Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:27 AM JST

PDB ID	:	5CFK
Title	:	Crystal structure of Proliferating Cell Nuclear Antigen from Leishmania donovani at 3.2 A resolution
Authors	:	Shukla, P.K.; Yadav, S.P.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2015-07-08
Resolution	:	3.20 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:

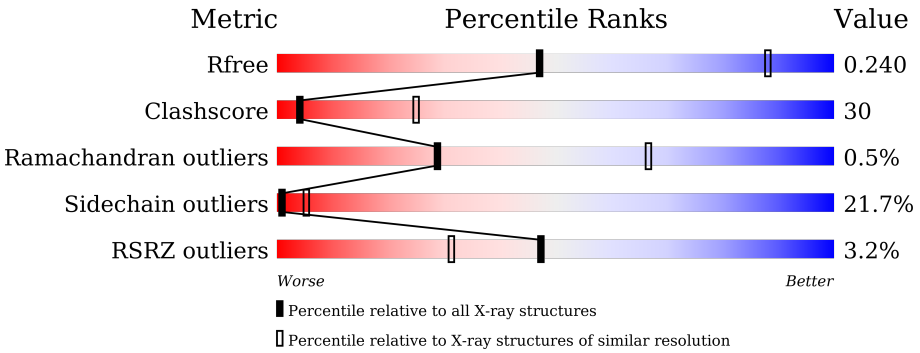
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	259	3% 51% 37% 9%
1	B	259	3% 48% 41% 7%
1	C	259	4% 43% 42% 12%
1	D	259	3% 42% 44% 12%
1	E	259	3% 50% 36% 12%
1	F	259	3% 44% 39% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11739 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 Proliferating cell nuclear antigen,Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	B	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	C	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	D	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	E	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			
1	F	253	Total	C	N	O	S	0	0	0
			1955	1230	325	385	15			

- Molecule 2 is water.

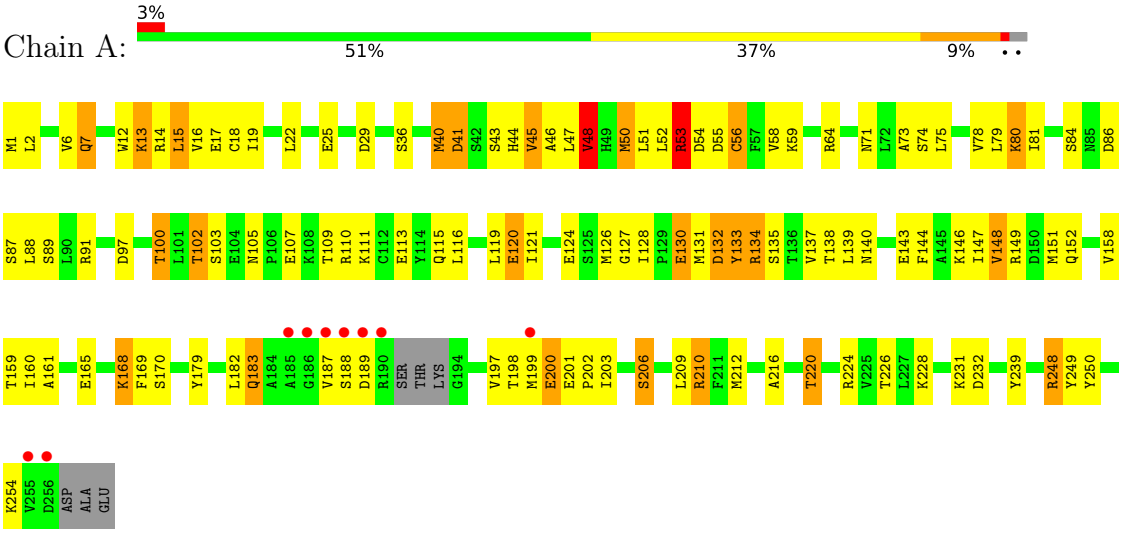
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	F	3	Total	O	0	0
			3	3		

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.

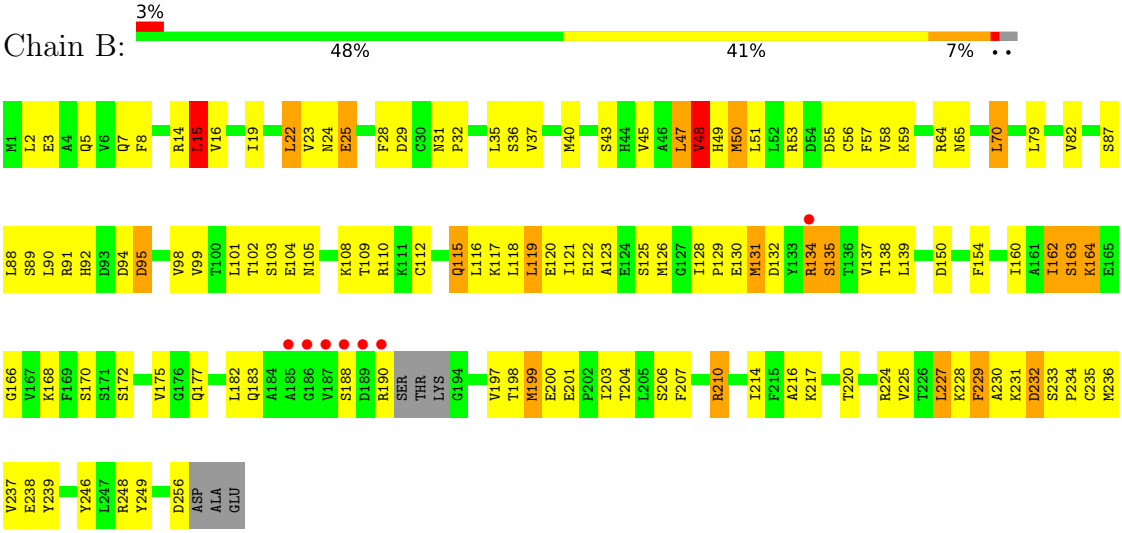
• Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

Chain A:



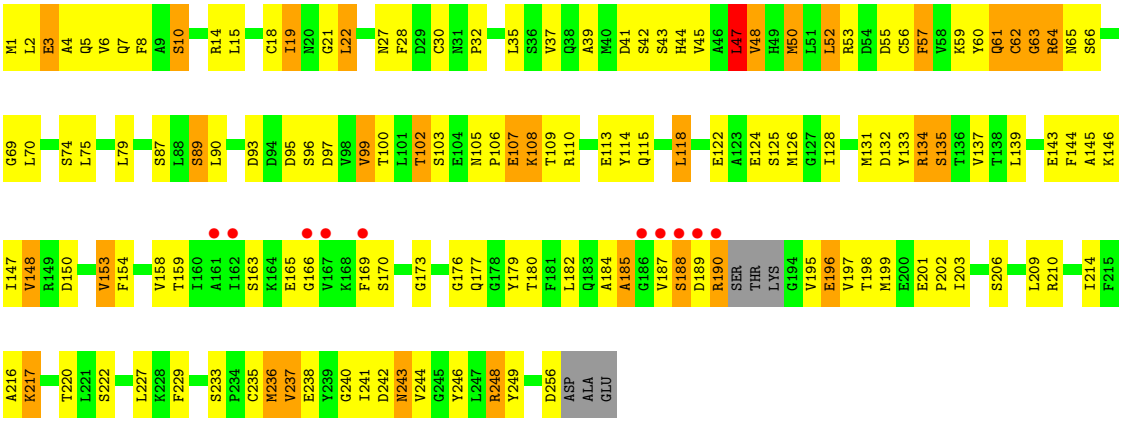
• Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

Chain B:

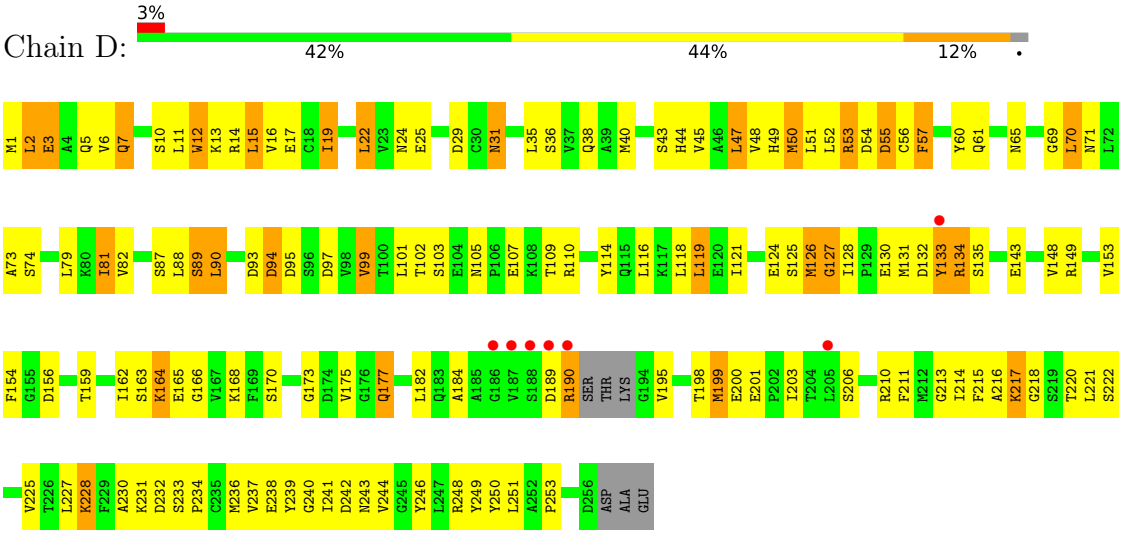


• Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

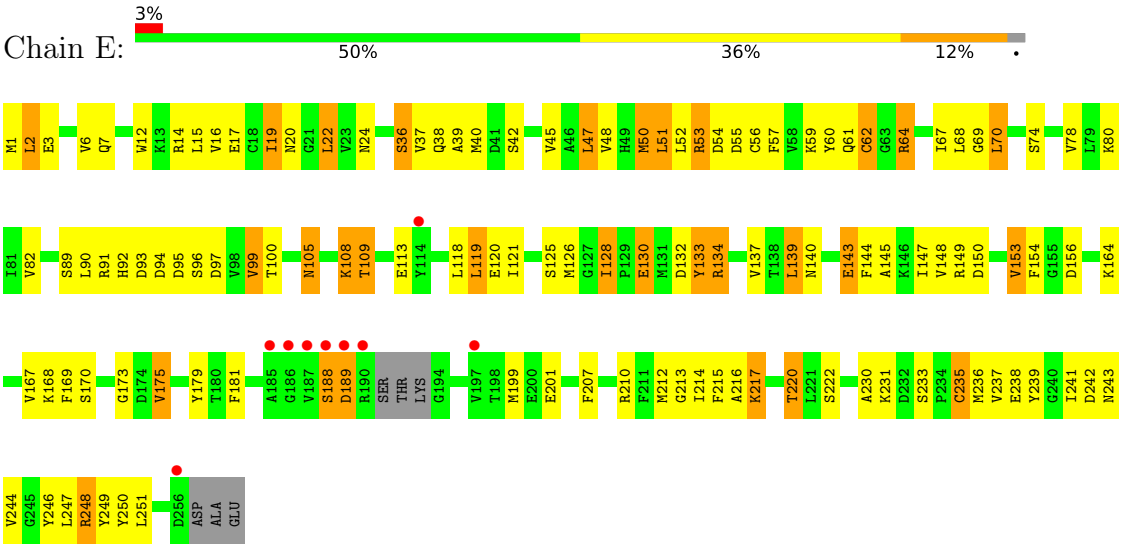
Chain C:



• Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

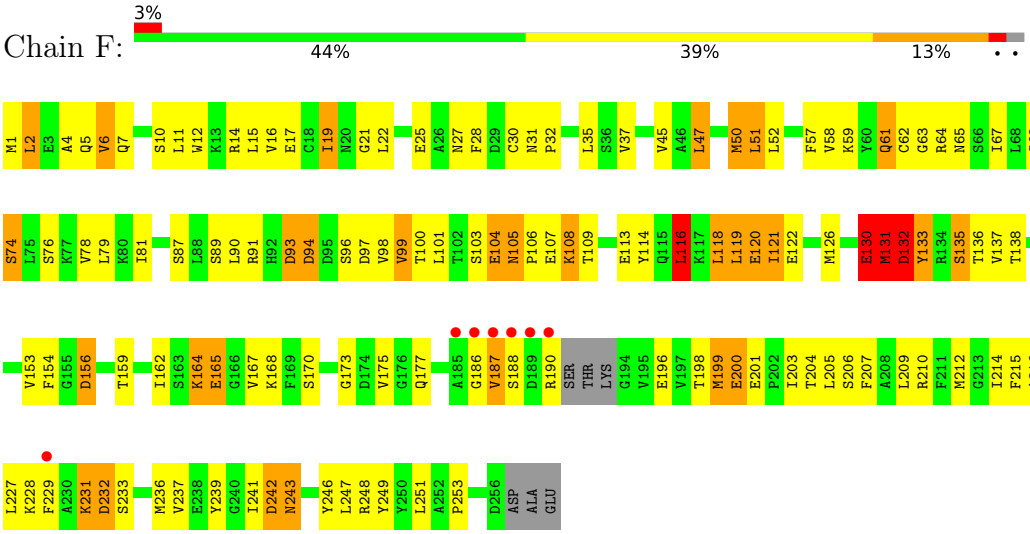


• Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen,Proliferating cell nuclear antigen

Chain F:


3%
44%
39%
13%
M1 L2 E3 A4 Q5 V6 Q7 S10 L11 W12 K13 R14 L15 V16 E17 C18 I19 N20 G21 L22 E25 A26 N27 F28 D29 C30 N31 P32 L35 S36 V37 V45 A46 L47 M50 L51 L52 F57 V58 K59 Y60 Q61 C62 G63 R64 N65 S66 I67 L68 G69 L70 N71 L72 A73
S74 L75 S76 K77 V78 L79 K80 I81 S87 L88 S89 L90 R91 H92 D93 D94 D95 S96 D97 V98 V99 T100 L101 T102 S103 E104 N105 P106 E107 K108 T109 E113 Y114 Q115 L116 K117 L118 L119 E120 I121 E122 M126 E130 M131 D132 Y133 R134 S135 T136 V137 T138 E143 I147 V148
V153 F154 G155 D156 T159 I162 S163 K164 E165 G166 V167 K168 F169 S170 G173 D174 V175 G176 Q177 A185 G186 V187 S188 D189 R190 SER THR LYS G194 V195 E196 V197 T198 M199 E200 E201 P202 I203 T204 L205 S206 F207 A208 L209 R210 F211 M212 G213 I214 F215 A216 K217 R224
L227 K228 F229 A230 K231 D232 S233 M236 V237 E238 Y239 G240 I241 D242 N243 Y246 L247 R248 Y249 Y250 L251 A252 P253 D256 ASP ALA GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.44Å 150.21Å 169.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 45.20 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.20) 99.6 (45.20-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.191 , 0.238 0.192 , 0.240	Depositor DCC
R_{free} test set	2854 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	93.7	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11739	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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	0.94	6/1983 (0.3%)	1.02	6/2675 (0.2%)
1	B	0.75	1/1983 (0.1%)	0.97	3/2675 (0.1%)
1	C	0.66	0/1983	0.99	6/2675 (0.2%)
1	D	0.72	2/1983 (0.1%)	0.92	2/2675 (0.1%)
1	E	0.66	0/1983	0.91	2/2675 (0.1%)
1	F	1.02	14/1983 (0.7%)	0.94	3/2675 (0.1%)
All	All	0.80	23/11898 (0.2%)	0.96	22/16050 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	130	GLU	CD-OE1	17.01	1.44	1.25
1	F	188	SER	CB-OG	13.46	1.59	1.42
1	A	120	GLU	CD-OE2	12.43	1.39	1.25
1	A	120	GLU	CD-OE1	10.33	1.37	1.25
1	D	190	ARG	C-O	10.13	1.42	1.23
1	F	130	GLU	CG-CD	9.44	1.66	1.51
1	F	130	GLU	CD-OE2	9.31	1.35	1.25
1	F	133	TYR	CE1-CZ	8.34	1.49	1.38
1	F	132	ASP	CB-CG	7.78	1.68	1.51
1	F	131	MET	CG-SD	7.07	1.99	1.81
1	A	120	GLU	CG-CD	6.83	1.62	1.51
1	B	117	LYS	CE-NZ	6.67	1.65	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	133	TYR	CG-CD1	6.60	1.47	1.39
1	F	133	TYR	CG-CD2	6.37	1.47	1.39
1	F	133	TYR	CE2-CZ	6.30	1.46	1.38
1	F	132	ASP	CG-OD1	6.29	1.39	1.25
1	A	133	TYR	CE1-CZ	6.03	1.46	1.38
1	F	130	GLU	C-O	5.79	1.34	1.23
1	A	132	ASP	CB-CG	5.33	1.62	1.51
1	F	132	ASP	CG-OD2	5.23	1.37	1.25
1	D	12	TRP	CD2-CE2	5.20	1.47	1.41
1	F	106	PRO	N-CD	5.19	1.55	1.47
1	A	132	ASP	CG-OD1	5.08	1.37	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	185	ALA	CB-CA-C	-11.64	92.64	110.10
1	B	48	VAL	CB-CA-C	-9.15	94.02	111.40
1	C	1	MET	CG-SD-CE	8.47	113.75	100.20
1	C	185	ALA	N-CA-C	7.63	131.62	111.00
1	A	13	LYS	CD-CE-NZ	-6.80	96.05	111.70
1	B	15	LEU	CB-CG-CD1	-6.72	99.57	111.00
1	F	131	MET	CG-SD-CE	6.23	110.17	100.20
1	A	15	LEU	CB-CG-CD1	-5.99	100.81	111.00
1	A	1	MET	CG-SD-CE	5.98	109.77	100.20
1	D	55	ASP	CB-CG-OD1	5.97	123.67	118.30
1	E	51	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	53	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	F	105	ASN	C-N-CD	5.69	140.34	128.40
1	E	55	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	47	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	48	VAL	CB-CA-C	-5.53	100.90	111.40
1	A	248	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	150	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	190	ARG	CA-C-O	-5.26	109.04	120.10
1	C	52	LEU	CB-CG-CD1	-5.20	102.17	111.00
1	F	116	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	48	VAL	CB-CA-C	-5.04	101.83	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	B	134	ARG	Peptide

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	1955	0	1948	75	0
1	B	1955	0	1948	102	0
1	C	1955	0	1948	122	0
1	D	1955	0	1948	142	0
1	E	1955	0	1948	112	0
1	F	1955	0	1948	155	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	F	3	0	0	1	0
All	All	11739	0	11688	699	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 30.

All (699) 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:E:241:ILE:HG21	1:E:244:VAL:HG22	1.27	1.17
1:F:51:LEU:HD23	1:F:246:TYR:CE1	1.82	1.14
1:B:131:MET:CG	1:B:132:ASP:HA	1.80	1.11
1:F:10:SER:HB3	1:F:14:ARG:NH1	1.66	1.09
1:D:134:ARG:HB3	1:D:200:GLU:HB2	1.28	1.08
1:E:50:MET:CE	1:E:52:LEU:HG	1.84	1.07
1:F:119:LEU:HB2	1:F:121:ILE:HG12	1.36	1.07
1:C:100:THR:HG22	1:C:115:GLN:HG2	1.35	1.06
1:F:10:SER:HB3	1:F:14:ARG:HH12	1.00	1.06
1:B:119:LEU:HA	1:B:120:GLU:HB2	1.37	1.06
1:F:130:GLU:HB3	1:F:131:MET:HG2	1.32	1.03
1:A:22:LEU:HD12	1:A:48:VAL:HG22	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ARG:CZ	1:E:201:GLU:HG3	1.89	1.02
1:E:241:ILE:CG2	1:E:244:VAL:HG22	1.89	1.02
1:D:134:ARG:HG3	1:D:200:GLU:HG3	1.39	1.00
1:B:40:MET:HG3	1:B:47:LEU:HD23	1.43	1.00
1:F:122:GLU:OE2	1:F:122:GLU:N	1.94	1.00
1:A:130:GLU:HB2	1:A:131:MET:HB2	1.43	0.99
1:E:241:ILE:HG21	1:E:244:VAL:CG2	1.90	0.99
1:C:4:ALA:HB1	1:C:57:PHE:CD2	1.99	0.97
1:F:99:VAL:HG12	1:F:118:LEU:HD22	1.42	0.97
1:E:118:LEU:C	1:E:119:LEU:HD23	1.85	0.96
1:F:241:ILE:HD12	1:F:246:TYR:HA	1.46	0.95
1:B:134:ARG:HH11	1:B:201:GLU:HG3	1.28	0.95
1:F:130:GLU:HB3	1:F:131:MET:CG	1.95	0.95
1:D:31:ASN:HD22	1:D:65:ASN:HB2	1.27	0.95
1:F:164:LYS:HE3	1:F:199:MET:HE1	1.46	0.95
1:D:19:ILE:HG22	1:D:48:VAL:HG11	1.49	0.94
1:D:184:ALA:HB2	1:D:195:VAL:HG12	1.47	0.94
1:B:134:ARG:HA	1:B:200:GLU:HB3	1.50	0.94
1:C:131:MET:HB2	1:C:132:ASP:HB2	1.50	0.93
1:F:119:LEU:HB2	1:F:121:ILE:CG1	1.98	0.92
1:E:50:MET:HE2	1:E:52:LEU:HG	1.48	0.92
1:A:130:GLU:HB2	1:A:131:MET:CB	1.98	0.92
1:B:131:MET:CB	1:B:132:ASP:HA	1.99	0.91
1:F:10:SER:CB	1:F:14:ARG:HH12	1.83	0.91
1:A:86:ASP:OD2	1:A:110:ARG:NH2	2.04	0.91
1:D:237:VAL:HG22	1:D:249:TYR:HB2	1.55	0.89
1:D:134:ARG:HG2	1:D:134:ARG:HH11	1.35	0.89
1:F:105:ASN:OD1	1:F:107:GLU:N	2.05	0.89
1:A:148:VAL:O	1:A:152:GLN:HG3	1.73	0.88
1:B:162:ILE:HG13	1:B:203:ILE:HG23	1.56	0.88
1:D:56:CYS:HB2	1:D:244:VAL:HB	1.56	0.88
1:F:5:GLN:HG2	1:F:58:VAL:CG2	2.04	0.88
1:B:119:LEU:CA	1:B:120:GLU:HB2	2.03	0.87
1:D:238:GLU:HG3	1:D:248:ARG:HD3	1.56	0.86
1:D:88:LEU:HD11	1:D:101:LEU:HD23	1.58	0.85
1:D:81:ILE:HD11	1:D:114:TYR:OH	1.75	0.84
1:F:16:VAL:HG21	1:F:79:LEU:CD1	2.06	0.84
1:C:22:LEU:HD12	1:C:48:VAL:CG2	2.08	0.84
1:B:131:MET:HG2	1:B:132:ASP:HA	1.58	0.84
1:F:104:GLU:HB3	1:F:108:LYS:HE2	1.59	0.84
1:B:134:ARG:HD3	1:B:201:GLU:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:VAL:HG21	1:F:79:LEU:HD12	1.57	0.83
1:B:134:ARG:NH1	1:B:201:GLU:HG3	1.92	0.83
1:F:51:LEU:HD23	1:F:246:TYR:HE1	1.37	0.83
1:A:132:ASP:HB3	1:A:134:ARG:HH11	1.41	0.83
1:C:132:ASP:OD1	1:C:133:TYR:N	2.12	0.83
1:B:31:ASN:HB3	1:B:32:PRO:CD	2.08	0.83
1:D:49:HIS:ND1	1:D:128:ILE:HD12	1.94	0.82
1:F:241:ILE:HD12	1:F:246:TYR:CA	2.09	0.82
1:F:105:ASN:O	1:F:108:LYS:HE3	1.78	0.82
1:C:41:ASP:OD2	1:C:43:SER:HB2	1.79	0.82
1:A:144:PHE:HZ	1:A:212:MET:CE	1.93	0.81
1:E:150:ASP:O	1:E:153:VAL:HG22	1.81	0.81
1:F:119:LEU:CB	1:F:121:ILE:HG12	2.10	0.81
1:B:131:MET:HB3	1:B:132:ASP:HB3	1.60	0.81
1:D:51:LEU:HB3	1:D:246:TYR:CE1	2.15	0.81
1:E:56:CYS:HB2	1:E:244:VAL:HB	1.61	0.80
1:D:134:ARG:HB3	1:D:200:GLU:CB	2.11	0.80
1:B:118:LEU:HD12	1:B:118:LEU:O	1.82	0.80
1:F:27:ASN:ND2	1:F:121:ILE:HB	1.97	0.79
1:B:131:MET:CB	1:B:132:ASP:CA	2.61	0.79
1:B:131:MET:HB3	1:B:132:ASP:CA	2.13	0.79
1:A:40:MET:SD	1:A:44:HIS:HD2	2.04	0.78
1:D:236:MET:HE3	1:D:238:GLU:HB2	1.64	0.78
1:E:139:LEU:HD11	1:E:144:PHE:HB2	1.64	0.78
1:E:119:LEU:HD23	1:E:119:LEU:N	1.98	0.78
1:F:93:ASP:O	1:F:96:SER:HB2	1.84	0.78
1:F:241:ILE:CD1	1:F:246:TYR:CA	2.62	0.78
1:E:22:LEU:HD12	1:E:48:VAL:CG2	2.15	0.77
1:F:31:ASN:HB3	1:F:65:ASN:ND2	1.98	0.77
1:A:132:ASP:HB3	1:A:134:ARG:NH1	1.99	0.77
1:A:159:THR:HA	1:A:206:SER:HB3	1.66	0.77
1:F:119:LEU:HA	1:F:120:GLU:HB3	1.67	0.77
1:A:22:LEU:CD1	1:A:48:VAL:HG22	2.15	0.76
1:C:21:GLY:O	1:C:214:ILE:HD12	1.85	0.76
1:D:134:ARG:HD3	1:D:199:MET:HA	1.68	0.76
1:C:150:ASP:O	1:C:153:VAL:HG22	1.86	0.76
1:D:241:ILE:HG22	1:D:244:VAL:HG22	1.68	0.76
1:D:119:LEU:HD23	1:D:119:LEU:N	2.01	0.75
1:B:31:ASN:HB3	1:B:32:PRO:HD2	1.68	0.75
1:B:119:LEU:HD23	1:B:119:LEU:N	2.02	0.75
1:F:119:LEU:N	1:F:119:LEU:HD23	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:MET:HE3	1:E:238:GLU:HB2	1.67	0.75
1:D:134:ARG:HG3	1:D:200:GLU:CG	2.16	0.74
1:E:70:LEU:HD23	1:E:99:VAL:HG11	1.69	0.74
1:E:236:MET:HE3	1:E:248:ARG:HG2	1.68	0.74
1:D:241:ILE:CG2	1:D:244:VAL:HG22	2.18	0.74
1:D:164:LYS:HG3	1:D:165:GLU:CG	2.17	0.74
1:F:27:ASN:HD21	1:F:121:ILE:HB	1.53	0.73
1:C:22:LEU:HD12	1:C:48:VAL:HG23	1.68	0.73
1:F:148:VAL:HG11	1:F:212:MET:HB3	1.69	0.73
1:E:246:TYR:CD2	1:E:248:ARG:HD2	2.22	0.73
1:D:74:SER:HB3	1:E:175:VAL:HG13	1.70	0.73
1:B:131:MET:HB3	1:B:132:ASP:CB	2.18	0.73
1:D:164:LYS:HG3	1:D:165:GLU:HG2	1.71	0.73
1:F:130:GLU:CG	1:F:131:MET:HA	2.19	0.73
1:F:69:GLY:HA3	1:F:121:ILE:CD1	2.18	0.72
1:D:134:ARG:HG2	1:D:134:ARG:NH1	1.99	0.72
1:F:200:GLU:HG2	1:F:200:GLU:O	1.89	0.72
1:D:134:ARG:CG	1:D:200:GLU:HG3	2.20	0.72
1:F:154:PHE:O	1:F:173:GLY:HA3	1.91	0.71
1:C:165:GLU:HA	1:C:184:ALA:HB3	1.73	0.71
1:E:246:TYR:CD2	1:E:248:ARG:CD	2.74	0.71
1:F:25:GLU:OE1	1:F:119:LEU:HD12	1.90	0.71
1:B:236:MET:HE3	1:B:238:GLU:HB2	1.74	0.70
1:D:49:HIS:ND1	1:D:128:ILE:CD1	2.53	0.70
1:F:69:GLY:CA	1:F:121:ILE:CD1	2.69	0.70
1:B:14:ARG:HD2	1:B:220:THR:HB	1.72	0.70
1:A:22:LEU:HD12	1:A:48:VAL:CG2	2.20	0.70
1:D:50:MET:CE	1:D:52:LEU:HG	2.20	0.70
1:F:241:ILE:CD1	1:F:246:TYR:C	2.60	0.70
1:F:119:LEU:HA	1:F:120:GLU:CB	2.21	0.70
1:A:75:LEU:HG	1:A:79:LEU:HD12	1.73	0.70
1:B:134:ARG:HD3	1:B:201:GLU:CG	2.22	0.69
1:B:48:VAL:HG13	1:B:249:TYR:CE1	2.27	0.69
1:C:201:GLU:HG2	1:C:202:PRO:HD2	1.73	0.69
1:A:110:ARG:HD3	1:D:143:GLU:OE1	1.91	0.69
1:D:118:LEU:C	1:D:119:LEU:HD23	2.12	0.69
1:D:50:MET:HE1	1:D:52:LEU:HG	1.75	0.69
1:A:216:ALA:HA	1:A:239:TYR:OH	1.93	0.69
1:F:207:PHE:HD2	1:F:251:LEU:HD23	1.58	0.69
1:E:134:ARG:NE	1:E:201:GLU:HG3	2.07	0.68
1:F:25:GLU:OE1	1:F:119:LEU:CD1	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:ARG:O	1:F:214:ILE:HG12	1.92	0.68
1:C:131:MET:CB	1:C:132:ASP:HB2	2.20	0.68
1:E:119:LEU:HA	1:E:120:GLU:HB2	1.74	0.68
1:B:134:ARG:HD3	1:B:201:GLU:CB	2.23	0.68
1:B:122:GLU:HG2	1:B:123:ALA:N	2.07	0.68
1:E:64:ARG:HH11	1:E:64:ARG:HB3	1.59	0.68
1:B:134:ARG:CD	1:B:201:GLU:HB2	2.23	0.68
1:C:133:TYR:HD2	1:C:134:ARG:H	1.41	0.68
1:A:14:ARG:HD2	1:A:220:THR:HB	1.74	0.68
1:B:94:ASP:O	1:B:95:ASP:OD1	2.11	0.68
1:C:242:ASP:C	1:C:243:ASN:HD22	1.97	0.68
1:B:3:GLU:HG3	1:B:91:ARG:HE	1.59	0.68
1:C:143:GLU:O	1:C:147:ILE:HG13	1.93	0.68
1:A:43:SER:OG	1:A:45:VAL:HG23	1.95	0.67
1:F:164:LYS:HG2	1:F:199:MET:HE1	1.77	0.67
1:B:135:SER:OG	1:B:203:ILE:HG21	1.94	0.67
1:C:243:ASN:HD22	1:C:243:ASN:N	1.91	0.67
1:E:64:ARG:HH11	1:E:64:ARG:CB	2.08	0.67
1:B:118:LEU:HD12	1:B:118:LEU:C	2.14	0.67
1:E:148:VAL:CG2	1:E:149:ARG:N	2.58	0.67
1:C:122:GLU:OE2	1:C:122:GLU:N	2.18	0.67
1:F:2:LEU:C	1:F:2:LEU:HD23	2.15	0.67
1:C:3:GLU:OE2	1:C:59:LYS:HE2	1.95	0.66
1:C:64:ARG:CB	1:C:64:ARG:HH11	2.08	0.66
1:D:1:MET:HB3	1:D:61:GLN:NE2	2.10	0.66
1:F:99:VAL:CG1	1:F:118:LEU:HD22	2.20	0.66
1:A:139:LEU:HD11	1:A:144:PHE:HB2	1.77	0.66
1:A:134:ARG:O	1:A:200:GLU:HB2	1.95	0.66
1:F:69:GLY:O	1:F:118:LEU:HB2	1.95	0.66
1:F:70:LEU:N	1:F:121:ILE:HD11	2.10	0.66
1:E:125:SER:OG	1:E:126:MET:N	2.25	0.66
1:E:230:ALA:HB3	1:E:233:SER:HB2	1.78	0.66
1:F:164:LYS:HG2	1:F:199:MET:CE	2.26	0.66
1:B:25:GLU:HB2	1:B:121:ILE:CD1	2.26	0.66
1:C:43:SER:O	1:C:44:HIS:HB2	1.96	0.66
1:D:2:LEU:HG	1:D:3:GLU:N	2.10	0.66
1:C:241:ILE:HG22	1:C:241:ILE:O	1.95	0.65
1:D:22:LEU:HD12	1:D:48:VAL:CG2	2.26	0.65
1:F:187:VAL:HG11	1:F:196:GLU:OE2	1.96	0.65
1:D:43:SER:O	1:D:45:VAL:HG23	1.96	0.65
1:A:168:LYS:HD2	1:A:179:TYR:CD1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:HD13	1:C:50:MET:HE2	1.78	0.65
1:B:53:ARG:O	1:B:56:CYS:HB3	1.97	0.65
1:E:96:SER:O	1:E:97:ASP:HB3	1.94	0.65
1:B:92:HIS:HD2	1:B:98:VAL:O	1.80	0.65
1:B:125:SER:OG	1:B:126:MET:N	2.27	0.65
1:D:51:LEU:HD23	1:D:246:TYR:HE1	1.62	0.65
1:E:210:ARG:O	1:E:214:ILE:HG12	1.98	0.64
1:E:215:PHE:CD1	1:E:249:TYR:CG	2.85	0.64
1:B:87:SER:O	1:B:103:SER:HA	1.97	0.64
1:C:135:SER:OG	1:C:203:ILE:HG21	1.97	0.64
1:E:56:CYS:CB	1:E:244:VAL:HB	2.27	0.64
1:A:165:GLU:O	1:A:183:GLN:HA	1.98	0.63
1:E:148:VAL:CG2	1:E:149:ARG:H	2.10	0.63
1:C:154:PHE:O	1:C:173:GLY:HA3	1.98	0.63
1:F:5:GLN:O	1:F:57:PHE:HD2	1.82	0.63
1:F:159:THR:OG1	1:F:206:SER:HB3	1.98	0.63
1:B:40:MET:HG3	1:B:47:LEU:CD2	2.24	0.63
1:C:57:PHE:CD1	1:C:57:PHE:N	2.67	0.63
1:A:71:ASN:HB2	1:A:119:LEU:HD11	1.80	0.63
1:F:164:LYS:CE	1:F:199:MET:HE1	2.26	0.63
1:A:100:THR:HG22	1:A:115:GLN:HG2	1.80	0.63
1:B:36:SER:HA	1:B:50:MET:O	1.99	0.62
1:D:134:ARG:HB2	1:D:200:GLU:CD	2.19	0.62
1:B:25:GLU:HB2	1:B:121:ILE:HD13	1.80	0.62
1:A:130:GLU:HB2	1:A:131:MET:CA	2.29	0.62
1:F:105:ASN:OD1	1:F:107:GLU:HB3	1.99	0.62
1:F:231:LYS:HE2	1:F:232:ASP:N	2.14	0.62
1:A:58:VAL:HG23	1:A:59:LYS:HG2	1.82	0.62
1:C:5:GLN:HB2	1:C:89:SER:OG	1.99	0.62
1:D:53:ARG:O	1:D:56:CYS:HB3	1.99	0.62
1:A:133:TYR:CD2	1:A:228:LYS:HD3	2.36	0.61
1:F:69:GLY:HA3	1:F:121:ILE:HG13	1.81	0.61
1:B:2:LEU:O	1:B:91:ARG:HA	2.01	0.61
1:D:16:VAL:HG21	1:D:79:LEU:CD1	2.30	0.61
1:D:22:LEU:HD12	1:D:48:VAL:HG22	1.82	0.61
1:D:135:SER:OG	1:D:203:ILE:HG21	2.01	0.61
1:D:241:ILE:HG21	1:D:244:VAL:CG2	2.31	0.61
1:C:62:CYS:O	1:C:63:GLY:C	2.39	0.60
1:F:69:GLY:CA	1:F:121:ILE:HD11	2.31	0.60
1:E:154:PHE:O	1:E:173:GLY:HA3	2.01	0.60
1:F:241:ILE:CD1	1:F:246:TYR:HA	2.24	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:HH11	1:C:64:ARG:CG	2.14	0.60
1:C:243:ASN:N	1:C:243:ASN:ND2	2.50	0.60
1:D:105:ASN:HD22	1:D:110:ARG:H	1.48	0.60
1:A:105:ASN:HD22	1:A:110:ARG:N	1.98	0.60
1:B:119:LEU:HA	1:B:120:GLU:CB	2.24	0.60
1:D:105:ASN:ND2	1:D:109:THR:HG23	2.17	0.60
1:F:51:LEU:HD23	1:F:246:TYR:CZ	2.35	0.60
1:F:138:THR:HG22	1:F:224:ARG:HH21	1.67	0.60
1:A:133:TYR:HD2	1:A:228:LYS:HD3	1.65	0.59
1:E:148:VAL:HG23	1:E:149:ARG:N	2.15	0.59
1:B:105:ASN:HB3	1:B:108:LYS:H	1.67	0.59
1:D:54:ASP:CB	1:D:60:TYR:CD2	2.85	0.59
1:F:119:LEU:CA	1:F:120:GLU:HB3	2.32	0.59
1:C:93:ASP:O	1:C:96:SER:HB2	2.02	0.59
1:D:5:GLN:HB2	1:D:89:SER:OG	2.02	0.59
1:C:10:SER:HB3	1:C:14:ARG:HH12	1.67	0.59
1:C:131:MET:HB3	1:C:132:ASP:HA	1.84	0.59
1:D:134:ARG:CB	1:D:200:GLU:HB2	2.19	0.59
1:E:69:GLY:O	1:E:118:LEU:HB2	2.01	0.59
1:F:107:GLU:HG3	1:F:109:THR:HG23	1.85	0.59
1:F:50:MET:HE3	1:F:52:LEU:HG	1.83	0.59
1:D:54:ASP:HB3	1:D:60:TYR:CE2	2.37	0.59
1:D:54:ASP:HB2	1:D:60:TYR:HD2	1.68	0.59
1:D:159:THR:OG1	1:D:206:SER:HB3	2.03	0.58
1:E:119:LEU:CA	1:E:120:GLU:HB2	2.33	0.58
1:B:90:LEU:HD13	1:B:101:LEU:HD21	1.86	0.58
1:D:164:LYS:HG3	1:D:165:GLU:HG3	1.84	0.58
1:C:4:ALA:HB1	1:C:57:PHE:CE2	2.39	0.58
1:D:1:MET:HB3	1:D:61:GLN:HE21	1.66	0.58
1:F:50:MET:CE	1:F:52:LEU:HG	2.33	0.58
1:F:130:GLU:HG3	1:F:131:MET:HA	1.85	0.58
1:F:5:GLN:HG2	1:F:58:VAL:HG23	1.84	0.58
1:B:7:GLN:NE2	1:B:8:PHE:CZ	2.72	0.58
1:D:134:ARG:HA	1:D:134:ARG:NE	2.19	0.58
1:F:241:ILE:HD13	1:F:246:TYR:N	2.19	0.58
1:A:50:MET:HG2	1:A:51:LEU:N	2.19	0.57
1:A:179:TYR:CE2	1:E:113:GLU:HB3	2.40	0.57
1:B:49:HIS:ND1	1:B:128:ILE:HD11	2.20	0.57
1:F:50:MET:HB2	1:F:247:LEU:HD12	1.86	0.57
1:E:19:ILE:HD11	1:E:37:VAL:HG11	1.85	0.57
1:C:182:LEU:HB3	1:C:195:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ILE:HD11	1:F:72:LEU:HD11	1.86	0.57
1:C:169:PHE:O	1:C:179:TYR:HA	2.04	0.57
1:D:107:GLU:HG2	1:D:109:THR:HG22	1.87	0.57
1:F:101:LEU:HD12	1:F:101:LEU:H	1.69	0.57
1:D:53:ARG:HB3	1:D:55:ASP:OD1	2.05	0.57
1:F:81:ILE:HD11	1:F:114:TYR:CZ	2.40	0.57
1:F:231:LYS:HE2	1:F:232:ASP:H	1.70	0.57
1:F:130:GLU:CB	1:F:131:MET:HA	2.35	0.56
1:F:156:ASP:OD1	1:F:156:ASP:N	2.38	0.56
1:C:15:LEU:HD22	1:C:50:MET:CE	2.35	0.56
1:E:246:TYR:CE2	1:E:248:ARG:NH1	2.73	0.56
1:F:5:GLN:HG2	1:F:58:VAL:HG22	1.86	0.56
1:F:69:GLY:C	1:F:121:ILE:HD11	2.26	0.56
1:A:105:ASN:HD22	1:A:110:ARG:H	1.54	0.56
1:D:105:ASN:HD22	1:D:110:ARG:N	2.03	0.56
1:E:246:TYR:CD2	1:E:248:ARG:HD3	2.41	0.56
1:C:165:GLU:HA	1:C:184:ALA:CB	2.36	0.56
1:E:74:SER:O	1:E:78:VAL:HG23	2.06	0.56
1:F:148:VAL:CG1	1:F:212:MET:HB3	2.34	0.56
1:C:102:THR:HG23	1:C:113:GLU:HG3	1.87	0.56
1:A:133:TYR:CD2	1:A:228:LYS:HB3	2.41	0.56
1:B:119:LEU:HB2	1:B:121:ILE:HG13	1.88	0.56
1:E:241:ILE:HD12	1:E:241:ILE:N	2.20	0.56
1:F:130:GLU:HG3	1:F:131:MET:HB3	1.88	0.55
1:C:133:TYR:CD2	1:C:134:ARG:N	2.72	0.55
1:F:50:MET:HG2	1:F:51:LEU:N	2.21	0.55
1:F:119:LEU:HB3	1:F:120:GLU:C	2.27	0.55
1:E:246:TYR:CE2	1:E:248:ARG:HD3	2.40	0.55
1:F:242:ASP:O	1:F:243:ASN:HB2	2.06	0.55
1:E:50:MET:CE	1:E:52:LEU:CG	2.73	0.55
1:B:172:SER:HB3	1:B:177:GLN:HG2	1.89	0.55
1:B:16:VAL:HG21	1:B:79:LEU:CD1	2.37	0.55
1:A:22:LEU:HD22	1:A:41:ASP:HB3	1.89	0.54
1:C:165:GLU:OE1	1:C:185:ALA:HB2	2.08	0.54
1:C:222:SER:HB2	1:C:240:GLY:O	2.07	0.54
1:D:210:ARG:O	1:D:214:ILE:HG12	2.07	0.54
1:F:119:LEU:CA	1:F:120:GLU:CB	2.85	0.54
1:B:172:SER:CB	1:B:177:GLN:HG2	2.38	0.54
1:D:31:ASN:ND2	1:D:65:ASN:HB2	2.09	0.54
1:D:40:MET:HE2	1:D:44:HIS:HA	1.89	0.54
1:D:71:ASN:OD1	1:D:73:ALA:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:B:130:GLU:N	2.41	0.54
1:C:131:MET:CB	1:C:132:ASP:CA	2.85	0.54
1:F:69:GLY:HA3	1:F:121:ILE:CG1	2.37	0.54
1:F:99:VAL:HG12	1:F:118:LEU:CD2	2.27	0.54
1:B:162:ILE:HG13	1:B:203:ILE:CG2	2.33	0.54
1:C:189:ASP:O	1:C:190:ARG:HB2	2.06	0.54
1:C:75:LEU:HG	1:C:79:LEU:HD12	1.88	0.54
1:C:22:LEU:HD12	1:C:48:VAL:HG22	1.86	0.54
1:E:236:MET:CE	1:E:238:GLU:HB2	2.34	0.54
1:B:115:GLN:HB2	1:F:177:GLN:HB2	1.90	0.54
1:D:31:ASN:HD22	1:D:65:ASN:CB	2.10	0.54
1:D:40:MET:HG2	1:D:47:LEU:CD2	2.38	0.54
1:C:56:CYS:HB2	1:C:244:VAL:HB	1.89	0.54
1:E:68:LEU:HD22	1:E:92:HIS:CD2	2.43	0.54
1:A:75:LEU:HG	1:A:79:LEU:CD1	2.38	0.53
1:C:131:MET:CB	1:C:132:ASP:CB	2.85	0.53
1:E:148:VAL:HG22	1:E:149:ARG:H	1.71	0.53
1:C:4:ALA:HB1	1:C:57:PHE:HD2	1.65	0.53
1:C:90:LEU:HD11	1:C:99:VAL:HG21	1.91	0.53
1:D:17:GLU:HB3	1:D:217:LYS:HE2	1.90	0.53
1:E:6:VAL:HG22	1:E:7:GLN:N	2.22	0.53
1:C:39:ALA:O	1:C:47:LEU:HD23	2.09	0.53
1:E:2:LEU:HD23	1:E:2:LEU:C	2.29	0.53
1:E:236:MET:CE	1:E:248:ARG:HG2	2.38	0.53
1:D:166:GLY:HA3	1:D:182:LEU:O	2.08	0.53
1:D:105:ASN:ND2	1:D:109:THR:CG2	2.72	0.53
1:C:57:PHE:N	1:C:57:PHE:HD1	2.06	0.53
1:C:108:LYS:CD	1:C:108:LYS:H	2.22	0.53
1:C:158:VAL:HB	1:C:209:LEU:HD21	1.90	0.53
1:D:241:ILE:CG2	1:D:244:VAL:CG2	2.86	0.53
1:C:30:CYS:SG	1:C:35:LEU:HD22	2.50	0.52
1:D:116:LEU:HD12	1:D:116:LEU:N	2.24	0.52
1:D:134:ARG:CB	1:D:200:GLU:CD	2.77	0.52
1:A:158:VAL:HB	1:A:209:LEU:HD21	1.91	0.52
1:C:187:VAL:HG13	1:C:188:SER:N	2.24	0.52
1:F:227:LEU:HD22	1:F:237:VAL:HG12	1.91	0.52
1:B:103:SER:HB3	1:B:112:CYS:HB2	1.90	0.52
1:B:119:LEU:CB	1:B:120:GLU:HB2	2.38	0.52
1:D:227:LEU:HD22	1:D:237:VAL:HG12	1.91	0.52
1:C:238:GLU:HG3	1:C:248:ARG:HD2	1.91	0.52
1:E:50:MET:HB2	1:E:247:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASP:HB3	1:D:60:TYR:CD2	2.44	0.52
1:D:228:LYS:HD2	1:D:236:MET:HE1	1.91	0.52
1:D:241:ILE:HG22	1:D:242:ASP:N	2.25	0.52
1:E:241:ILE:N	1:E:241:ILE:CD1	2.73	0.52
1:E:169:PHE:O	1:E:179:TYR:HA	2.10	0.52
1:E:246:TYR:HD2	1:E:248:ARG:CD	2.22	0.52
1:F:6:VAL:HG11	1:F:12:TRP:CD1	2.45	0.52
1:D:246:TYR:HD2	1:D:248:ARG:HB2	1.74	0.52
1:E:89:SER:HB3	1:E:91:ARG:HH21	1.75	0.52
1:C:15:LEU:HD11	1:C:52:LEU:HD21	1.92	0.51
1:C:32:PRO:HG3	1:C:62:CYS:O	2.10	0.51
1:D:70:LEU:HD23	1:D:99:VAL:HG11	1.92	0.51
1:F:47:LEU:O	1:F:249:TYR:HA	2.10	0.51
1:F:241:ILE:HD13	1:F:246:TYR:CA	2.41	0.51
1:F:30:CYS:SG	1:F:35:LEU:CD2	2.98	0.51
1:C:196:GLU:O	1:C:197:VAL:HG23	2.10	0.51
1:E:119:LEU:HB3	1:E:120:GLU:HB2	1.92	0.51
1:B:43:SER:O	1:B:45:VAL:HG23	2.11	0.51
1:B:53:ARG:HB3	1:B:55:ASP:OD1	2.11	0.51
1:F:205:LEU:HD22	1:F:253:PRO:HB3	1.92	0.51
1:C:6:VAL:HG22	1:C:7:GLN:N	2.25	0.51
1:A:144:PHE:HZ	1:A:212:MET:HE2	1.72	0.51
1:C:132:ASP:C	1:C:133:TYR:CD1	2.84	0.51
1:E:92:HIS:ND1	1:E:93:ASP:N	2.57	0.51
1:F:1:MET:N	1:F:94:ASP:OD2	2.43	0.51
1:F:69:GLY:CA	1:F:121:ILE:HD12	2.39	0.51
1:B:105:ASN:HD22	1:B:110:ARG:H	1.58	0.51
1:C:27:ASN:HA	1:C:69:GLY:HA2	1.93	0.51
1:C:132:ASP:O	1:C:133:TYR:CD1	2.64	0.51
1:F:31:ASN:HB2	1:F:32:PRO:HD3	1.92	0.51
1:B:119:LEU:HB3	1:B:120:GLU:HB2	1.93	0.51
1:C:22:LEU:HD22	1:C:41:ASP:HB3	1.93	0.51
1:C:176:GLY:C	1:C:177:GLN:HG3	2.31	0.51
1:E:215:PHE:CE1	1:E:249:TYR:HB3	2.46	0.51
1:B:228:LYS:HD2	1:B:236:MET:HE1	1.93	0.50
1:C:64:ARG:CG	1:C:64:ARG:NH1	2.73	0.50
1:A:139:LEU:HD23	1:A:139:LEU:H	1.76	0.50
1:B:37:VAL:HG23	1:B:50:MET:HE2	1.92	0.50
1:C:5:GLN:O	1:C:57:PHE:HB3	2.11	0.50
1:E:6:VAL:HG11	1:E:12:TRP:CD1	2.47	0.50
1:F:135:SER:OG	1:F:203:ILE:HG21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ARG:NH1	1:E:201:GLU:HG3	2.26	0.50
1:F:11:LEU:O	1:F:11:LEU:HD12	2.11	0.50
1:F:71:ASN:HB3	1:F:74:SER:OG	2.11	0.50
1:A:161:ALA:HB3	1:A:168:LYS:HB3	1.92	0.50
1:C:15:LEU:CD1	1:C:50:MET:HE2	2.42	0.50
1:E:145:ALA:HA	1:E:216:ALA:HB1	1.93	0.50
1:C:105:ASN:HB3	1:C:108:LYS:HA	1.93	0.50
1:F:4:ALA:O	1:F:90:LEU:N	2.45	0.50
1:F:200:GLU:O	1:F:201:GLU:HG2	2.12	0.50
1:B:28:PHE:CE1	1:B:70:LEU:HD11	2.45	0.50
1:D:57:PHE:N	1:D:57:PHE:CD1	2.80	0.50
1:F:31:ASN:HB2	1:F:32:PRO:CD	2.42	0.50
1:F:130:GLU:CB	1:F:131:MET:CA	2.90	0.50
1:C:30:CYS:HB2	1:C:66:SER:O	2.12	0.49
1:C:210:ARG:O	1:C:214:ILE:HG12	2.13	0.49
1:D:14:ARG:HD2	1:D:220:THR:HB	1.93	0.49
1:F:87:SER:O	1:F:103:SER:HA	2.12	0.49
1:D:246:TYR:CE2	1:D:248:ARG:CZ	2.94	0.49
1:C:201:GLU:HG2	1:C:202:PRO:CD	2.40	0.49
1:B:5:GLN:HB2	1:B:89:SER:OG	2.12	0.49
1:C:179:TYR:CE2	1:F:113:GLU:HB3	2.47	0.49
1:D:54:ASP:CB	1:D:60:TYR:HD2	2.24	0.49
1:E:246:TYR:HD2	1:E:248:ARG:HD2	1.72	0.49
1:F:5:GLN:O	1:F:57:PHE:CD2	2.63	0.49
1:D:134:ARG:CG	1:D:200:GLU:CG	2.86	0.49
1:E:59:LYS:O	1:E:60:TYR:HB2	2.12	0.49
1:F:143:GLU:O	1:F:147:ILE:HG13	2.12	0.49
1:A:7:GLN:O	1:A:87:SER:HA	2.13	0.49
1:B:154:PHE:HB3	1:B:172:SER:HA	1.93	0.49
1:C:124:GLU:HG2	1:C:125:SER:N	2.28	0.49
1:F:28:PHE:CD1	1:F:37:VAL:HG22	2.48	0.49
1:F:246:TYR:CE2	1:F:248:ARG:CZ	2.95	0.49
1:B:57:PHE:CD1	1:B:57:PHE:N	2.80	0.49
1:E:188:SER:OG	1:E:189:ASP:HB3	2.12	0.49
1:D:19:ILE:CG2	1:D:48:VAL:HG11	2.34	0.49
1:C:100:THR:CG2	1:C:115:GLN:HG2	2.25	0.49
1:D:211:PHE:HA	1:D:214:ILE:HG12	1.94	0.49
1:D:215:PHE:CD1	1:D:249:TYR:CD1	3.01	0.49
1:F:119:LEU:HB3	1:F:120:GLU:HB3	1.93	0.49
1:F:203:ILE:CG1	1:F:204:THR:N	2.75	0.48
1:E:140:ASN:HB3	1:E:143:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:TYR:HE1	1:E:62:CYS:HB2	1.78	0.48
1:F:98:VAL:HG13	1:F:116:LEU:O	2.12	0.48
1:B:228:LYS:HD2	1:B:236:MET:CE	2.43	0.48
1:D:133:TYR:CD2	1:D:230:ALA:HB1	2.49	0.48
1:E:67:ILE:O	1:E:68:LEU:HD23	2.12	0.48
1:F:30:CYS:SG	1:F:35:LEU:HD21	2.53	0.48
1:B:58:VAL:HG23	1:B:59:LYS:H	1.78	0.48
1:D:124:GLU:OE1	1:D:124:GLU:HA	2.12	0.48
1:E:15:LEU:O	1:E:19:ILE:HG22	2.13	0.48
1:F:162:ILE:HD11	1:F:229:PHE:CE1	2.48	0.48
1:B:216:ALA:HA	1:B:239:TYR:OH	2.14	0.48
1:C:18:CYS:HB3	1:C:249:TYR:OH	2.13	0.48
1:D:134:ARG:CB	1:D:200:GLU:CG	2.91	0.48
1:A:201:GLU:HB3	1:A:202:PRO:HD2	1.95	0.48
1:D:236:MET:SD	1:D:248:ARG:HD2	2.53	0.48
1:F:207:PHE:CD2	1:F:251:LEU:HD23	2.45	0.48
1:C:118:LEU:HD12	1:C:118:LEU:H	1.78	0.48
1:E:64:ARG:NH1	1:E:64:ARG:HA	2.29	0.48
1:C:15:LEU:HD22	1:C:50:MET:HE2	1.95	0.48
1:D:45:VAL:HG12	1:D:45:VAL:O	2.12	0.48
1:E:133:TYR:CD1	1:E:133:TYR:C	2.87	0.48
1:E:241:ILE:HG22	1:E:244:VAL:HG22	1.84	0.48
1:A:53:ARG:O	1:A:56:CYS:HB3	2.14	0.47
1:A:102:THR:HG23	1:A:113:GLU:HG3	1.95	0.47
1:D:56:CYS:CB	1:D:244:VAL:HB	2.38	0.47
1:B:129:PRO:C	1:B:130:GLU:OE1	2.52	0.47
1:C:158:VAL:HG13	1:C:158:VAL:O	2.14	0.47
1:D:16:VAL:HG21	1:D:79:LEU:HD11	1.96	0.47
1:D:199:MET:HG2	1:D:200:GLU:N	2.29	0.47
1:D:203:ILE:HG23	1:D:203:ILE:O	2.14	0.47
1:E:143:GLU:O	1:E:147:ILE:HG13	2.15	0.47
1:B:16:VAL:HG21	1:B:79:LEU:HD12	1.97	0.47
1:C:55:ASP:C	1:C:55:ASP:OD1	2.53	0.47
1:D:164:LYS:CG	1:D:165:GLU:HG3	2.43	0.47
1:E:128:ILE:HG22	1:E:130:GLU:HG3	1.95	0.47
1:B:15:LEU:CD1	1:B:50:MET:SD	3.03	0.47
1:B:98:VAL:HG12	1:B:99:VAL:N	2.29	0.47
1:B:163:SER:O	1:B:164:LYS:C	2.53	0.47
1:C:10:SER:HB3	1:C:14:ARG:NH1	2.30	0.47
1:C:99:VAL:HG12	1:C:118:LEU:HD23	1.96	0.47
1:C:144:PHE:O	1:C:148:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:O	1:C:210:ARG:C	2.53	0.47
1:E:6:VAL:CG2	1:E:7:GLN:N	2.78	0.47
1:E:40:MET:HG2	1:E:47:LEU:HD22	1.97	0.47
1:E:207:PHE:CE2	1:E:235:CYS:SG	3.08	0.47
1:F:130:GLU:HB3	1:F:131:MET:CB	2.44	0.47
1:F:206:SER:C	1:F:207:PHE:CD1	2.88	0.47
1:A:126:MET:HG3	1:A:127:GLY:H	1.80	0.47
1:A:197:VAL:HG12	1:A:198:THR:N	2.29	0.47
1:B:227:LEU:HA	1:B:236:MET:O	2.15	0.47
1:C:43:SER:HB2	1:C:45:VAL:HG12	1.96	0.47
1:D:218:GLY:O	1:D:221:LEU:HB2	2.15	0.47
1:E:14:ARG:HD2	1:E:220:THR:HB	1.97	0.47
1:E:118:LEU:O	1:E:119:LEU:HD23	2.12	0.47
1:F:15:LEU:O	1:F:19:ILE:HG23	2.14	0.47
1:C:60:TYR:CD1	1:C:61:GLN:N	2.83	0.47
1:C:131:MET:HB3	1:C:132:ASP:CA	2.44	0.47
1:E:118:LEU:C	1:E:118:LEU:HD12	2.35	0.47
1:F:19:ILE:HD11	1:F:72:LEU:CD1	2.45	0.47
1:A:160:ILE:HG12	1:A:169:PHE:CD1	2.50	0.47
1:F:16:VAL:CG2	1:F:79:LEU:CD1	2.88	0.47
1:F:243:ASN:HD22	1:F:243:ASN:HA	1.57	0.46
1:B:229:PHE:N	1:B:229:PHE:CD1	2.84	0.46
1:D:54:ASP:HB2	1:D:60:TYR:CD2	2.48	0.46
1:D:69:GLY:O	1:D:118:LEU:HB2	2.15	0.46
1:D:213:GLY:O	1:D:214:ILE:C	2.52	0.46
1:B:231:LYS:O	1:B:232:ASP:HB2	2.13	0.46
1:D:130:GLU:OE2	1:D:130:GLU:N	2.48	0.46
1:B:177:GLN:O	1:C:114:TYR:HA	2.16	0.46
1:E:230:ALA:O	1:E:231:LYS:C	2.54	0.46
1:F:4:ALA:O	1:F:89:SER:HA	2.16	0.46
1:A:22:LEU:CD1	1:A:48:VAL:CG2	2.88	0.46
1:B:82:VAL:HG11	1:B:88:LEU:HD13	1.98	0.46
1:C:187:VAL:O	1:C:188:SER:C	2.53	0.46
1:A:47:LEU:HD23	1:A:250:TYR:CD1	2.50	0.46
1:A:138:THR:HG23	1:A:226:THR:OG1	2.15	0.46
1:F:153:VAL:O	1:F:175:VAL:HG21	2.15	0.46
1:C:28:PHE:CD1	1:C:37:VAL:HG22	2.51	0.46
1:D:40:MET:HG2	1:D:47:LEU:HD22	1.98	0.46
1:C:237:VAL:HG22	1:C:249:TYR:HB2	1.97	0.46
1:D:6:VAL:HG22	1:D:7:GLN:N	2.30	0.46
1:F:94:ASP:OD1	1:F:94:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ALA:HA	1:C:216:ALA:HB1	1.98	0.46
1:E:78:VAL:O	1:E:82:VAL:HG23	2.16	0.46
1:E:90:LEU:HD12	1:E:90:LEU:HA	1.62	0.46
1:C:135:SER:OG	1:C:203:ILE:CG2	2.64	0.45
1:D:241:ILE:CG2	1:D:242:ASP:N	2.79	0.45
1:E:57:PHE:CD1	1:E:57:PHE:N	2.82	0.45
1:F:212:MET:O	1:F:215:PHE:HB2	2.16	0.45
1:B:15:LEU:HD13	1:B:50:MET:SD	2.57	0.45
1:E:60:TYR:CE1	1:E:62:CYS:HB2	2.51	0.45
1:E:237:VAL:HG22	1:E:249:TYR:HB2	1.99	0.45
1:B:182:LEU:HD23	1:C:110:ARG:HB2	1.97	0.45
1:E:2:LEU:HD23	1:E:3:GLU:N	2.30	0.45
1:F:119:LEU:HB2	1:F:121:ILE:HG13	1.91	0.45
1:A:140:ASN:HB3	1:A:143:GLU:HB3	1.99	0.45
1:B:28:PHE:CD1	1:B:28:PHE:N	2.82	0.45
1:D:216:ALA:HA	1:D:239:TYR:OH	2.17	0.45
1:F:130:GLU:HG3	1:F:131:MET:CB	2.46	0.45
1:A:209:LEU:O	1:A:210:ARG:C	2.55	0.45
1:C:87:SER:O	1:C:103:SER:HA	2.16	0.45
1:D:50:MET:HE2	1:D:52:LEU:HG	1.96	0.45
1:E:22:LEU:HD12	1:E:48:VAL:HG23	1.95	0.45
1:A:55:ASP:OD1	1:A:55:ASP:N	2.48	0.45
1:D:225:VAL:HG21	1:D:239:TYR:CZ	2.52	0.45
1:F:21:GLY:O	1:F:214:ILE:HD12	2.17	0.45
1:F:35:LEU:HD12	1:F:57:PHE:CZ	2.52	0.45
1:A:2:LEU:O	1:A:91:ARG:HA	2.17	0.45
1:A:46:ALA:HA	1:A:250:TYR:O	2.16	0.45
1:B:131:MET:HG2	1:B:132:ASP:CA	2.38	0.45
1:C:227:LEU:HB2	1:C:229:PHE:HE1	1.81	0.45
1:D:132:ASP:C	1:D:133:TYR:HD1	2.20	0.45
1:E:216:ALA:HA	1:E:239:TYR:OH	2.16	0.45
1:C:217:LYS:O	1:C:220:THR:HG23	2.17	0.45
1:C:246:TYR:CD1	1:C:248:ARG:NE	2.85	0.45
1:D:11:LEU:HG	1:D:15:LEU:HD12	1.98	0.45
1:E:60:TYR:CD1	1:E:61:GLN:N	2.84	0.44
1:A:12:TRP:O	1:A:16:VAL:HG23	2.16	0.44
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.83	0.44
1:B:51:LEU:HB3	1:B:246:TYR:CE2	2.51	0.44
1:E:36:SER:HA	1:E:50:MET:O	2.18	0.44
1:F:94:ASP:CB	2:F:303:HOH:O	2.65	0.44
1:F:241:ILE:HG22	1:F:242:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:LEU:CB	1:F:120:GLU:HB3	2.47	0.44
1:A:130:GLU:CB	1:A:131:MET:CA	2.92	0.44
1:B:199:MET:HG3	1:B:201:GLU:O	2.17	0.44
1:B:207:PHE:CZ	1:B:235:CYS:HB3	2.52	0.44
1:D:12:TRP:O	1:D:16:VAL:HG23	2.17	0.44
1:D:40:MET:CE	1:D:44:HIS:HA	2.47	0.44
1:E:16:VAL:HA	1:E:19:ILE:HG23	2.00	0.44
1:C:133:TYR:O	1:C:134:ARG:HB2	2.18	0.44
1:C:187:VAL:CG1	1:C:188:SER:N	2.80	0.44
1:E:16:VAL:O	1:E:20:ASN:HB2	2.16	0.44
1:E:242:ASP:OD1	1:E:242:ASP:N	2.50	0.44
1:A:78:VAL:O	1:A:81:ILE:HG12	2.18	0.44
1:B:35:LEU:O	1:B:51:LEU:HD12	2.18	0.44
1:B:134:ARG:HD3	1:B:201:GLU:HG3	1.97	0.44
1:D:133:TYR:CD1	1:D:133:TYR:N	2.85	0.44
1:D:230:ALA:O	1:D:231:LYS:C	2.55	0.44
1:B:230:ALA:HB3	1:B:233:SER:HB3	1.99	0.44
1:C:189:ASP:O	1:C:190:ARG:HD3	2.17	0.44
1:E:246:TYR:CE2	1:E:248:ARG:CD	3.00	0.44
1:A:40:MET:HG3	1:A:47:LEU:HD12	1.99	0.44
1:A:48:VAL:HG13	1:A:249:TYR:CE1	2.53	0.44
1:B:160:ILE:O	1:B:204:THR:HA	2.18	0.44
1:D:236:MET:CE	1:D:238:GLU:HB2	2.41	0.44
1:E:70:LEU:CD2	1:E:99:VAL:HG11	2.41	0.44
1:F:61:GLN:HE21	1:F:61:GLN:HB3	1.58	0.44
1:C:7:GLN:NE2	1:C:8:PHE:CE1	2.86	0.43
1:C:132:ASP:HB3	1:C:133:TYR:HD1	1.83	0.43
1:F:98:VAL:HA	1:F:118:LEU:CD2	2.47	0.43
1:A:71:ASN:OD1	1:A:73:ALA:HB3	2.18	0.43
1:C:64:ARG:NH1	1:C:64:ARG:HG2	2.32	0.43
1:D:215:PHE:CD1	1:D:249:TYR:CG	3.07	0.43
1:E:105:ASN:OD1	1:E:109:THR:HG23	2.18	0.43
1:F:1:MET:N	1:F:94:ASP:CG	2.71	0.43
1:C:180:THR:HG22	1:C:182:LEU:HD12	2.00	0.43
1:D:164:LYS:HA	1:D:199:MET:HE1	2.00	0.43
1:E:148:VAL:HG21	1:E:213:GLY:HA2	1.99	0.43
1:F:74:SER:O	1:F:78:VAL:HG23	2.18	0.43
1:B:28:PHE:CE1	1:B:70:LEU:CD1	3.02	0.43
1:E:38:GLN:HE21	1:E:38:GLN:HB2	1.61	0.43
1:B:55:ASP:OD1	1:B:55:ASP:N	2.52	0.43
1:F:186:GLY:HA3	1:F:187:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LEU:HB3	1:D:250:TYR:HB2	2.01	0.43
1:F:79:LEU:HD23	1:F:79:LEU:HA	1.80	0.43
1:A:144:PHE:O	1:A:148:VAL:HG13	2.18	0.43
1:C:15:LEU:HD22	1:C:50:MET:HE3	2.01	0.43
1:D:154:PHE:O	1:D:173:GLY:HA3	2.18	0.43
1:E:119:LEU:CB	1:E:120:GLU:HB2	2.49	0.43
1:F:215:PHE:CE1	1:F:249:TYR:HB3	2.53	0.43
1:D:222:SER:HB2	1:D:240:GLY:O	2.18	0.43
1:E:6:VAL:CG2	1:E:7:GLN:H	2.32	0.43
1:F:241:ILE:HD12	1:F:241:ILE:H	1.83	0.43
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.87	0.43
1:A:144:PHE:CZ	1:A:212:MET:HE2	2.50	0.43
1:B:166:GLY:HA2	1:B:183:GLN:HA	2.01	0.43
1:C:236:MET:HE3	1:C:248:ARG:HG3	2.01	0.43
1:D:105:ASN:ND2	1:D:110:ARG:HB3	2.34	0.43
1:D:153:VAL:O	1:D:175:VAL:HG21	2.17	0.43
1:E:50:MET:HE1	1:E:52:LEU:HG	1.87	0.43
1:F:246:TYR:CZ	1:F:248:ARG:NH2	2.87	0.43
1:B:210:ARG:O	1:B:214:ILE:HG13	2.18	0.42
1:C:196:GLU:OE2	1:C:196:GLU:N	2.52	0.42
1:D:81:ILE:HD11	1:D:114:TYR:HH	1.82	0.42
1:D:233:SER:O	1:D:253:PRO:HG3	2.19	0.42
1:D:237:VAL:CG2	1:D:249:TYR:HB2	2.37	0.42
1:F:30:CYS:O	1:F:65:ASN:HA	2.19	0.42
1:A:50:MET:CE	1:A:52:LEU:HG	2.50	0.42
1:C:124:GLU:O	1:C:125:SER:HB2	2.20	0.42
1:C:139:LEU:HD23	1:C:139:LEU:N	2.33	0.42
1:D:3:GLU:HA	1:D:90:LEU:O	2.19	0.42
1:D:93:ASP:O	1:D:94:ASP:C	2.58	0.42
1:D:107:GLU:OE1	1:D:107:GLU:N	2.43	0.42
1:D:148:VAL:HG23	1:D:149:ARG:N	2.34	0.42
1:D:246:TYR:CE2	1:D:248:ARG:NH2	2.87	0.42
1:D:246:TYR:CZ	1:D:248:ARG:NH2	2.87	0.42
1:C:62:CYS:O	1:C:63:GLY:O	2.36	0.42
1:C:131:MET:CB	1:C:132:ASP:HA	2.45	0.42
1:D:135:SER:HA	1:D:199:MET:HB2	2.00	0.42
1:D:246:TYR:CD2	1:D:248:ARG:HB2	2.53	0.42
1:C:60:TYR:HE1	1:C:62:CYS:HB2	1.85	0.42
1:D:87:SER:O	1:D:103:SER:HA	2.19	0.42
1:D:156:ASP:OD1	1:D:156:ASP:N	2.51	0.42
1:E:38:GLN:O	1:E:39:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ARG:O	1:E:56:CYS:HB3	2.20	0.42
1:F:69:GLY:HA2	1:F:121:ILE:HD12	2.02	0.42
1:F:101:LEU:HD12	1:F:101:LEU:N	2.32	0.42
1:A:6:VAL:HG22	1:A:7:GLN:N	2.34	0.42
1:C:132:ASP:O	1:C:133:TYR:CG	2.72	0.42
1:E:67:ILE:C	1:E:68:LEU:HD23	2.40	0.42
1:B:92:HIS:CD2	1:B:98:VAL:O	2.67	0.42
1:E:236:MET:CE	1:E:238:GLU:OE1	2.68	0.42
1:F:133:TYR:CG	1:F:228:LYS:HB3	2.55	0.42
1:B:175:VAL:HG13	1:C:74:SER:HB3	2.00	0.42
1:C:106:PRO:O	1:C:107:GLU:CD	2.57	0.42
1:E:17:GLU:HB3	1:E:217:LYS:HE2	2.01	0.42
1:A:12:TRP:CD1	1:A:88:LEU:HD23	2.54	0.42
1:C:19:ILE:HG21	1:C:19:ILE:HD13	1.51	0.42
1:C:122:GLU:H	1:C:122:GLU:CD	2.10	0.42
1:D:24:ASN:OD1	1:D:24:ASN:N	2.48	0.42
1:D:234:PRO:HA	1:D:251:LEU:O	2.19	0.42
1:F:51:LEU:CD2	1:F:246:TYR:HE1	2.18	0.42
1:D:19:ILE:HG23	1:D:19:ILE:HD13	1.66	0.42
1:A:147:ILE:CD1	1:A:182:LEU:HD11	2.50	0.41
1:A:147:ILE:O	1:A:151:MET:HG2	2.20	0.41
1:B:138:THR:HA	1:B:225:VAL:O	2.19	0.41
1:C:166:GLY:HA2	1:C:182:LEU:O	2.20	0.41
1:F:2:LEU:HD23	1:F:2:LEU:O	2.20	0.41
1:F:98:VAL:HA	1:F:118:LEU:HD23	2.02	0.41
1:F:104:GLU:HB3	1:F:108:LYS:CE	2.42	0.41
1:C:146:LYS:HD3	1:C:150:ASP:OD2	2.20	0.41
1:D:13:LYS:HD2	1:D:82:VAL:O	2.20	0.41
1:F:215:PHE:CD1	1:F:249:TYR:CG	3.08	0.41
1:D:118:LEU:CA	1:D:119:LEU:HD23	2.49	0.41
1:E:15:LEU:CD2	1:E:247:LEU:HD13	2.50	0.41
1:F:17:GLU:HB3	1:F:217:LYS:HE3	2.01	0.41
1:C:22:LEU:CD1	1:C:48:VAL:HG23	2.45	0.41
1:F:236:MET:SD	1:F:248:ARG:HG2	2.61	0.41
1:A:115:GLN:HB2	1:D:177:GLN:HG3	2.02	0.41
1:E:140:ASN:HB3	1:E:143:GLU:CB	2.51	0.41
1:F:5:GLN:HA	1:F:89:SER:HA	2.02	0.41
1:A:135:SER:OG	1:A:203:ILE:HG21	2.20	0.41
1:B:197:VAL:HG12	1:B:199:MET:HE2	2.03	0.41
1:C:118:LEU:HD12	1:C:118:LEU:N	2.33	0.41
1:D:134:ARG:HH11	1:D:134:ARG:CG	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:HA	1:A:189:ASP:HA	1.72	0.41
1:B:134:ARG:HA	1:B:200:GLU:CB	2.36	0.41
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.84	0.41
1:D:19:ILE:HD12	1:D:19:ILE:HG21	1.70	0.41
1:E:68:LEU:HD13	1:E:92:HIS:HD2	1.86	0.41
1:A:6:VAL:CG2	1:A:7:GLN:N	2.84	0.41
1:B:37:VAL:HG23	1:B:50:MET:CE	2.51	0.41
1:B:119:LEU:HB3	1:B:120:GLU:CB	2.50	0.41
1:E:105:ASN:HB3	1:E:108:LYS:N	2.36	0.41
1:E:153:VAL:HG23	1:E:154:PHE:CD1	2.56	0.41
1:F:132:ASP:OD1	1:F:133:TYR:N	2.54	0.41
1:F:209:LEU:HD23	1:F:209:LEU:HA	1.80	0.41
1:B:22:LEU:HD23	1:B:23:VAL:HG13	2.02	0.41
1:E:89:SER:CB	1:E:91:ARG:HH21	2.33	0.41
1:E:235:CYS:O	1:E:250:TYR:HA	2.21	0.41
1:F:5:GLN:HE21	1:F:58:VAL:HG21	1.85	0.41
1:F:27:ASN:OD1	1:F:67:ILE:HG22	2.20	0.41
1:F:186:GLY:HA2	1:F:187:VAL:HA	1.91	0.41
1:D:225:VAL:CG2	1:D:239:TYR:CE2	3.04	0.40
1:A:17:GLU:O	1:A:18:CYS:C	2.60	0.40
1:A:25:GLU:HB2	1:A:121:ILE:HD11	2.04	0.40
1:B:233:SER:O	1:B:234:PRO:C	2.58	0.40
1:D:246:TYR:CD2	1:D:248:ARG:CZ	3.05	0.40
1:E:147:ILE:HG13	1:E:147:ILE:H	1.60	0.40
1:B:134:ARG:HH11	1:B:201:GLU:CG	2.12	0.40
1:F:165:GLU:N	1:F:165:GLU:OE2	2.54	0.40
1:D:126:MET:C	1:D:127:GLY:O	2.58	0.40
1:D:131:MET:HB3	1:D:133:TYR:HE1	1.86	0.40
1:F:216:ALA:HA	1:F:239:TYR:OH	2.21	0.40
1:A:201:GLU:CB	1:A:202:PRO:HD2	2.51	0.40
1:D:81:ILE:HD11	1:D:114:TYR:CZ	2.56	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	249/259 (96%)	228 (92%)	21 (8%)	0	100	100
1	B	249/259 (96%)	227 (91%)	22 (9%)	0	100	100
1	C	249/259 (96%)	216 (87%)	32 (13%)	1 (0%)	34	69
1	D	249/259 (96%)	221 (89%)	26 (10%)	2 (1%)	19	58
1	E	249/259 (96%)	217 (87%)	29 (12%)	3 (1%)	13	49
1	F	249/259 (96%)	219 (88%)	29 (12%)	1 (0%)	34	69
All	All	1494/1554 (96%)	1328 (89%)	159 (11%)	7 (0%)	29	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	63	GLY
1	D	127	GLY
1	E	54	ASP
1	D	95	ASP
1	E	2	LEU
1	F	63	GLY
1	E	175	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	220/225 (98%)	172 (78%)	48 (22%)	1	5
1	B	220/225 (98%)	179 (81%)	41 (19%)	1	8
1	C	220/225 (98%)	172 (78%)	48 (22%)	1	5
1	D	220/225 (98%)	174 (79%)	46 (21%)	1	6
1	E	220/225 (98%)	170 (77%)	50 (23%)	1	4
1	F	220/225 (98%)	166 (76%)	54 (24%)	0	2
All	All	1320/1350 (98%)	1033 (78%)	287 (22%)	1	5

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	13	LYS
1	A	15	LEU
1	A	19	ILE
1	A	29	ASP
1	A	36	SER
1	A	40	MET
1	A	41	ASP
1	A	45	VAL
1	A	48	VAL
1	A	50	MET
1	A	53	ARG
1	A	54	ASP
1	A	56	CYS
1	A	64	ARG
1	A	74	SER
1	A	80	LYS
1	A	84	SER
1	A	89	SER
1	A	97	ASP
1	A	100	THR
1	A	102	THR
1	A	103	SER
1	A	107	GLU
1	A	109	THR
1	A	111	LYS
1	A	116	LEU
1	A	120	GLU
1	A	128	ILE
1	A	130	GLU
1	A	134	ARG
1	A	137	VAL
1	A	146	LYS
1	A	148	VAL
1	A	149	ARG
1	A	168	LYS
1	A	170	SER
1	A	183	GLN
1	A	187	VAL
1	A	199	MET
1	A	200	GLU
1	A	206	SER

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Mol	Chain	Res	Type
1	A	210	ARG
1	A	220	THR
1	A	231	LYS
1	A	232	ASP
1	A	248	ARG
1	A	254	LYS
1	B	15	LEU
1	B	19	ILE
1	B	22	LEU
1	B	24	ASN
1	B	25	GLU
1	B	29	ASP
1	B	47	LEU
1	B	48	VAL
1	B	50	MET
1	B	64	ARG
1	B	65	ASN
1	B	70	LEU
1	B	95	ASP
1	B	102	THR
1	B	104	GLU
1	B	109	THR
1	B	115	GLN
1	B	116	LEU
1	B	119	LEU
1	B	131	MET
1	B	135	SER
1	B	137	VAL
1	B	139	LEU
1	B	162	ILE
1	B	163	SER
1	B	164	LYS
1	B	168	LYS
1	B	170	SER
1	B	188	SER
1	B	190	ARG
1	B	198	THR
1	B	199	MET
1	B	206	SER
1	B	210	ARG
1	B	217	LYS
1	B	227	LEU

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Mol	Chain	Res	Type
1	B	229	PHE
1	B	232	ASP
1	B	237	VAL
1	B	248	ARG
1	B	256	ASP
1	C	2	LEU
1	C	3	GLU
1	C	10	SER
1	C	19	ILE
1	C	22	LEU
1	C	42	SER
1	C	47	LEU
1	C	50	MET
1	C	53	ARG
1	C	57	PHE
1	C	61	GLN
1	C	62	CYS
1	C	64	ARG
1	C	65	ASN
1	C	70	LEU
1	C	89	SER
1	C	95	ASP
1	C	97	ASP
1	C	99	VAL
1	C	102	THR
1	C	107	GLU
1	C	108	LYS
1	C	109	THR
1	C	118	LEU
1	C	126	MET
1	C	128	ILE
1	C	134	ARG
1	C	135	SER
1	C	137	VAL
1	C	148	VAL
1	C	153	VAL
1	C	159	THR
1	C	163	SER
1	C	170	SER
1	C	188	SER
1	C	190	ARG
1	C	196	GLU

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Mol	Chain	Res	Type
1	C	198	THR
1	C	199	MET
1	C	206	SER
1	C	217	LYS
1	C	233	SER
1	C	235	CYS
1	C	236	MET
1	C	237	VAL
1	C	243	ASN
1	C	248	ARG
1	C	256	ASP
1	D	2	LEU
1	D	3	GLU
1	D	7	GLN
1	D	10	SER
1	D	15	LEU
1	D	19	ILE
1	D	22	LEU
1	D	25	GLU
1	D	29	ASP
1	D	31	ASN
1	D	35	LEU
1	D	36	SER
1	D	38	GLN
1	D	47	LEU
1	D	50	MET
1	D	53	ARG
1	D	57	PHE
1	D	70	LEU
1	D	81	ILE
1	D	89	SER
1	D	90	LEU
1	D	94	ASP
1	D	97	ASP
1	D	99	VAL
1	D	102	THR
1	D	119	LEU
1	D	121	ILE
1	D	125	SER
1	D	126	MET
1	D	133	TYR
1	D	134	ARG

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Mol	Chain	Res	Type
1	D	162	ILE
1	D	163	SER
1	D	164	LYS
1	D	168	LYS
1	D	170	SER
1	D	177	GLN
1	D	189	ASP
1	D	190	ARG
1	D	198	THR
1	D	199	MET
1	D	201	GLU
1	D	217	LYS
1	D	228	LYS
1	D	232	ASP
1	D	243	ASN
1	E	1	MET
1	E	19	ILE
1	E	22	LEU
1	E	24	ASN
1	E	36	SER
1	E	42	SER
1	E	45	VAL
1	E	47	LEU
1	E	50	MET
1	E	51	LEU
1	E	53	ARG
1	E	62	CYS
1	E	64	ARG
1	E	70	LEU
1	E	80	LYS
1	E	94	ASP
1	E	95	ASP
1	E	99	VAL
1	E	100	THR
1	E	105	ASN
1	E	108	LYS
1	E	109	THR
1	E	119	LEU
1	E	121	ILE
1	E	128	ILE
1	E	130	GLU
1	E	132	ASP

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Mol	Chain	Res	Type
1	E	133	TYR
1	E	134	ARG
1	E	137	VAL
1	E	139	LEU
1	E	143	GLU
1	E	153	VAL
1	E	156	ASP
1	E	164	LYS
1	E	167	VAL
1	E	168	LYS
1	E	170	SER
1	E	181	PHE
1	E	188	SER
1	E	189	ASP
1	E	199	MET
1	E	212	MET
1	E	217	LYS
1	E	220	THR
1	E	222	SER
1	E	235	CYS
1	E	243	ASN
1	E	248	ARG
1	E	251	LEU
1	F	2	LEU
1	F	6	VAL
1	F	7	GLN
1	F	19	ILE
1	F	22	LEU
1	F	45	VAL
1	F	47	LEU
1	F	50	MET
1	F	51	LEU
1	F	59	LYS
1	F	61	GLN
1	F	62	CYS
1	F	64	ARG
1	F	70	LEU
1	F	74	SER
1	F	76	SER
1	F	91	ARG
1	F	93	ASP
1	F	94	ASP

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Mol	Chain	Res	Type
1	F	97	ASP
1	F	99	VAL
1	F	100	THR
1	F	104	GLU
1	F	108	LYS
1	F	116	LEU
1	F	118	LEU
1	F	119	LEU
1	F	120	GLU
1	F	121	ILE
1	F	126	MET
1	F	130	GLU
1	F	131	MET
1	F	132	ASP
1	F	135	SER
1	F	136	THR
1	F	137	VAL
1	F	148	VAL
1	F	156	ASP
1	F	164	LYS
1	F	165	GLU
1	F	167	VAL
1	F	168	LYS
1	F	170	SER
1	F	187	VAL
1	F	190	ARG
1	F	198	THR
1	F	199	MET
1	F	200	GLU
1	F	217	LYS
1	F	231	LYS
1	F	232	ASP
1	F	233	SER
1	F	242	ASP
1	F	243	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	44	HIS
1	A	49	HIS

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Mol	Chain	Res	Type
1	A	105	ASN
1	A	115	GLN
1	A	243	ASN
1	B	7	GLN
1	B	31	ASN
1	B	92	HIS
1	B	183	GLN
1	C	7	GLN
1	C	31	ASN
1	C	44	HIS
1	C	115	GLN
1	C	183	GLN
1	C	243	ASN
1	D	27	ASN
1	D	31	ASN
1	D	38	GLN
1	D	61	GLN
1	D	105	ASN
1	D	115	GLN
1	D	183	GLN
1	D	243	ASN
1	E	20	ASN
1	E	38	GLN
1	E	44	HIS
1	E	49	HIS
1	E	115	GLN
1	E	243	ASN
1	F	44	HIS
1	F	61	GLN
1	F	115	GLN
1	F	243	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	253/259 (97%)	0.05	9 (3%)	42	27	57, 85, 159, 259	0
1	B	253/259 (97%)	-0.05	7 (2%)	53	37	57, 89, 164, 215	0
1	C	253/259 (97%)	0.08	10 (3%)	38	25	60, 97, 165, 261	0
1	D	253/259 (97%)	0.07	7 (2%)	53	37	68, 102, 166, 249	0
1	E	253/259 (97%)	0.13	9 (3%)	42	27	69, 105, 178, 235	0
1	F	253/259 (97%)	0.04	7 (2%)	53	37	67, 108, 169, 244	0
All	All	1518/1554 (97%)	0.05	49 (3%)	47	31	57, 98, 169, 261	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	VAL	8.2
1	A	186	GLY	8.1
1	A	188	SER	7.2
1	F	188	SER	7.2
1	F	187	VAL	6.4
1	A	187	VAL	6.3
1	D	188	SER	6.3
1	D	190	ARG	6.3
1	A	256	ASP	6.1
1	E	186	GLY	5.7
1	E	187	VAL	5.3
1	C	188	SER	5.1
1	C	189	ASP	4.8
1	E	188	SER	4.8
1	A	189	ASP	4.7
1	C	187	VAL	4.5
1	B	187	VAL	4.4
1	F	189	ASP	4.3
1	D	189	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	186	GLY	3.9
1	E	189	ASP	3.8
1	C	186	GLY	3.8
1	A	190	ARG	3.4
1	E	185	ALA	3.3
1	C	167	VAL	3.2
1	B	188	SER	3.1
1	A	255	VAL	3.1
1	D	133	TYR	3.0
1	B	186	GLY	3.0
1	B	134	ARG	2.9
1	B	190	ARG	2.9
1	F	185	ALA	2.8
1	B	189	ASP	2.6
1	C	166	GLY	2.6
1	A	185	ALA	2.6
1	D	186	GLY	2.6
1	B	185	ALA	2.6
1	E	256	ASP	2.6
1	E	190	ARG	2.5
1	A	199	MET	2.5
1	E	114	TYR	2.3
1	C	161	ALA	2.3
1	C	190	ARG	2.2
1	F	229	PHE	2.2
1	F	190	ARG	2.2
1	D	205	LEU	2.1
1	C	162	ILE	2.1
1	C	169	PHE	2.1
1	E	197	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.