Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID	:	1G8Y
Title	:	CRYSTAL STRUCTURE OF THE HEXAMERIC REPLICATIVE HELICASE REPA OF PLASMID RSF1010
Authors	:	Niedenzu, T.; Roeleke, D.; Bains, G.; Scherzinger, E.; Saenger, W.
Deposited on	:	2000-11-21
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

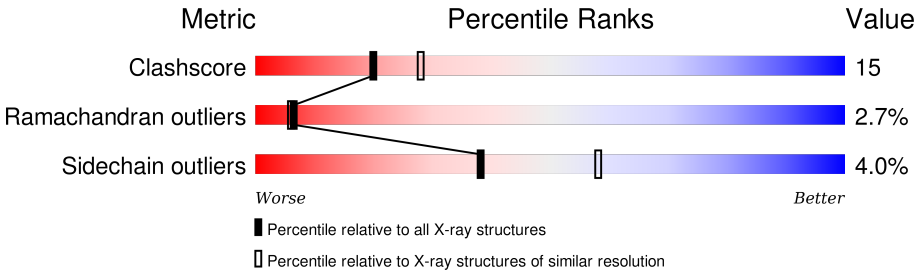
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	62% 23% • 13%
1	B	279	60% 22% 5% 13%
1	C	279	62% 21% • 13%
1	D	279	63% 21% • 13%
1	E	279	62% 22% • 13%
1	F	279	66% 19% •• 13%
1	G	279	62% 20% • 13%

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Mol	Chain	Length	Quality of chain
1	H	279	
1	I	279	
1	J	279	
1	K	279	
1	L	279	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22536 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 REGULATORY PROTEIN REPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	B	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	C	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	D	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	E	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	F	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	G	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	H	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	I	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	J	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	K	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			
1	L	242	Total	C	N	O	S	0	0	0
			1838	1170	327	333	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	40	Total	O	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	40	Total O 40 40	0	0
2	D	39	Total O 39 39	0	0
2	E	41	Total O 41 41	0	0
2	F	39	Total O 39 39	0	0
2	G	41	Total O 41 41	0	0
2	H	38	Total O 38 38	0	0
2	I	41	Total O 41 41	0	0
2	J	41	Total O 41 41	0	0
2	K	38	Total O 38 38	0	0
2	L	41	Total O 41 41	0	0

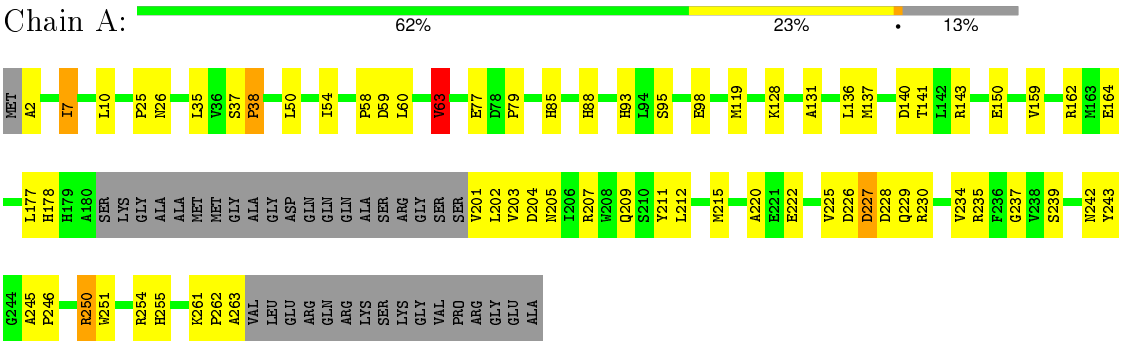
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

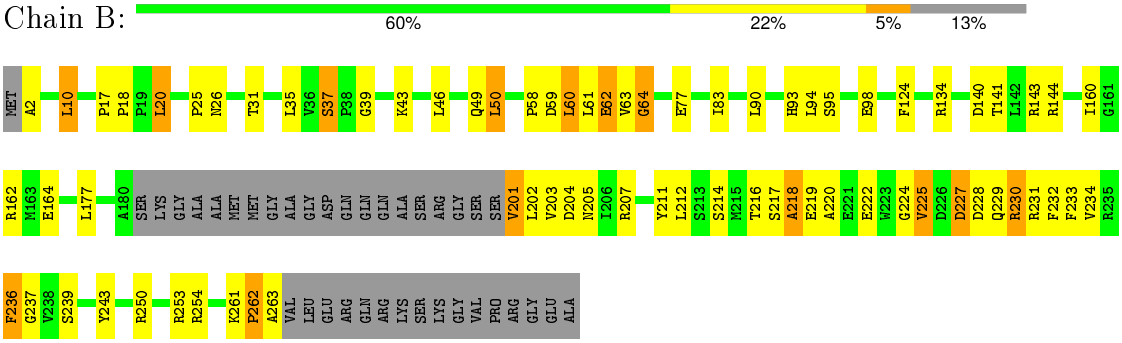
• Molecule 1: REGULATORY PROTEIN REPA

Chain A:



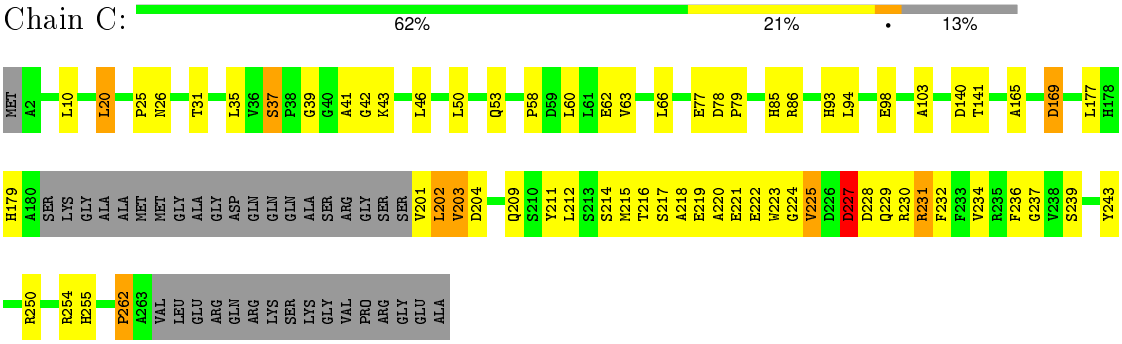
• Molecule 1: REGULATORY PROTEIN REPA

Chain B:



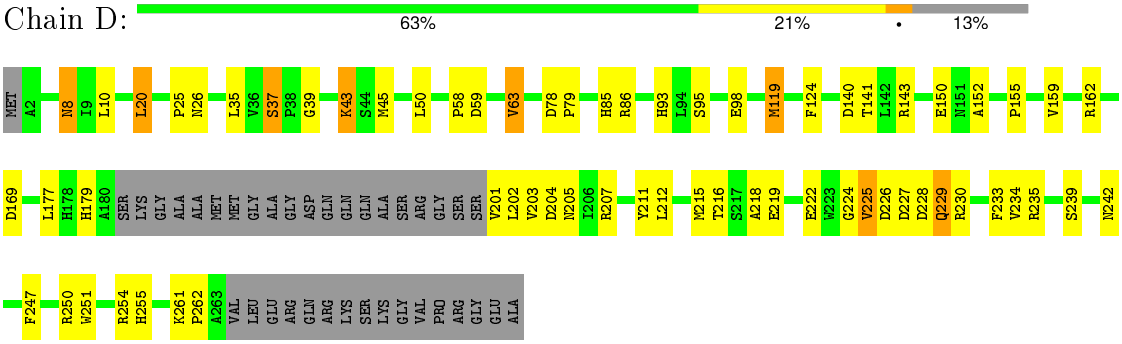
• Molecule 1: REGULATORY PROTEIN REPA

Chain C:



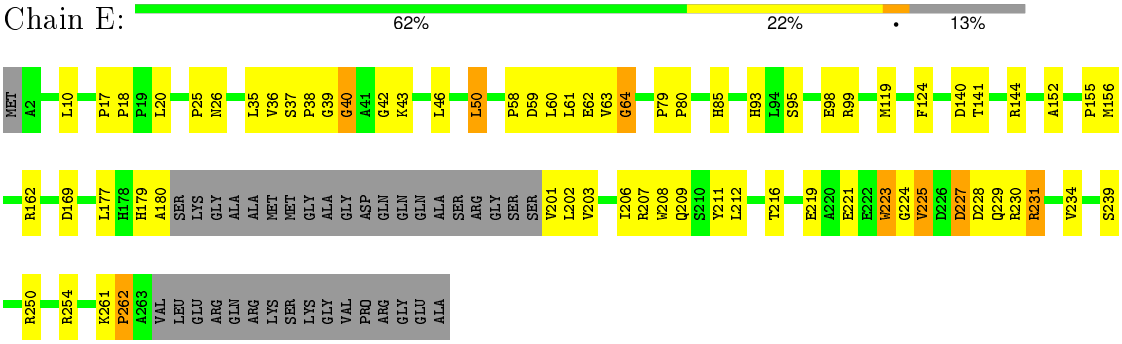
• Molecule 1: REGULATORY PROTEIN REPA

Chain D:



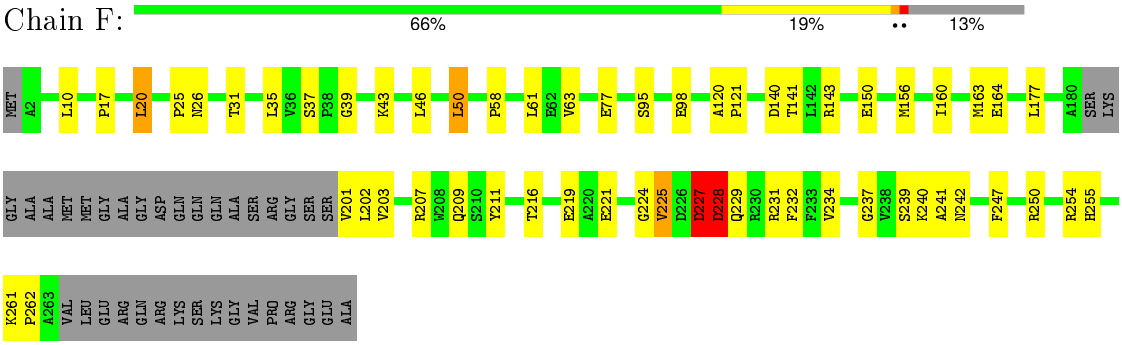
• Molecule 1: REGULATORY PROTEIN REPA

Chain E:



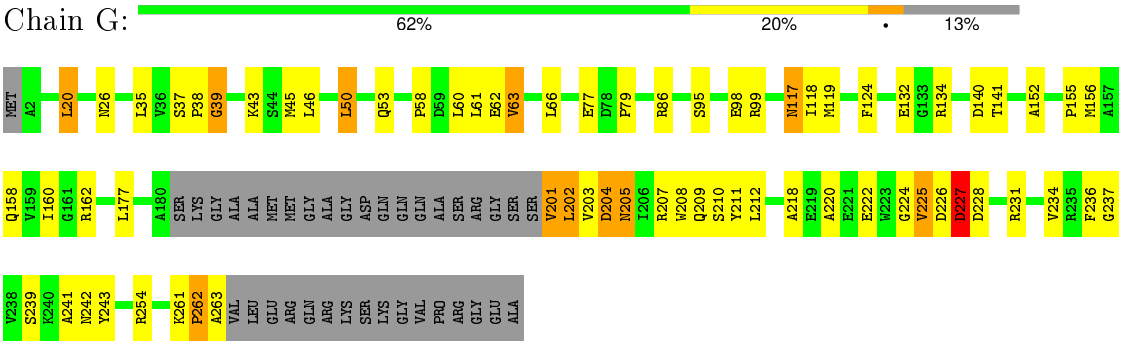
• Molecule 1: REGULATORY PROTEIN REPA

Chain F:



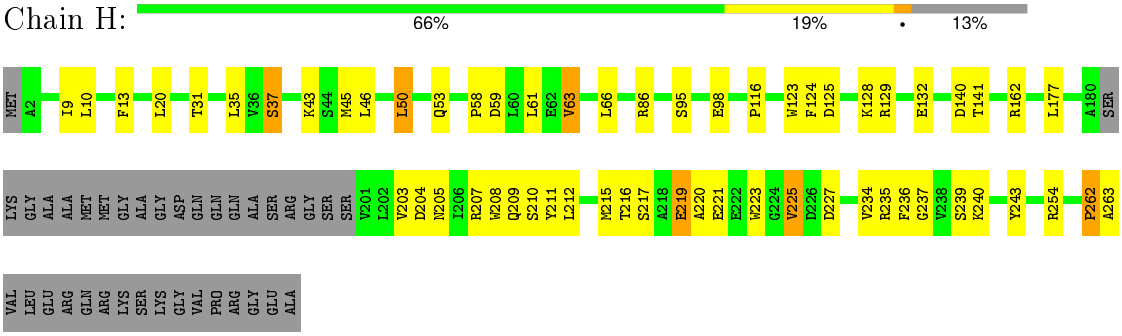
• Molecule 1: REGULATORY PROTEIN REPA

Chain G:



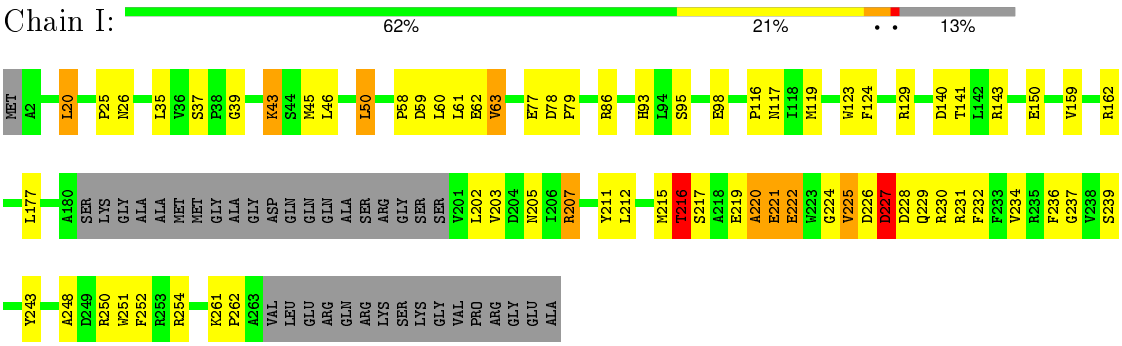
• Molecule 1: REGULATORY PROTEIN REPA

Chain H:



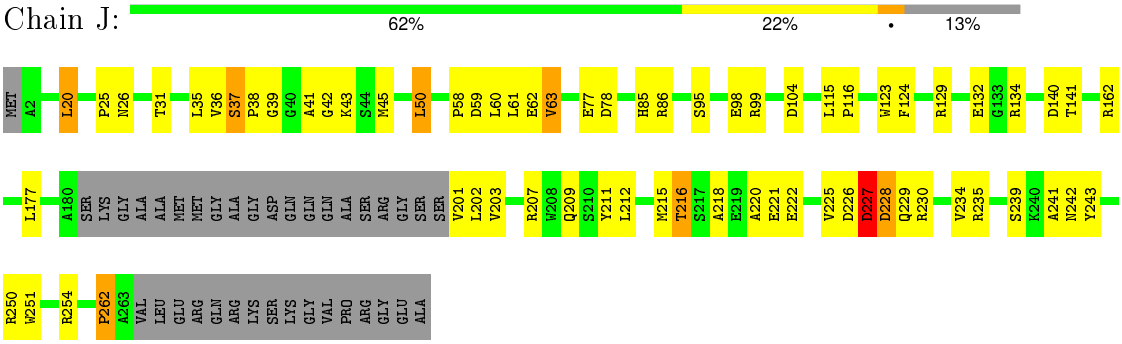
• Molecule 1: REGULATORY PROTEIN REPA

Chain I:



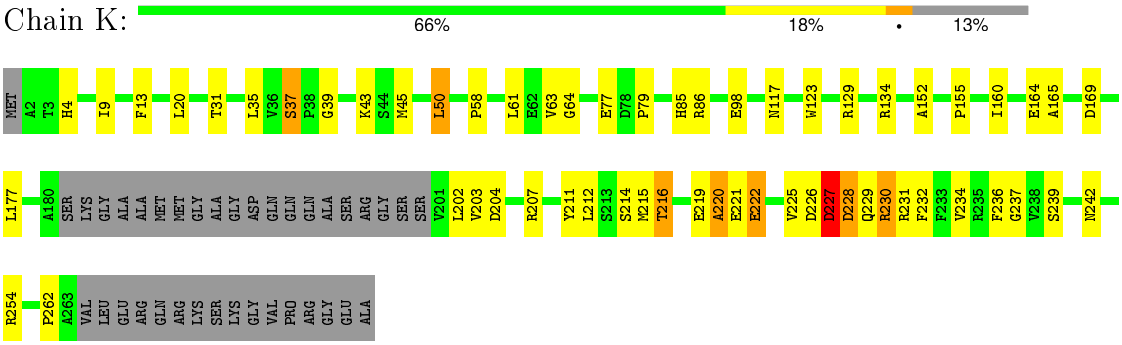
• Molecule 1: REGULATORY PROTEIN REPA

Chain J:



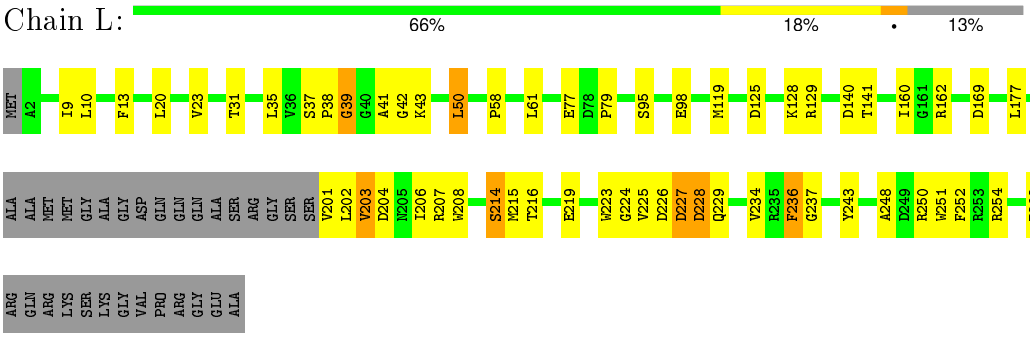
• Molecule 1: REGULATORY PROTEIN REPA

Chain K:



• Molecule 1: REGULATORY PROTEIN REPA

Chain L:


66%
18%
13%
MET A2 I9 L10 F13 L20 V23 T31 L35 V36 S37 P38 G39 G40 A41 G42 K43 L50 P58 L61 E77 D78 P79 S95 E98 M119 D125 K128 R129 D140 T141 I160 G161 R162 D169 L177 A180 SER LYS GLY
ALA ALA MET MET GLY ALA GLY ASP GLN GLN GLN ALA SER ARG GLY SER SER V201 L202 V203 D204 N205 I206 R207 W208 S214 M215 T216 E219 W223 G224 V225 D226 D227 D228 Q229 V234 R235 F236 G237 Y243 A248 D249 R250 W251 F252 R253 R254 P262 A263 VAL LEU GLU
ARG GLN ARG LYS SER LYS GLY VAL PRO ARG GLY GLU ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.43Å 179.16Å 116.29Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.0 (30.00-2.40)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22536	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

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	0.49	0/1884	0.67	1/2564 (0.0%)
1	B	0.47	0/1884	0.67	1/2564 (0.0%)
1	C	0.49	0/1884	0.69	1/2564 (0.0%)
1	D	0.50	0/1884	0.68	1/2564 (0.0%)
1	E	0.47	0/1884	0.66	0/2564
1	F	0.48	0/1884	0.71	1/2564 (0.0%)
1	G	0.53	0/1884	0.71	2/2564 (0.1%)
1	H	0.53	0/1884	0.71	1/2564 (0.0%)
1	I	0.48	0/1884	0.68	1/2564 (0.0%)
1	J	0.54	0/1884	0.73	3/2564 (0.1%)
1	K	0.50	0/1884	0.69	1/2564 (0.0%)
1	L	0.49	0/1884	0.68	0/2564
All	All	0.50	0/22608	0.69	13/30768 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	63	VAL	N-CA-C	-7.81	89.92	111.00
1	J	63	VAL	N-CA-C	-7.54	90.65	111.00
1	J	134	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	C	63	VAL	N-CA-C	-6.08	94.57	111.00
1	J	104	ASP	N-CA-C	-6.03	94.73	111.00
1	G	134	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	H	63	VAL	N-CA-C	-5.80	95.34	111.00
1	I	63	VAL	N-CA-C	-5.75	95.47	111.00
1	F	63	VAL	N-CA-C	-5.60	95.88	111.00
1	D	63	VAL	N-CA-C	-5.37	96.51	111.00
1	K	134	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	63	VAL	N-CA-C	-5.11	97.21	111.00
1	B	134	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1838	0	1819	57	0
1	B	1838	0	1819	68	0
1	C	1838	0	1819	60	0
1	D	1838	0	1819	57	0
1	E	1838	0	1819	57	0
1	F	1838	0	1819	49	0
1	G	1838	0	1819	58	0
1	H	1838	0	1819	49	0
1	I	1838	0	1819	73	0
1	J	1838	0	1819	56	0
1	K	1838	0	1819	50	0
1	L	1838	0	1819	54	0
2	A	41	0	0	2	0
2	B	40	0	0	0	0
2	C	40	0	0	1	0
2	D	39	0	0	0	0
2	E	41	0	0	1	0
2	F	39	0	0	0	0
2	G	41	0	0	0	0
2	H	38	0	0	0	0
2	I	41	0	0	0	0
2	J	41	0	0	1	0
2	K	38	0	0	1	0
2	L	41	0	0	2	0
All	All	22536	0	21828	649	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 15.

All (649) 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:F:203:VAL:HG23	1:F:209:GLN:HE22	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.19	1.05
1:B:250:ARG:HG3	1:B:250:ARG:HH11	1.31	0.95
1:H:203:VAL:HG23	1:H:209:GLN:HE22	1.33	0.94
1:B:62:GLU:HB2	1:B:262:PRO:HG3	1.56	0.88
1:F:203:VAL:HG23	1:F:209:GLN:NE2	1.89	0.87
1:B:216:THR:HG22	1:B:230:ARG:HH21	1.41	0.85
1:H:234:VAL:CG1	1:H:254:ARG:HH21	1.90	0.85
1:B:216:THR:HA	1:B:230:ARG:HE	1.43	0.84
1:I:95:SER:OG	1:I:98:GLU:HG3	1.77	0.84
1:E:250:ARG:HH11	1:E:250:ARG:HG3	1.42	0.83
1:A:250:ARG:HH11	1:A:250:ARG:CG	1.91	0.82
1:C:201:VAL:HB	1:C:203:VAL:HG12	1.61	0.80
1:K:231:ARG:HH11	1:K:232:PHE:HE2	1.33	0.77
1:E:95:SER:OG	1:E:98:GLU:HG3	1.85	0.77
1:J:201:VAL:HG23	1:J:203:VAL:HG12	1.66	0.77
1:L:202:LEU:HD22	1:L:202:LEU:H	1.49	0.77
1:L:250:ARG:HG3	1:L:250:ARG:HH11	1.48	0.76
1:G:203:VAL:HG23	1:G:209:GLN:OE1	1.86	0.76
1:D:250:ARG:HG3	1:D:250:ARG:HH11	1.49	0.76
1:K:220:ALA:HA	1:K:225:VAL:HG23	1.68	0.75
1:L:95:SER:OG	1:L:98:GLU:HG3	1.87	0.74
1:C:216:THR:HB	1:C:219:GLU:H	1.52	0.74
1:I:50:LEU:HD13	1:I:61:LEU:HD12	1.69	0.74
1:H:203:VAL:HG23	1:H:209:GLN:NE2	2.02	0.74
1:B:95:SER:OG	1:B:98:GLU:HG3	1.87	0.74
1:K:216:THR:HA	1:K:230:ARG:HE	1.51	0.74
1:I:43:LYS:HB3	1:I:177:LEU:HD13	1.70	0.73
1:F:216:THR:OG1	1:F:219:GLU:HG3	1.87	0.73
1:J:37:SER:HB2	1:J:212:LEU:O	1.88	0.73
1:G:45:MET:HE1	1:G:86:ARG:HG3	1.71	0.73
1:F:95:SER:OG	1:F:98:GLU:HG3	1.88	0.72
1:L:43:LYS:HB3	1:L:177:LEU:HD13	1.71	0.72
1:D:39:GLY:HA2	1:D:43:LYS:NZ	2.03	0.72
1:K:221:GLU:O	1:K:222:GLU:HB2	1.89	0.72
1:J:207:ARG:HB3	1:J:242:ASN:HD21	1.54	0.71
1:C:231:ARG:HD2	1:C:232:PHE:CE1	2.25	0.71
1:A:250:ARG:HG3	1:A:250:ARG:NH1	2.01	0.71
1:H:234:VAL:HG11	1:H:254:ARG:HH21	1.53	0.71
1:G:203:VAL:HG13	1:G:204:ASP:OD2	1.90	0.71
1:A:119:MET:HE2	1:A:162:ARG:HD2	1.73	0.71
1:B:62:GLU:HB2	1:B:262:PRO:CG	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LYS:HB3	1:F:177:LEU:HD13	1.74	0.69
1:C:43:LYS:HZ1	1:C:179:HIS:CE1	2.10	0.69
1:E:211:TYR:HD2	1:E:239:SER:HB2	1.57	0.69
1:B:93:HIS:HD2	1:B:261:LYS:HE3	1.57	0.69
1:I:93:HIS:HD2	1:I:261:LYS:HE3	1.58	0.69
1:E:59:ASP:OD2	1:E:63:VAL:O	2.10	0.69
1:J:211:TYR:HD2	1:J:239:SER:HB2	1.58	0.68
1:C:43:LYS:HB3	1:C:177:LEU:HD13	1.75	0.68
1:G:211:TYR:HD2	1:G:239:SER:HB2	1.59	0.67
1:L:58:PRO:HG3	1:L:98:GLU:CD	2.14	0.67
1:I:45:MET:HE1	1:I:86:ARG:HG3	1.75	0.67
1:I:221:GLU:O	1:I:222:GLU:HB2	1.93	0.67
1:J:207:ARG:HB3	1:J:242:ASN:ND2	2.10	0.67
1:J:45:MET:HE1	1:J:86:ARG:HG2	1.77	0.67
1:C:216:THR:HG22	1:C:218:ALA:H	1.59	0.67
1:C:35:LEU:HB3	1:C:177:LEU:HD22	1.75	0.67
1:E:119:MET:HE2	1:E:162:ARG:HD2	1.77	0.67
1:G:95:SER:OG	1:G:98:GLU:HG3	1.95	0.67
1:B:216:THR:HG22	1:B:230:ARG:NH2	2.10	0.66
1:H:58:PRO:HG3	1:H:98:GLU:CD	2.16	0.66
1:L:119:MET:HE2	1:L:162:ARG:HD2	1.78	0.66
1:C:211:TYR:HD2	1:C:239:SER:HB2	1.61	0.66
1:G:201:VAL:HG23	1:G:203:VAL:HG12	1.78	0.66
1:C:37:SER:HB2	1:C:212:LEU:O	1.95	0.66
1:G:207:ARG:HB3	1:G:242:ASN:HD21	1.61	0.65
1:K:234:VAL:CG1	1:K:254:ARG:HH21	2.10	0.65
1:K:211:TYR:CD2	1:K:239:SER:HB2	2.31	0.65
1:G:207:ARG:HB3	1:G:242:ASN:ND2	2.11	0.65
1:D:211:TYR:HD2	1:D:239:SER:HB2	1.61	0.65
1:J:234:VAL:CG1	1:J:254:ARG:HH21	2.10	0.64
1:B:203:VAL:HG13	1:B:204:ASP:OD2	1.97	0.64
1:B:46:LEU:HD22	1:B:212:LEU:HD13	1.80	0.64
1:L:58:PRO:HG3	1:L:98:GLU:OE2	1.98	0.64
1:K:43:LYS:HB3	1:K:177:LEU:HD13	1.77	0.64
1:B:43:LYS:HB3	1:B:177:LEU:HD13	1.78	0.64
1:J:202:LEU:N	1:J:202:LEU:HD12	2.13	0.64
1:I:93:HIS:CD2	1:I:261:LYS:HE3	2.33	0.63
1:G:234:VAL:HG11	1:G:254:ARG:HH21	1.63	0.63
1:B:250:ARG:HH11	1:B:250:ARG:CG	2.08	0.63
1:L:219:GLU:OE1	1:L:251:TRP:HH2	1.81	0.63
1:F:203:VAL:CG2	1:F:209:GLN:HE22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:VAL:HG13	1:H:254:ARG:HH21	1.64	0.63
1:D:37:SER:HB2	1:D:212:LEU:O	1.99	0.63
1:C:203:VAL:HG13	1:C:204:ASP:OD2	1.97	0.63
1:H:43:LYS:HB3	1:H:177:LEU:HD13	1.78	0.63
1:I:119:MET:HE2	1:I:162:ARG:HD2	1.80	0.63
1:E:216:THR:HA	1:E:230:ARG:NH2	2.13	0.63
1:I:205:ASN:HD22	1:I:205:ASN:N	1.96	0.63
1:J:207:ARG:HD2	1:K:77:GLU:HB3	1.81	0.62
1:F:231:ARG:HG3	1:F:232:PHE:CD1	2.34	0.62
1:F:227:ASP:C	1:F:229:GLN:H	2.01	0.62
1:C:78:ASP:OD1	1:C:86:ARG:NH2	2.33	0.62
1:F:201:VAL:HB	1:F:203:VAL:HG12	1.82	0.62
1:H:53:GLN:NE2	1:H:66:LEU:HD12	2.14	0.62
1:A:60:LEU:O	1:A:262:PRO:HD3	1.99	0.62
1:A:207:ARG:HD2	1:B:77:GLU:O	1.98	0.62
1:A:95:SER:OG	1:A:98:GLU:HG3	2.00	0.62
1:D:255:HIS:CE1	1:D:261:LYS:HD3	2.35	0.62
1:H:234:VAL:CG1	1:H:254:ARG:NH2	2.62	0.61
1:G:205:ASN:H	1:G:205:ASN:HD22	1.48	0.61
1:B:58:PRO:HG3	1:B:98:GLU:OE2	2.00	0.61
1:G:77:GLU:O	1:L:207:ARG:HD2	2.00	0.61
1:B:216:THR:CA	1:B:230:ARG:HE	2.12	0.61
1:L:234:VAL:CG1	1:L:254:ARG:HH21	2.13	0.61
1:C:211:TYR:CD2	1:C:239:SER:HB2	2.35	0.61
1:A:205:ASN:ND2	1:B:143:ARG:HG2	2.15	0.61
1:K:211:TYR:HD2	1:K:239:SER:HB2	1.64	0.61
1:I:216:THR:HG22	1:I:230:ARG:HH12	1.65	0.61
1:C:20:LEU:HD13	1:D:85:HIS:CD2	2.35	0.61
1:I:234:VAL:CG1	1:I:254:ARG:HH21	2.14	0.61
1:K:37:SER:HB2	1:K:212:LEU:O	2.00	0.61
1:A:85:HIS:CD2	1:F:20:LEU:HD13	2.36	0.61
1:I:35:LEU:HB3	1:I:177:LEU:HD22	1.83	0.60
1:I:58:PRO:HG3	1:I:98:GLU:OE2	2.01	0.60
1:H:125:ASP:O	1:H:129:ARG:HG3	2.01	0.60
1:K:215:MET:HG3	1:K:219:GLU:HB2	1.83	0.60
1:H:211:TYR:CD2	1:H:239:SER:HB2	2.36	0.60
1:D:228:ASP:O	1:D:229:GLN:HG2	2.02	0.60
1:L:227:ASP:C	1:L:229:GLN:H	2.05	0.60
1:G:79:PRO:HG3	1:L:31:THR:CG2	2.32	0.60
1:I:207:ARG:HD2	1:J:77:GLU:O	2.02	0.60
1:B:216:THR:HA	1:B:230:ARG:NE	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:LEU:HD13	1:K:61:LEU:CD1	2.32	0.60
1:G:43:LYS:HB3	1:G:177:LEU:HD13	1.84	0.60
1:H:203:VAL:HG13	1:H:204:ASP:OD2	2.02	0.59
1:E:43:LYS:NZ	1:E:179:HIS:ND1	2.51	0.59
1:B:124:PHE:CD1	1:B:162:ARG:HD3	2.37	0.59
1:B:37:SER:OG	1:B:43:LYS:HG3	2.02	0.59
1:G:234:VAL:CG1	1:G:254:ARG:HH21	2.15	0.59
1:B:60:LEU:O	1:B:262:PRO:HD3	2.02	0.59
1:F:160:ILE:O	1:F:164:GLU:HG3	2.03	0.59
1:I:215:MET:HB2	1:I:251:TRP:CZ3	2.38	0.59
1:J:220:ALA:HB1	1:J:225:VAL:O	2.02	0.59
1:C:202:LEU:HD12	1:C:202:LEU:N	2.18	0.59
1:B:160:ILE:O	1:B:164:GLU:HG3	2.02	0.58
1:H:45:MET:CE	1:H:86:ARG:HG2	2.34	0.58
1:C:46:LEU:HD22	1:C:212:LEU:HD13	1.86	0.58
1:G:119:MET:HE2	1:G:162:ARG:HD2	1.85	0.58
1:L:214:SER:HA	1:L:234:VAL:HG12	1.86	0.58
1:D:224:GLY:O	1:D:225:VAL:O	2.21	0.58
1:C:58:PRO:HG3	1:C:98:GLU:CD	2.23	0.58
1:G:211:TYR:CD2	1:G:239:SER:HB2	2.37	0.58
1:A:234:VAL:CG1	1:A:254:ARG:HH21	2.17	0.58
1:K:234:VAL:HG13	1:K:254:ARG:HH21	1.69	0.57
1:B:234:VAL:HG13	1:B:254:ARG:HH21	1.69	0.57
1:A:35:LEU:HB3	1:A:177:LEU:HD22	1.86	0.57
1:J:31:THR:CG2	1:K:79:PRO:HG3	2.34	0.57
1:A:215:MET:SD	1:A:230:ARG:HB2	2.44	0.57
1:J:218:ALA:O	1:J:222:GLU:HG3	2.04	0.57
1:I:250:ARG:HH11	1:I:250:ARG:HG3	1.70	0.57
1:E:227:ASP:C	1:E:229:GLN:H	2.06	0.57
1:B:234:VAL:CG1	1:B:254:ARG:HH21	2.17	0.57
1:F:234:VAL:HG13	1:F:254:ARG:HH21	1.70	0.57
1:E:211:TYR:CD2	1:E:239:SER:HB2	2.38	0.57
1:F:231:ARG:HG3	1:F:232:PHE:HD1	1.69	0.57
1:A:250:ARG:NH1	1:A:250:ARG:CG	2.60	0.57
1:J:226:ASP:O	1:J:229:GLN:HB2	2.05	0.57
1:G:220:ALA:O	1:G:224:GLY:O	2.23	0.57
1:L:160:ILE:HD11	1:L:202:LEU:HD12	1.86	0.57
1:E:37:SER:HB3	1:E:43:LYS:HG2	1.86	0.56
1:H:50:LEU:HD13	1:H:61:LEU:HD12	1.87	0.56
1:I:45:MET:CE	1:I:86:ARG:HG3	2.34	0.56
1:D:119:MET:CE	1:D:159:VAL:HA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLU:HB2	1:E:262:PRO:HG3	1.87	0.56
1:E:36:VAL:CG1	1:E:180:ALA:HB2	2.35	0.56
1:D:39:GLY:HA2	1:D:43:LYS:HZ1	1.70	0.56
1:A:215:MET:HB2	1:A:251:TRP:HZ3	1.68	0.56
1:E:250:ARG:HG3	1:E:250:ARG:NH1	2.18	0.56
1:J:45:MET:CE	1:J:86:ARG:HG2	2.35	0.56
1:H:203:VAL:HG13	1:H:204:ASP:N	2.20	0.56
1:D:35:LEU:HB3	1:D:177:LEU:HD22	1.87	0.56
1:H:35:LEU:HB3	1:H:177:LEU:HD22	1.88	0.56
1:J:58:PRO:HG3	1:J:98:GLU:CD	2.27	0.56
1:L:125:ASP:OD1	1:L:129:ARG:NH1	2.39	0.56
1:C:62:GLU:HB2	1:C:262:PRO:HG3	1.88	0.56
1:D:235:ARG:HD2	1:D:251:TRP:CZ2	2.41	0.55
1:B:253:ARG:HB2	1:B:263:ALA:HB3	1.88	0.55
1:J:211:TYR:CD2	1:J:239:SER:HB2	2.39	0.55
1:I:215:MET:O	1:I:230:ARG:HB2	2.07	0.55
1:A:215:MET:HB2	1:A:251:TRP:CZ3	2.41	0.55
1:J:220:ALA:C	1:J:222:GLU:H	2.09	0.55
1:E:201:VAL:HG23	1:E:203:VAL:HG12	1.88	0.55
1:D:20:LEU:HD13	1:E:85:HIS:CD2	2.41	0.55
1:K:45:MET:CE	1:K:86:ARG:HG2	2.37	0.55
1:K:216:THR:CA	1:K:230:ARG:HE	2.19	0.55
1:G:45:MET:CE	1:G:86:ARG:HG3	2.36	0.55
1:D:43:LYS:NZ	1:D:43:LYS:HB2	2.22	0.55
1:B:233:PHE:CE2	1:B:253:ARG:HG3	2.42	0.55
1:B:93:HIS:CD2	1:B:261:LYS:HE3	2.39	0.55
1:H:45:MET:HE1	1:H:86:ARG:HG2	1.89	0.55
1:G:117:ASN:HD21	1:G:119:MET:HB2	1.72	0.55
1:I:226:ASP:O	1:I:229:GLN:HB2	2.07	0.55
1:F:228:ASP:HA	1:F:231:ARG:HH12	1.72	0.54
1:C:227:ASP:C	1:C:229:GLN:H	2.11	0.54
1:D:8:ASN:HD22	1:D:8:ASN:C	2.10	0.54
1:B:201:VAL:HG23	1:B:202:LEU:H	1.72	0.54
1:A:79:PRO:HG3	1:F:31:THR:CG2	2.37	0.54
1:C:231:ARG:HD2	1:C:232:PHE:CD1	2.42	0.54
1:D:211:TYR:CD2	1:D:239:SER:HB2	2.40	0.54
1:K:35:LEU:HB3	1:K:177:LEU:HD22	1.89	0.54
1:I:205:ASN:N	1:I:205:ASN:ND2	2.56	0.54
1:E:62:GLU:CD	1:E:262:PRO:HG2	2.28	0.54
1:H:216:THR:HB	1:H:219:GLU:OE2	2.08	0.54
1:L:227:ASP:O	1:L:229:GLN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:MET:HG3	1:D:219:GLU:HB2	1.89	0.54
1:J:43:LYS:HB3	1:J:177:LEU:HD13	1.90	0.54
1:A:211:TYR:CD2	1:A:239:SER:HB2	2.43	0.54
1:F:35:LEU:HB3	1:F:177:LEU:HD22	1.88	0.54
1:L:236:PHE:CG	1:L:237:GLY:N	2.75	0.54
1:I:216:THR:HG22	1:I:230:ARG:NH1	2.23	0.54
1:E:35:LEU:HB3	1:E:177:LEU:HD22	1.90	0.54
1:J:227:ASP:C	1:J:229:GLN:H	2.11	0.54
1:K:45:MET:HE1	1:K:86:ARG:HG2	1.88	0.54
1:I:236:PHE:CG	1:I:237:GLY:N	2.74	0.54
1:E:234:VAL:CG1	1:E:254:ARG:HH21	2.20	0.54
1:L:202:LEU:HD22	1:L:202:LEU:N	2.22	0.54
1:I:234:VAL:HG13	1:I:254:ARG:HH21	1.71	0.54
1:H:125:ASP:OD1	1:H:129:ARG:HD2	2.08	0.54
1:D:215:MET:HB2	1:D:251:TRP:CZ3	2.42	0.54
1:I:217:SER:O	1:I:220:ALA:HB3	2.08	0.54
1:B:227:ASP:C	1:B:229:GLN:H	2.10	0.54
1:J:95:SER:O	1:J:99:ARG:HG3	2.09	0.53
1:K:227:ASP:C	1:K:229:GLN:H	2.11	0.53
1:D:152:ALA:O	1:D:155:PRO:HD2	2.08	0.53
1:H:211:TYR:HD2	1:H:239:SER:HB2	1.72	0.53
1:E:46:LEU:HD22	1:E:212:LEU:HD13	1.90	0.53
1:G:218:ALA:O	1:G:222:GLU:HG3	2.08	0.53
1:J:250:ARG:HH11	1:J:250:ARG:HG3	1.72	0.53
1:D:43:LYS:HZ1	1:D:179:HIS:CE1	2.25	0.53
1:E:124:PHE:CD1	1:E:162:ARG:HD3	2.44	0.53
1:B:214:SER:HA	1:B:234:VAL:HG12	1.91	0.53
1:J:35:LEU:HB3	1:J:177:LEU:HD22	1.88	0.53
1:I:216:THR:C	1:I:230:ARG:HH11	2.11	0.53
1:D:215:MET:HB2	1:D:251:TRP:HZ3	1.73	0.53
1:A:7:ILE:HD12	1:B:83:ILE:CG2	2.37	0.53
1:D:39:GLY:HA2	1:D:43:LYS:HZ2	1.72	0.53
1:F:227:ASP:C	1:F:229:GLN:N	2.61	0.53
1:G:155:PRO:HA	1:G:158:GLN:HE21	1.74	0.53
1:B:216:THR:O	1:B:218:ALA:N	2.41	0.53
1:L:227:ASP:C	1:L:229:GLN:N	2.62	0.53
1:F:227:ASP:O	1:F:229:GLN:N	2.41	0.53
1:L:201:VAL:HG23	1:L:203:VAL:HG12	1.90	0.53
1:H:124:PHE:CD1	1:H:162:ARG:HD3	2.44	0.53
1:F:46:LEU:O	1:F:50:LEU:HD22	2.08	0.53
1:L:248:ALA:O	1:L:250:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ALA:HA	1:L:129:ARG:NH2	2.24	0.52
1:H:219:GLU:C	1:H:221:GLU:H	2.12	0.52
1:K:9:ILE:HG22	1:K:13:PHE:CE1	2.44	0.52
1:F:255:HIS:CE1	1:F:261:LYS:HD3	2.43	0.52
1:J:202:LEU:CD1	1:J:202:LEU:N	2.72	0.52
1:A:202:LEU:HD12	1:A:202:LEU:N	2.24	0.52
1:K:202:LEU:HD12	1:K:202:LEU:N	2.24	0.52
1:H:215:MET:SD	1:H:225:VAL:HG21	2.50	0.52
1:L:50:LEU:HD13	1:L:61:LEU:HD12	1.91	0.52
1:E:216:THR:OG1	1:E:219:GLU:HG3	2.09	0.52
1:D:119:MET:HE1	1:D:159:VAL:HA	1.91	0.52
1:K:220:ALA:HA	1:K:225:VAL:CG2	2.37	0.52
1:H:129:ARG:HA	1:H:132:GLU:HG3	1.92	0.52
1:G:35:LEU:HB3	1:G:177:LEU:HD22	1.91	0.52
1:C:227:ASP:C	1:C:229:GLN:N	2.63	0.52
1:D:58:PRO:HG3	1:D:98:GLU:CD	2.30	0.52
1:B:50:LEU:HD13	1:B:61:LEU:HD12	1.91	0.52
1:F:25:PRO:O	1:F:26:ASN:HB2	2.10	0.52
1:D:93:HIS:CD2	1:D:261:LYS:HD2	2.45	0.52
1:L:203:VAL:HG13	1:L:204:ASP:N	2.25	0.52
1:A:164:GLU:HG2	2:A:312:HOH:O	2.09	0.52
1:G:201:VAL:CG2	1:G:203:VAL:HG12	2.38	0.52
1:I:227:ASP:O	1:I:229:GLN:N	2.43	0.52
1:B:211:TYR:CD2	1:B:239:SER:HB2	2.45	0.52
1:G:160:ILE:HD11	1:G:202:LEU:HB2	1.92	0.52
1:G:124:PHE:CD1	1:G:162:ARG:HD3	2.45	0.52
1:E:234:VAL:HG13	1:E:254:ARG:HH21	1.75	0.52
1:I:216:THR:HG22	1:I:217:SER:H	1.76	0.51
1:A:211:TYR:HD2	1:A:239:SER:HB2	1.74	0.51
1:J:216:THR:HA	1:J:230:ARG:HE	1.75	0.51
1:H:59:ASP:OD2	1:H:63:VAL:O	2.28	0.51
1:G:79:PRO:HG3	1:L:31:THR:HG21	1.93	0.51
1:G:119:MET:HE2	1:G:119:MET:HA	1.92	0.51
1:H:219:GLU:O	1:H:223:TRP:HD1	1.92	0.51
1:H:31:THR:CG2	1:I:79:PRO:HG3	2.41	0.51
1:K:236:PHE:CG	1:K:237:GLY:N	2.78	0.51
1:B:35:LEU:HB3	1:B:177:LEU:HD22	1.92	0.51
1:E:38:PRO:O	1:E:40:GLY:N	2.42	0.51
1:E:207:ARG:HD2	1:F:77:GLU:HB3	1.93	0.51
1:A:59:ASP:OD2	1:A:63:VAL:O	2.28	0.51
1:J:234:VAL:HG13	1:J:254:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:VAL:HG23	1:H:225:VAL:O	2.11	0.51
1:C:220:ALA:HB1	1:C:225:VAL:O	2.10	0.51
1:C:201:VAL:HB	1:C:203:VAL:CG1	2.37	0.51
1:F:207:ARG:HB3	1:F:242:ASN:ND2	2.26	0.51
1:H:37:SER:HB2	1:H:212:LEU:O	2.10	0.51
1:B:49:GLN:HG2	1:B:90:LEU:HD13	1.93	0.51
1:G:37:SER:HB3	1:G:43:LYS:CG	2.40	0.51
1:G:118:ILE:HG23	1:G:119:MET:HE3	1.92	0.51
1:B:20:LEU:HD13	1:C:85:HIS:CD2	2.45	0.51
1:E:50:LEU:HD13	1:E:61:LEU:HD12	1.92	0.51
1:J:201:VAL:CG2	1:J:203:VAL:HG12	2.38	0.50
1:H:50:LEU:HD13	1:H:61:LEU:CD1	2.41	0.50
1:H:125:ASP:OD2	1:H:129:ARG:NH1	2.45	0.50
1:J:95:SER:OG	1:J:98:GLU:HG3	2.11	0.50
1:C:216:THR:HB	1:C:219:GLU:HG3	1.94	0.50
1:F:219:GLU:C	1:F:221:GLU:H	2.15	0.50
1:E:60:LEU:O	1:E:262:PRO:HD3	2.11	0.50
1:C:62:GLU:CD	1:C:262:PRO:HG2	2.32	0.50
1:E:224:GLY:O	1:E:225:VAL:HG22	2.11	0.50
1:L:250:ARG:HG3	1:L:250:ARG:NH1	2.22	0.50
1:F:58:PRO:HG3	1:F:98:GLU:CD	2.31	0.50
1:B:204:ASP:C	1:B:205:ASN:HD22	2.15	0.50
1:A:207:ARG:HB3	1:A:242:ASN:ND2	2.27	0.50
1:C:203:VAL:HG23	1:C:209:GLN:NE2	2.26	0.50
1:C:216:THR:CB	1:C:219:GLU:HG3	2.42	0.50
1:G:117:ASN:ND2	1:G:119:MET:H	2.10	0.50
1:A:215:MET:SD	1:A:225:VAL:HG21	2.52	0.50
1:D:218:ALA:O	1:D:222:GLU:HG3	2.11	0.50
1:C:31:THR:CG2	1:D:79:PRO:HG3	2.41	0.50
1:B:207:ARG:HD2	1:C:77:GLU:HB3	1.93	0.50
1:H:203:VAL:HG13	1:H:204:ASP:H	1.76	0.50
1:J:203:VAL:HG23	1:J:209:GLN:NE2	2.27	0.50
1:C:202:LEU:N	1:C:202:LEU:CD1	2.75	0.50
1:E:203:VAL:HG23	1:E:209:GLN:NE2	2.27	0.50
1:J:62:GLU:HB2	1:J:262:PRO:HG3	1.92	0.50
1:D:169:ASP:OD1	1:I:129:ARG:NH2	2.45	0.50
1:I:46:LEU:HD22	1:I:212:LEU:HD13	1.94	0.50
1:B:250:ARG:NH1	1:B:250:ARG:HG3	2.10	0.50
1:E:58:PRO:HG3	1:E:98:GLU:OE2	2.12	0.50
1:L:119:MET:CE	1:L:162:ARG:HD2	2.42	0.50
1:G:117:ASN:C	1:G:117:ASN:HD22	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:THR:CG2	1:I:230:ARG:HH12	2.25	0.49
1:A:220:ALA:HA	1:A:225:VAL:HG23	1.95	0.49
1:I:202:LEU:HD12	1:I:202:LEU:N	2.27	0.49
1:K:31:THR:CG2	1:L:79:PRO:HG3	2.42	0.49
1:F:234:VAL:CG1	1:F:254:ARG:HH21	2.24	0.49
1:L:219:GLU:O	1:L:223:TRP:HD1	1.95	0.49
1:E:36:VAL:HG12	1:E:180:ALA:HB2	1.94	0.49
1:A:201:VAL:CG2	1:A:203:VAL:HG12	2.43	0.49
1:K:207:ARG:HB3	1:K:242:ASN:ND2	2.28	0.49
1:B:10:LEU:HD13	1:C:103:ALA:CB	2.41	0.49
1:E:95:SER:O	1:E:99:ARG:HG3	2.11	0.49
1:I:50:LEU:HD13	1:I:61:LEU:CD1	2.40	0.49
1:G:224:GLY:O	1:G:225:VAL:O	2.29	0.49
1:D:59:ASP:OD2	1:D:63:VAL:O	2.31	0.49
1:A:54:ILE:HD12	1:A:136:LEU:HD22	1.95	0.49
1:C:216:THR:OG1	1:C:219:GLU:HG3	2.12	0.49
1:G:95:SER:O	1:G:99:ARG:HG3	2.13	0.49
1:I:119:MET:HE3	1:I:159:VAL:HA	1.95	0.49
1:G:205:ASN:N	1:G:205:ASN:HD22	2.11	0.49
1:J:129:ARG:HA	1:J:132:GLU:HG3	1.93	0.49
1:E:231:ARG:HG2	1:E:231:ARG:HH11	1.78	0.49
1:C:215:MET:HB3	1:C:230:ARG:O	2.13	0.49
1:K:214:SER:HA	1:K:234:VAL:HG12	1.94	0.49
1:J:227:ASP:C	1:J:229:GLN:N	2.66	0.49
1:A:178:HIS:CD2	1:A:202:LEU:HD22	2.48	0.49
1:C:216:THR:HG22	1:C:217:SER:N	2.27	0.49
1:L:42:GLY:HA2	2:L:1438:HOH:O	2.13	0.49
1:B:63:VAL:O	1:B:64:GLY:O	2.31	0.49
1:C:250:ARG:HH11	1:C:250:ARG:HG3	1.78	0.49
1:B:231:ARG:CZ	1:B:232:PHE:HE1	2.26	0.48
1:F:211:TYR:CD2	1:F:239:SER:HB2	2.48	0.48
1:B:220:ALA:C	1:B:222:GLU:H	2.15	0.48
1:B:250:ARG:NH1	1:B:250:ARG:CG	2.72	0.48
1:C:43:LYS:NZ	1:C:179:HIS:CE1	2.81	0.48
1:C:220:ALA:C	1:C:222:GLU:H	2.17	0.48
1:D:43:LYS:HZ2	1:D:43:LYS:HB2	1.77	0.48
1:B:225:VAL:HG11	1:B:233:PHE:CE1	2.48	0.48
1:G:37:SER:HB3	1:G:43:LYS:HD3	1.95	0.48
1:C:224:GLY:O	1:C:225:VAL:O	2.31	0.48
1:D:201:VAL:HB	1:D:203:VAL:HG12	1.95	0.48
1:E:93:HIS:CD2	1:E:261:LYS:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:VAL:HG11	1:H:254:ARG:NH2	2.23	0.48
1:L:215:MET:HB2	1:L:251:TRP:CZ3	2.48	0.48
1:C:234:VAL:CG1	1:C:254:ARG:HH21	2.26	0.48
1:D:25:PRO:O	1:D:26:ASN:HB2	2.14	0.48
1:B:2:ALA:HA	1:K:129:ARG:HH21	1.79	0.48
1:J:124:PHE:CD1	1:J:162:ARG:HD3	2.49	0.48
1:G:62:GLU:C	1:G:63:VAL:O	2.47	0.48
1:A:140:ASP:HA	1:A:141:THR:HA	1.70	0.48
1:L:234:VAL:HG13	1:L:254:ARG:HH21	1.77	0.48
1:D:203:VAL:HG13	1:D:204:ASP:N	2.27	0.48
1:J:59:ASP:OD2	1:J:63:VAL:O	2.32	0.48
1:L:35:LEU:HB3	1:L:177:LEU:HD22	1.95	0.48
1:G:38:PRO:O	1:G:39:GLY:C	2.52	0.48
1:D:45:MET:HE2	1:D:86:ARG:HD3	1.96	0.47
1:K:117:ASN:O	1:K:123:TRP:HB2	2.15	0.47
1:G:204:ASP:OD2	1:G:204:ASP:N	2.47	0.47
1:E:43:LYS:HB3	1:E:177:LEU:HD13	1.96	0.47
1:C:227:ASP:O	1:C:229:GLN:N	2.47	0.47
1:H:220:ALA:O	1:H:221:GLU:HG3	2.14	0.47
1:A:202:LEU:CD1	1:A:202:LEU:N	2.77	0.47
1:I:224:GLY:O	1:I:225:VAL:O	2.33	0.47
1:I:231:ARG:HG3	1:I:232:PHE:CE1	2.49	0.47
1:B:59:ASP:OD2	1:B:64:GLY:O	2.31	0.47
1:C:231:ARG:HD2	1:C:232:PHE:CZ	2.49	0.47
1:E:206:ILE:HG22	1:E:208:TRP:H	1.79	0.47
1:A:226:ASP:O	1:A:229:GLN:HB2	2.14	0.47
1:L:202:LEU:CD2	1:L:202:LEU:H	2.23	0.47
1:D:37:SER:O	1:D:179:HIS:HA	2.15	0.47
1:K:234:VAL:HG11	1:K:254:ARG:HH21	1.79	0.47
1:I:234:VAL:CG1	1:I:254:ARG:NH2	2.77	0.47
1:I:248:ALA:O	1:I:250:ARG:NH1	2.47	0.47
1:I:211:TYR:CD2	1:I:239:SER:HB2	2.49	0.47
1:E:140:ASP:HA	1:E:141:THR:HA	1.65	0.47
1:L:37:SER:HB3	1:L:43:LYS:CG	2.44	0.47
1:F:224:GLY:O	1:F:225:VAL:O	2.33	0.47
1:G:211:TYR:CE1	1:G:236:PHE:O	2.69	0.46
1:K:234:VAL:CG1	1:K:254:ARG:NH2	2.77	0.46
1:E:144:ARG:HH11	1:E:144:ARG:HG2	1.81	0.46
1:D:143:ARG:NH1	1:D:150:GLU:HG3	2.30	0.46
1:A:119:MET:HE3	1:A:159:VAL:HA	1.96	0.46
1:F:26:ASN:HB3	1:F:241:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:CD2	1:A:261:LYS:HD2	2.50	0.46
1:K:234:VAL:HG11	1:K:254:ARG:NH2	2.30	0.46
1:K:216:THR:HG22	1:K:230:ARG:HH21	1.81	0.46
1:A:220:ALA:C	1:A:222:GLU:H	2.19	0.46
1:I:236:PHE:HB2	1:I:252:PHE:HE1	1.80	0.46
1:J:60:LEU:O	1:J:262:PRO:HD3	2.16	0.46
1:E:144:ARG:NH1	1:E:144:ARG:HG2	2.31	0.46
1:I:143:ARG:NH1	1:I:150:GLU:HG3	2.30	0.46
1:C:53:GLN:NE2	1:C:66:LEU:HD12	2.30	0.46
1:L:140:ASP:HA	1:L:141:THR:HA	1.68	0.46
1:G:58:PRO:HG3	1:G:98:GLU:CD	2.36	0.46
1:A:205:ASN:HD21	1:B:143:ARG:HG2	1.78	0.46
1:I:230:ARG:C	1:I:232:PHE:H	2.17	0.46
1:J:235:ARG:HD2	1:J:251:TRP:CH2	2.51	0.46
1:A:131:ALA:HB2	1:A:137:MET:HE3	1.97	0.46
1:B:93:HIS:HD2	1:B:261:LYS:CE	2.28	0.46
1:B:236:PHE:CG	1:B:237:GLY:N	2.83	0.46
1:I:20:LEU:HD13	1:J:85:HIS:CD2	2.51	0.46
1:D:124:PHE:CD1	1:D:162:ARG:HD3	2.51	0.46
1:H:9:ILE:HG22	1:H:13:PHE:CE1	2.51	0.46
1:I:215:MET:HB2	1:I:251:TRP:CH2	2.51	0.46
1:I:217:SER:N	1:I:230:ARG:HH11	2.14	0.46
1:L:141:THR:HB	1:L:177:LEU:O	2.15	0.46
1:J:50:LEU:HD13	1:J:61:LEU:CD1	2.46	0.46
1:A:262:PRO:O	1:A:263:ALA:C	2.54	0.45
1:C:60:LEU:O	1:C:262:PRO:HD3	2.15	0.45
1:A:255:HIS:CE1	1:A:261:LYS:HD3	2.52	0.45
1:J:116:PRO:HA	1:J:123:TRP:CE2	2.51	0.45
1:K:160:ILE:O	1:K:164:GLU:HG3	2.16	0.45
1:C:214:SER:HA	1:C:234:VAL:HG12	1.97	0.45
1:I:93:HIS:HD2	1:I:261:LYS:CE	2.27	0.45
1:A:58:PRO:HG3	1:A:98:GLU:OE2	2.16	0.45
1:G:37:SER:HB3	1:G:43:LYS:CD	2.46	0.45
1:D:219:GLU:CD	1:D:219:GLU:H	2.20	0.45
1:G:53:GLN:NE2	1:G:66:LEU:HD12	2.32	0.45
1:K:215:MET:SD	1:K:225:VAL:HG21	2.57	0.45
1:J:226:ASP:O	1:J:227:ASP:O	2.35	0.45
1:F:140:ASP:HA	1:F:141:THR:HA	1.73	0.45
1:D:119:MET:HE2	1:D:159:VAL:HG22	1.97	0.45
1:I:140:ASP:HA	1:I:141:THR:HA	1.75	0.45
1:D:216:THR:HA	1:D:230:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:VAL:HG11	1:L:254:ARG:HH21	1.81	0.45
1:E:201:VAL:CG2	1:E:203:VAL:HG12	2.46	0.45
1:D:95:SER:OG	1:D:98:GLU:HG3	2.17	0.45
1:F:143:ARG:NH1	1:F:150:GLU:HG3	2.32	0.45
1:A:143:ARG:NH1	1:A:150:GLU:HG3	2.32	0.45
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.81	0.45
1:G:50:LEU:HD13	1:G:61:LEU:CD1	2.46	0.45
1:K:220:ALA:CA	1:K:225:VAL:HG23	2.44	0.45
1:G:117:ASN:HD22	1:G:119:MET:H	1.65	0.45
1:A:203:VAL:HG13	1:A:204:ASP:N	2.32	0.45
1:B:2:ALA:HA	1:K:129:ARG:NH2	2.32	0.45
1:A:255:HIS:CE1	1:A:261:LYS:HB2	2.52	0.45
1:G:46:LEU:HD22	1:G:212:LEU:HD13	1.97	0.45
1:H:116:PRO:HA	1:H:123:TRP:CE2	2.52	0.45
1:I:227:ASP:C	1:I:229:GLN:N	2.71	0.44
1:A:203:VAL:HG23	1:A:209:GLN:OE1	2.17	0.44
1:K:58:PRO:HB3	1:K:98:GLU:OE2	2.17	0.44
1:H:208:TRP:CH2	1:H:210:SER:HB3	2.52	0.44
1:D:202:LEU:N	1:D:202:LEU:CD1	2.80	0.44
1:E:63:VAL:O	1:E:64:GLY:O	2.34	0.44
1:A:7:ILE:HD12	1:B:83:ILE:HG21	1.99	0.44
1:B:31:THR:CG2	1:C:79:PRO:HG3	2.47	0.44
1:E:25:PRO:O	1:E:26:ASN:HB2	2.17	0.44
1:F:141:THR:HB	1:F:177:LEU:O	2.17	0.44
1:B:205:ASN:HD22	1:B:205:ASN:N	2.16	0.44
1:K:227:ASP:O	1:K:229:GLN:N	2.51	0.44
1:L:9:ILE:HG22	1:L:13:PHE:CE1	2.52	0.44
1:G:20:LEU:HD12	1:G:20:LEU:HA	1.80	0.44
1:A:234:VAL:HG11	1:A:254:ARG:HH21	1.83	0.44
1:F:211:TYR:HD2	1:F:239:SER:HB2	1.83	0.44
1:I:116:PRO:HA	1:I:123:TRP:CE2	2.52	0.44
1:C:216:THR:O	1:C:230:ARG:HD2	2.18	0.44
1:H:236:PHE:CG	1:H:237:GLY:N	2.86	0.44
1:B:25:PRO:O	1:B:26:ASN:HB2	2.16	0.44
1:D:250:ARG:HG3	1:D:250:ARG:NH1	2.26	0.44
1:L:37:SER:OG	1:L:41:ALA:HB3	2.17	0.44
1:H:140:ASP:HA	1:H:141:THR:HA	1.82	0.44
1:D:234:VAL:CG1	1:D:254:ARG:HH21	2.30	0.44
1:H:207:ARG:NH1	1:I:77:GLU:OE1	2.50	0.44
1:J:227:ASP:O	1:J:229:GLN:N	2.50	0.44
1:G:26:ASN:HB3	1:G:241:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:PRO:HG3	1:I:98:GLU:CD	2.38	0.44
1:L:58:PRO:CG	1:L:98:GLU:CD	2.86	0.44
1:I:50:LEU:HA	1:I:50:LEU:HD12	1.87	0.44
1:E:169:ASP:OD1	1:H:129:ARG:NH2	2.51	0.44
1:A:25:PRO:O	1:A:26:ASN:HB2	2.18	0.44
1:L:160:ILE:HD13	1:L:206:ILE:HD11	2.00	0.44
1:B:243:TYR:OH	1:C:78:ASP:OD2	2.36	0.44
1:I:219:GLU:O	1:I:220:ALA:C	2.55	0.44
1:C:93:HIS:C	1:C:94:LEU:HD12	2.38	0.44
1:L:128:LYS:NZ	1:L:169:ASP:OD2	2.37	0.44
1:C:219:GLU:O	1:C:223:TRP:HD1	2.01	0.43
1:I:37:SER:HB3	1:I:43:LYS:CG	2.47	0.43
1:A:58:PRO:HG3	1:A:98:GLU:CD	2.39	0.43
1:I:117:ASN:O	1:I:123:TRP:HB2	2.19	0.43
1:G:140:ASP:HA	1:G:141:THR:HA	1.80	0.43
1:L:228:ASP:OD1	1:L:229:GLN:HG2	2.17	0.43
1:F:160:ILE:HA	1:F:163:MET:HE2	2.00	0.43
1:E:231:ARG:HG2	1:E:231:ARG:NH1	2.34	0.43
1:G:37:SER:HB3	1:G:43:LYS:HG3	1.99	0.43
1:K:203:VAL:HG13	1:K:204:ASP:OD1	2.17	0.43
1:I:25:PRO:O	1:I:26:ASN:HB2	2.17	0.43
1:H:95:SER:OG	1:H:98:GLU:HG3	2.18	0.43
1:D:205:ASN:HB3	1:E:144:ARG:HH22	1.83	0.43
1:E:156:MET:CE	1:E:202:LEU:HD11	2.49	0.43
1:J:36:VAL:HG12	1:J:37:SER:N	2.34	0.43
1:D:43:LYS:HD2	1:D:177:LEU:HB3	2.01	0.43
1:I:216:THR:CG2	1:I:230:ARG:NH1	2.80	0.43
1:D:226:ASP:O	1:D:229:GLN:HB2	2.19	0.43
1:B:60:LEU:HD11	1:B:94:LEU:CD1	2.49	0.43
1:J:215:MET:O	1:J:230:ARG:HB3	2.19	0.43
1:E:144:ARG:HA	1:E:144:ARG:HD3	1.80	0.43
1:D:207:ARG:HB3	1:D:242:ASN:ND2	2.34	0.43
1:K:152:ALA:HB1	1:K:155:PRO:HD2	1.99	0.43
1:B:224:GLY:O	1:B:225:VAL:C	2.57	0.43
1:H:243:TYR:OH	1:I:78:ASP:OD2	2.37	0.43
1:D:247:PHE:CZ	1:D:250:ARG:NH1	2.86	0.43
1:L:43:LYS:HB3	1:L:177:LEU:CD1	2.43	0.43
1:I:216:THR:CA	1:I:230:ARG:HH11	2.32	0.43
1:E:227:ASP:O	1:E:228:ASP:HB3	2.18	0.43
1:D:58:PRO:HG3	1:D:98:GLU:OE2	2.19	0.43
1:F:228:ASP:HA	1:F:231:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:LEU:HD22	1:H:212:LEU:HD13	2.01	0.43
1:B:262:PRO:O	1:B:263:ALA:C	2.56	0.42
1:F:58:PRO:HG3	1:F:98:GLU:OE2	2.19	0.42
1:I:119:MET:CE	1:I:159:VAL:HA	2.48	0.42
1:A:77:GLU:O	1:F:207:ARG:HD2	2.19	0.42
1:L:38:PRO:O	1:L:39:GLY:C	2.56	0.42
1:L:23:VAL:HA	2:L:1416:HOH:O	2.19	0.42
1:A:245:ALA:O	1:A:246:PRO:C	2.57	0.42
1:F:209:GLN:HB3	1:F:240:LYS:HB3	2.00	0.42
1:H:209:GLN:HB3	1:H:240:LYS:HB3	2.00	0.42
1:A:222:GLU:O	1:A:222:GLU:HG2	2.19	0.42
1:D:140:ASP:HA	1:D:141:THR:HA	1.73	0.42
1:E:223:TRP:N	1:E:223:TRP:CD1	2.87	0.42
1:J:25:PRO:O	1:J:26:ASN:HB2	2.19	0.42
1:B:37:SER:HB2	1:B:212:LEU:O	2.19	0.42
1:L:215:MET:HB2	1:L:251:TRP:HZ3	1.84	0.42
1:C:202:LEU:H	1:C:202:LEU:CD1	2.33	0.42
1:H:216:THR:HG22	1:H:217:SER:N	2.34	0.42
1:K:227:ASP:C	1:K:229:GLN:N	2.72	0.42
1:G:152:ALA:O	1:G:155:PRO:HD2	2.19	0.42
1:I:202:LEU:N	1:I:202:LEU:CD1	2.82	0.42
1:H:262:PRO:O	1:H:263:ALA:O	2.38	0.42
1:C:217:SER:HA	1:C:230:ARG:CD	2.49	0.42
1:K:226:ASP:O	1:K:227:ASP:O	2.37	0.42
1:F:50:LEU:HD13	1:F:61:LEU:HD12	2.00	0.42
1:E:50:LEU:HA	1:E:50:LEU:HD12	1.87	0.42
1:C:42:GLY:HA2	2:C:538:HOH:O	2.20	0.42
1:E:79:PRO:O	1:E:80:PRO:C	2.57	0.42
1:J:42:GLY:HA2	2:J:1238:HOH:O	2.19	0.42
1:E:37:SER:HB3	1:E:43:LYS:CG	2.50	0.42
1:H:45:MET:HE2	1:H:86:ARG:HG2	2.00	0.42
1:F:207:ARG:HB3	1:F:242:ASN:HD22	1.84	0.42
1:K:227:ASP:O	1:K:228:ASP:CG	2.58	0.42
1:B:17:PRO:HA	1:B:18:PRO:HD3	1.91	0.42
1:J:227:ASP:O	1:J:228:ASP:CG	2.58	0.42
1:J:50:LEU:HD12	1:J:50:LEU:HA	1.96	0.42
1:F:250:ARG:HH11	1:F:250:ARG:HG3	1.84	0.42
1:G:236:PHE:CG	1:G:237:GLY:N	2.86	0.42
1:L:219:GLU:OE1	1:L:251:TRP:CH2	2.68	0.42
1:L:234:VAL:CG1	1:L:254:ARG:NH2	2.80	0.42
1:K:165:ALA:O	1:K:169:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:LEU:HD13	1:K:85:HIS:CD2	2.55	0.42
1:I:60:LEU:C	1:I:62:GLU:N	2.73	0.42
1:I:46:LEU:HD12	1:I:61:LEU:HD11	2.02	0.42
1:C:46:LEU:HD21	1:C:236:PHE:CE1	2.55	0.42
1:I:124:PHE:CE1	1:I:162:ARG:HB3	2.55	0.42
1:C:201:VAL:HG21	1:C:204:ASP:CG	2.40	0.42
1:E:219:GLU:C	1:E:221:GLU:H	2.21	0.42
1:E:227:ASP:C	1:E:229:GLN:N	2.73	0.42
1:D:219:GLU:HA	1:D:222:GLU:OE2	2.20	0.42
1:J:62:GLU:C	1:J:63:VAL:O	2.53	0.42
1:G:262:PRO:O	1:G:263:ALA:C	2.58	0.42
1:C:140:ASP:HA	1:C:141:THR:HA	1.68	0.42
1:F:37:SER:HB3	1:F:43:LYS:CG	2.50	0.41
1:B:140:ASP:HA	1:B:141:THR:HA	1.73	0.41
1:F:120:ALA:HA	1:F:121:PRO:HD3	1.91	0.41
1:F:202:LEU:HD12	1:F:202:LEU:C	2.41	0.41
1:B:224:GLY:O	1:B:225:VAL:O	2.37	0.41
1:C:203:VAL:HG13	1:C:204:ASP:N	2.34	0.41
1:J:140:ASP:HA	1:J:141:THR:HA	1.75	0.41
1:C:25:PRO:O	1:C:26:ASN:HB2	2.20	0.41
1:A:212:LEU:HA	1:A:235:ARG:O	2.21	0.41
1:C:231:ARG:C	1:C:231:ARG:HD3	2.40	0.41
1:K:50:LEU:HD13	1:K:61:LEU:HD12	2.01	0.41
1:G:156:MET:CE	1:G:202:LEU:HD23	2.50	0.41
1:B:20:LEU:HD12	1:B:20:LEU:HA	1.96	0.41
1:D:234:VAL:HG11	1:D:254:ARG:HH21	1.84	0.41
1:B:219:GLU:H	1:B:219:GLU:CD	2.23	0.41
1:J:86:ARG:HG3	1:J:86:ARG:NH1	2.34	0.41
1:I:230:ARG:HG3	1:I:231:ARG:N	2.35	0.41
1:F:156:MET:O	1:F:160:ILE:HG13	2.20	0.41
1:C:31:THR:HG22	1:D:79:PRO:HG3	2.02	0.41
1:F:247:PHE:CZ	1:F:250:ARG:NH1	2.89	0.41
1:C:165:ALA:O	1:C:169:ASP:HB2	2.21	0.41
1:I:227:ASP:C	1:I:229:GLN:H	2.23	0.41
1:E:17:PRO:HA	1:E:18:PRO:HD3	1.87	0.41
1:G:226:ASP:C	1:G:227:ASP:O	2.59	0.41
1:A:88:HIS:CG	1:F:17:PRO:HD3	2.56	0.41
1:I:59:ASP:CG	1:I:59:ASP:O	2.58	0.41
1:I:43:LYS:HB3	1:I:177:LEU:CD1	2.47	0.41
1:A:79:PRO:HG3	1:F:31:THR:HG22	2.02	0.41
1:J:115:LEU:N	1:J:116:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:GLY:HA2	2:E:738:HOH:O	2.20	0.41
1:B:216:THR:C	1:B:230:ARG:HE	2.24	0.41
1:F:228:ASP:OD1	1:F:228:ASP:O	2.39	0.41
1:L:236:PHE:HB2	1:L:252:PHE:HE1	1.85	0.41
1:K:207:ARG:NH1	1:L:77:GLU:OE1	2.52	0.41
1:L:37:SER:HB3	1:L:43:LYS:HG3	2.03	0.41
1:B:227:ASP:C	1:B:229:GLN:N	2.73	0.41
1:D:78:ASP:OD1	1:D:86:ARG:NH2	2.53	0.41
1:I:211:TYR:HD2	1:I:239:SER:HB2	1.86	0.41
1:G:60:LEU:O	1:G:262:PRO:HD3	2.21	0.41
1:I:58:PRO:HD3	1:I:98:GLU:HB3	2.03	0.40
1:I:230:ARG:C	1:I:232:PHE:N	2.74	0.40
1:J:201:VAL:HB	1:J:202:LEU:H	1.70	0.40
1:J:37:SER:HA	1:J:38:PRO:HD3	1.90	0.40
1:H:58:PRO:HG3	1:H:98:GLU:OE2	2.20	0.40
1:I:219:GLU:N	1:I:219:GLU:CD	2.75	0.40
1:D:225:VAL:HG11	1:D:233:PHE:CE1	2.56	0.40
1:G:227:ASP:O	1:G:228:ASP:CG	2.60	0.40
1:K:4:HIS:HE1	2:K:1329:HOH:O	2.05	0.40
1:E:152:ALA:HB1	1:E:155:PRO:HD2	2.03	0.40
1:K:254:ARG:HB2	1:K:254:ARG:HE	1.76	0.40
1:L:206:ILE:HG22	1:L:208:TRP:O	2.22	0.40
1:J:78:ASP:OD1	1:J:86:ARG:NH2	2.52	0.40
1:G:205:ASN:ND2	1:G:205:ASN:N	2.69	0.40
1:A:35:LEU:HD23	1:A:177:LEU:HD22	2.04	0.40
1:E:203:VAL:CG2	1:E:209:GLN:NE2	2.84	0.40
1:I:59:ASP:OD2	1:I:63:VAL:O	2.39	0.40
2:A:401:HOH:O	1:B:144:ARG:HD2	2.21	0.40
1:G:208:TRP:CH2	1:G:210:SER:HB3	2.56	0.40
1:K:226:ASP:N	1:K:226:ASP:OD1	2.53	0.40
1:J:26:ASN:HB3	1:J:241:ALA:HB1	2.04	0.40
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.74	0.40
1:D:10:LEU:HA	1:D:10:LEU:HD12	1.74	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	238/279 (85%)	215 (90%)	19 (8%)	4 (2%)	11 14
1	B	238/279 (85%)	214 (90%)	15 (6%)	9 (4%)	4 3
1	C	238/279 (85%)	215 (90%)	13 (6%)	10 (4%)	3 2
1	D	238/279 (85%)	221 (93%)	14 (6%)	3 (1%)	15 21
1	E	238/279 (85%)	220 (92%)	13 (6%)	5 (2%)	9 10
1	F	238/279 (85%)	220 (92%)	12 (5%)	6 (2%)	7 7
1	G	238/279 (85%)	222 (93%)	12 (5%)	4 (2%)	11 14
1	H	238/279 (85%)	219 (92%)	15 (6%)	4 (2%)	11 14
1	I	238/279 (85%)	212 (89%)	16 (7%)	10 (4%)	3 2
1	J	238/279 (85%)	222 (93%)	10 (4%)	6 (2%)	7 7
1	K	238/279 (85%)	216 (91%)	14 (6%)	8 (3%)	5 4
1	L	238/279 (85%)	215 (90%)	15 (6%)	8 (3%)	5 4
All	All	2856/3348 (85%)	2611 (91%)	168 (6%)	77 (3%)	6 6

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	B	217	SER
1	B	218	ALA
1	B	225	VAL
1	C	225	VAL
1	D	225	VAL
1	E	39	GLY
1	E	225	VAL
1	F	225	VAL
1	F	237	GLY
1	G	225	VAL
1	H	225	VAL

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Mol	Chain	Res	Type
1	I	222	GLU
1	I	225	VAL
1	I	227	ASP
1	I	228	ASP
1	J	39	GLY
1	J	227	ASP
1	K	39	GLY
1	K	222	GLU
1	K	227	ASP
1	L	203	VAL
1	L	225	VAL
1	L	228	ASP
1	A	227	ASP
1	B	64	GLY
1	B	227	ASP
1	C	39	GLY
1	C	41	ALA
1	C	227	ASP
1	E	64	GLY
1	F	39	GLY
1	F	227	ASP
1	F	228	ASP
1	G	39	GLY
1	G	227	ASP
1	H	227	ASP
1	I	39	GLY
1	I	216	THR
1	I	220	ALA
1	J	262	PRO
1	K	228	ASP
1	L	39	GLY
1	A	237	GLY
1	B	39	GLY
1	B	262	PRO
1	C	228	ASP
1	C	262	PRO
1	D	229	GLN
1	H	205	ASN
1	I	43	LYS
1	K	220	ALA
1	K	262	PRO
1	L	262	PRO

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Mol	Chain	Res	Type
1	C	221	GLU
1	C	255	HIS
1	F	262	PRO
1	G	262	PRO
1	J	221	GLU
1	J	228	ASP
1	L	216	THR
1	B	236	PHE
1	D	262	PRO
1	E	262	PRO
1	H	262	PRO
1	I	262	PRO
1	J	41	ALA
1	K	63	VAL
1	B	60	LEU
1	C	203	VAL
1	E	40	GLY
1	L	236	PHE
1	C	237	GLY
1	I	203	VAL
1	L	224	GLY
1	K	64	GLY
1	A	63	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	186/212 (88%)	177 (95%)	9 (5%)	31	49
1	B	186/212 (88%)	178 (96%)	8 (4%)	35	55
1	C	186/212 (88%)	177 (95%)	9 (5%)	31	49
1	D	186/212 (88%)	179 (96%)	7 (4%)	40	60
1	E	186/212 (88%)	180 (97%)	6 (3%)	46	68
1	F	186/212 (88%)	181 (97%)	5 (3%)	52	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	186/212 (88%)	174 (94%)	12 (6%)	21 33
1	H	186/212 (88%)	179 (96%)	7 (4%)	40 60
1	I	186/212 (88%)	179 (96%)	7 (4%)	40 60
1	J	186/212 (88%)	180 (97%)	6 (3%)	46 68
1	K	186/212 (88%)	180 (97%)	6 (3%)	46 68
1	L	186/212 (88%)	179 (96%)	7 (4%)	40 60
All	All	2232/2544 (88%)	2143 (96%)	89 (4%)	38 58

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	37	SER
1	A	38	PRO
1	A	50	LEU
1	A	128	LYS
1	A	227	ASP
1	A	228	ASP
1	A	243	TYR
1	A	250	ARG
1	B	10	LEU
1	B	20	LEU
1	B	37	SER
1	B	50	LEU
1	B	62	GLU
1	B	201	VAL
1	B	228	ASP
1	B	230	ARG
1	C	10	LEU
1	C	20	LEU
1	C	37	SER
1	C	50	LEU
1	C	169	ASP
1	C	202	LEU
1	C	227	ASP
1	C	231	ARG
1	C	243	TYR
1	D	8	ASN
1	D	20	LEU
1	D	37	SER

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Mol	Chain	Res	Type
1	D	43	LYS
1	D	50	LEU
1	D	119	MET
1	D	227	ASP
1	E	10	LEU
1	E	20	LEU
1	E	50	LEU
1	E	223	TRP
1	E	227	ASP
1	E	231	ARG
1	F	10	LEU
1	F	20	LEU
1	F	50	LEU
1	F	227	ASP
1	F	228	ASP
1	G	20	LEU
1	G	50	LEU
1	G	117	ASN
1	G	132	GLU
1	G	201	VAL
1	G	202	LEU
1	G	204	ASP
1	G	205	ASN
1	G	227	ASP
1	G	231	ARG
1	G	243	TYR
1	G	261	LYS
1	H	10	LEU
1	H	20	LEU
1	H	37	SER
1	H	50	LEU
1	H	128	LYS
1	H	219	GLU
1	H	235	ARG
1	I	20	LEU
1	I	50	LEU
1	I	207	ARG
1	I	216	THR
1	I	221	GLU
1	I	227	ASP
1	I	243	TYR
1	J	20	LEU

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Mol	Chain	Res	Type
1	J	37	SER
1	J	50	LEU
1	J	216	THR
1	J	227	ASP
1	J	243	TYR
1	K	20	LEU
1	K	37	SER
1	K	50	LEU
1	K	216	THR
1	K	227	ASP
1	K	230	ARG
1	L	10	LEU
1	L	20	LEU
1	L	50	LEU
1	L	214	SER
1	L	226	ASP
1	L	227	ASP
1	L	243	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	205	ASN
1	A	242	ASN
1	A	255	HIS
1	B	93	HIS
1	B	158	GLN
1	B	205	ASN
1	C	53	GLN
1	C	209	GLN
1	C	229	GLN
1	C	242	ASN
1	D	8	ASN
1	D	93	HIS
1	D	242	ASN
1	D	255	HIS
1	E	93	HIS
1	E	209	GLN
1	F	158	GLN
1	F	209	GLN
1	F	242	ASN

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Mol	Chain	Res	Type
1	F	255	HIS
1	G	93	HIS
1	G	117	ASN
1	G	158	GLN
1	G	205	ASN
1	G	242	ASN
1	H	53	GLN
1	H	209	GLN
1	I	93	HIS
1	I	205	ASN
1	J	158	GLN
1	J	209	GLN
1	J	242	ASN
1	J	255	HIS
1	K	158	GLN
1	K	242	ASN
1	L	53	GLN
1	L	158	GLN
1	L	242	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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