:O	1:C:36:LEU:N	2.51	0.41
1:C:62:SER:HB3	1:C:71:ILE:CD1	2.48	0.41
1:D:6:TYR:HD2	1:D:71:ILE:CG1	2.32	0.41
1:E:172:VAL:HG23	1:E:191:LEU:CD1	2.50	0.41
1:G:85:LEU:HD21	1:G:125:ILE:CD1	2.50	0.41
1:G:94:GLN:HE21	1:G:189:GLY:HA2	1.85	0.41
1:C:189:GLY:O	1:C:242:ARG:NH2	2.54	0.41
1:H:205:LEU:HD23	1:H:205:LEU:HA	1.89	0.41
1:C:82:GLU:HG3	1:C:154:VAL:HG22	2.02	0.41
1:C:94:GLN:NE2	1:C:189:GLY:HA2	2.36	0.41
1:H:175:ALA:HB1	1:H:177:GLU:HG2	2.03	0.41
1:C:235:LEU:O	1:C:239:VAL:HG23	2.20	0.41
1:D:3:GLU:HG3	1:D:76:PRO:HB3	2.03	0.41
1:D:156:ASN:HB3	1:D:159:ARG:CB	2.51	0.41
1:D:142:ALA:HB1	1:D:145:ALA:HB3	2.03	0.40
1:H:167:GLU:O	1:H:190:ARG:NH1	2.54	0.40
1:C:54:ASN:ND2	1:C:57:TYR:HB2	2.35	0.40
1:D:141:VAL:O	1:D:141:VAL:CG1	2.69	0.40
1:E:96:PHE:HB2	1:E:242:ARG:NH1	2.36	0.40
1:A:104:THR:C	1:A:132:ALA:HB2	2.42	0.40
1:C:28:LEU:HD22	1:C:55:ARG:HH11	1.86	0.40
1:F:85:LEU:HB3	1:F:86:PRO:HD3	2.04	0.40
1:B:79:GLN:NE2	1:B:79:GLN:HA	2.36	0.40
1:B:85:LEU:HD23	1:B:163:MSE:CE	2.52	0.40
1:B:155:THR:HG22	1:B:156:ASN:N	2.37	0.40
1:F:27:ILE:HG13	1:F:52:LEU:CD2	2.51	0.40
1:A:209:HIS:HA	1:B:204:ARG:CD	2.51	0.40
1:G:85:LEU:CD1	1:G:152:ILE:HD13	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	240/253 (95%)	218 (91%)	17 (7%)	5 (2%)	7 11
1	B	242/253 (96%)	215 (89%)	24 (10%)	3 (1%)	13 24
1	C	240/253 (95%)	221 (92%)	15 (6%)	4 (2%)	9 16
1	D	242/253 (96%)	223 (92%)	18 (7%)	1 (0%)	34 54
1	E	164/253 (65%)	157 (96%)	6 (4%)	1 (1%)	25 43
1	F	251/253 (99%)	226 (90%)	19 (8%)	6 (2%)	6 9
1	G	164/253 (65%)	159 (97%)	5 (3%)	0	100 100
1	H	248/253 (98%)	233 (94%)	13 (5%)	2 (1%)	19 35
All	All	1791/2024 (88%)	1652 (92%)	117 (6%)	22 (1%)	13 24

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	C	129	ASP
1	C	178	ALA
1	A	62	SER
1	B	179	ASP
1	C	132	ALA
1	D	55	ARG
1	F	223	SER
1	H	199	GLY
1	A	61	LYS
1	B	39	LEU
1	F	199	GLY
1	B	13	ALA
1	E	130	ARG
1	F	-9	SER
1	F	72	ALA
1	A	54	ASN

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Mol	Chain	Res	Type
1	F	221	SER
1	F	10	ALA
1	H	222	VAL
1	A	66	VAL
1	C	103	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	197/198 (100%)	184 (93%)	13 (7%)	16 32
1	B	199/198 (100%)	178 (89%)	21 (11%)	6 13
1	C	197/198 (100%)	182 (92%)	15 (8%)	13 25
1	D	199/198 (100%)	184 (92%)	15 (8%)	13 26
1	E	134/198 (68%)	122 (91%)	12 (9%)	9 19
1	F	206/198 (104%)	187 (91%)	19 (9%)	9 18
1	G	134/198 (68%)	123 (92%)	11 (8%)	11 22
1	H	204/198 (103%)	194 (95%)	10 (5%)	25 47
All	All	1470/1584 (93%)	1354 (92%)	116 (8%)	12 24

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	20	GLU
1	A	31	ARG
1	A	57	TYR
1	A	79	GLN
1	A	92	LEU
1	A	93	ASP
1	A	126	VAL
1	A	154	VAL
1	A	177	GLU

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Mol	Chain	Res	Type
1	A	222	VAL
1	A	235	LEU
1	A	242	ARG
1	B	8	ILE
1	B	12	GLN
1	B	14	LEU
1	B	28	LEU
1	B	55	ARG
1	B	58	LEU
1	B	63	ASP
1	B	83	ASN
1	B	96	PHE
1	B	135	ASN
1	B	143	CYS
1	B	147	GLU
1	B	154	VAL
1	B	182	LEU
1	B	187	MSE
1	B	200	GLU
1	B	218	MSE
1	B	221	SER
1	B	225	LEU
1	B	226	ASN
1	B	235	LEU
1	C	4	MSE
1	C	15	LEU
1	C	20	GLU
1	C	73	ARG
1	C	84	ASP
1	C	92	LEU
1	C	93	ASP
1	C	130	ARG
1	C	134	LEU
1	C	143	CYS
1	C	166	GLU
1	C	190	ARG
1	C	224	SER
1	C	235	LEU
1	C	242	ARG
1	D	6	TYR
1	D	15	LEU
1	D	33	ASP

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Mol	Chain	Res	Type
1	D	92	LEU
1	D	147	GLU
1	D	154	VAL
1	D	156	ASN
1	D	162	ARG
1	D	166	GLU
1	D	177	GLU
1	D	187	MSE
1	D	205	LEU
1	D	226	ASN
1	D	227	VAL
1	D	235	LEU
1	E	79	GLN
1	E	83	ASN
1	E	92	LEU
1	E	94	GLN
1	E	143	CYS
1	E	147	GLU
1	E	166	GLU
1	E	191	LEU
1	E	205	LEU
1	E	225	LEU
1	E	235	LEU
1	E	243	SER
1	F	4	MSE
1	F	5	ILE
1	F	12	GLN
1	F	20	GLU
1	F	28	LEU
1	F	39	LEU
1	F	41	HIS
1	F	63	ASP
1	F	71	ILE
1	F	73	ARG
1	F	79	GLN
1	F	92	LEU
1	F	148	SER
1	F	151	LEU
1	F	154	VAL
1	F	193	LEU
1	F	225	LEU
1	F	235	LEU

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Mol	Chain	Res	Type
1	F	242	ARG
1	G	79	GLN
1	G	93	ASP
1	G	97	LEU
1	G	133	GLN
1	G	134	LEU
1	G	143	CYS
1	G	167	GLU
1	G	205	LEU
1	G	225	LEU
1	G	235	LEU
1	G	242	ARG
1	H	-6	VAL
1	H	28	LEU
1	H	63	ASP
1	H	143	CYS
1	H	147	GLU
1	H	162	ARG
1	H	198	GLU
1	H	200	GLU
1	H	235	LEU
1	H	240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	94	GLN
1	A	156	ASN
1	B	79	GLN
1	B	81	GLN
1	B	94	GLN
1	B	135	ASN
1	C	23	GLN
1	C	46	GLN
1	C	79	GLN
1	C	81	GLN
1	C	94	GLN
1	D	81	GLN
1	E	79	GLN
1	E	133	GLN
1	F	12	GLN

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Mol	Chain	Res	Type
1	F	46	GLN
1	F	51	GLN
1	F	54	ASN
1	F	94	GLN
1	F	133	GLN
1	G	94	GLN
1	H	51	GLN
1	H	79	GLN
1	H	133	GLN
1	H	165	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 monosaccharides 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, 95^{th} 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	235/253 (92%)	0.41	21 (8%) 9 9	23, 53, 106, 116	1 (0%)
1	B	236/253 (93%)	0.44	17 (7%) 15 16	27, 55, 74, 116	0
1	C	235/253 (92%)	0.34	12 (5%) 28 29	21, 53, 91, 106	0
1	D	236/253 (93%)	0.28	14 (5%) 22 23	20, 45, 82, 96	0
1	E	160/253 (63%)	-0.09	2 (1%) 77 79	21, 40, 63, 83	0
1	F	245/253 (96%)	0.77	40 (16%) 1 1	19, 42, 118, 126	0
1	G	160/253 (63%)	0.07	4 (2%) 57 61	26, 46, 69, 86	0
1	H	242/253 (95%)	0.23	15 (6%) 20 21	19, 43, 97, 115	0
All	All	1749/2024 (86%)	0.34	125 (7%) 16 16	19, 47, 96, 126	1 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	27	ILE	8.3
1	C	31	ARG	8.2
1	F	36	LEU	7.9
1	F	54	ASN	7.4
1	F	39	LEU	7.3
1	F	69	GLY	7.2
1	F	34	LYS	7.1
1	F	37	LEU	7.1
1	F	64	GLY	7.0
1	F	52	LEU	6.9
1	F	56	GLN	6.5
1	H	35	ARG	6.0
1	F	53	ALA	6.0
1	F	30	GLY	5.6
1	F	28	LEU	5.4
1	A	17	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	12	GLN	5.2
1	F	57	TYR	5.2
1	A	36	LEU	5.1
1	F	6	TYR	5.1
1	H	36	LEU	4.9
1	H	39	LEU	4.7
1	F	41	HIS	4.6
1	F	67	HIS	4.6
1	D	27	ILE	4.6
1	F	70	ILE	4.4
1	F	71	ILE	4.2
1	F	11	VAL	4.2
1	F	31	ARG	4.1
1	H	40	ILE	4.1
1	F	58	LEU	4.0
1	C	17	ARG	3.8
1	C	63	ASP	3.8
1	A	66	VAL	3.7
1	F	18	ALA	3.7
1	F	10	ALA	3.6
1	B	78	ARG	3.6
1	H	41	HIS	3.6
1	B	18	ALA	3.6
1	D	222	VAL	3.5
1	C	36	LEU	3.5
1	H	-6	VAL	3.5
1	A	58	LEU	3.5
1	H	30	GLY	3.4
1	H	71	ILE	3.4
1	D	34	LYS	3.4
1	F	32	GLU	3.3
1	A	35	ARG	3.3
1	C	199	GLY	3.3
1	D	72	ALA	3.3
1	H	37	LEU	3.3
1	A	67	HIS	3.2
1	H	33	ASP	3.2
1	H	57	TYR	3.2
1	F	25	VAL	3.2
1	H	31	ARG	3.2
1	A	6	TYR	3.0
1	G	79	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	57	TYR	3.0
1	F	15	LEU	2.9
1	F	68	GLN	2.9
1	D	-1	HIS	2.9
1	A	54	ASN	2.9
1	A	53	ALA	2.9
1	A	55	ARG	2.8
1	B	25	VAL	2.8
1	H	28	LEU	2.8
1	C	66	VAL	2.8
1	G	149	VAL	2.8
1	C	60	GLU	2.8
1	D	64	GLY	2.8
1	B	9	HIS	2.8
1	F	220	GLY	2.7
1	B	31	ARG	2.7
1	H	55	ARG	2.7
1	B	-1	HIS	2.7
1	A	221	SER	2.7
1	A	31	ARG	2.7
1	C	77	GLY	2.7
1	F	35	ARG	2.6
1	C	35	ARG	2.6
1	B	72	ALA	2.6
1	D	54	ASN	2.6
1	F	29	LYS	2.5
1	B	49	VAL	2.5
1	A	77	GLY	2.5
1	F	51	GLN	2.5
1	D	33	ASP	2.5
1	B	61	LYS	2.4
1	F	9	HIS	2.4
1	A	129	ASP	2.4
1	B	69	GLY	2.4
1	D	65	ALA	2.4
1	A	73	ARG	2.4
1	B	14	LEU	2.4
1	F	16	GLU	2.4
1	C	34	LYS	2.4
1	B	39	LEU	2.4
1	G	85	LEU	2.4
1	F	66	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	5	ILE	2.3
1	F	14	LEU	2.3
1	B	17	ARG	2.3
1	A	64	GLY	2.3
1	B	36	LEU	2.3
1	B	5	ILE	2.3
1	C	219	ALA	2.3
1	A	29	LYS	2.3
1	H	-7	LEU	2.3
1	D	78	ARG	2.2
1	D	6	TYR	2.2
1	A	38	PRO	2.2
1	C	55	ARG	2.1
1	B	91	SER	2.1
1	G	145	ALA	2.1
1	B	40	ILE	2.1
1	F	224	SER	2.1
1	D	30	GLY	2.1
1	D	28	LEU	2.1
1	E	136	ALA	2.1
1	A	68	GLN	2.1
1	E	78	ARG	2.0
1	F	50	ILE	2.0
1	A	78	ARG	2.0
1	A	74	VAL	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 monosaccharides 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.