



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:38 AM GMT

PDB ID : 3P16  
Title : Crystal structure of DNA polymerase III sliding clamp  
Authors : Gui, W.J.; Lin, S.Q.; Chen, Y.Y.; Zhang, X.E.; Bi, L.J.; Jiang, T.  
Deposited on : 2010-09-30  
Resolution : 2.89 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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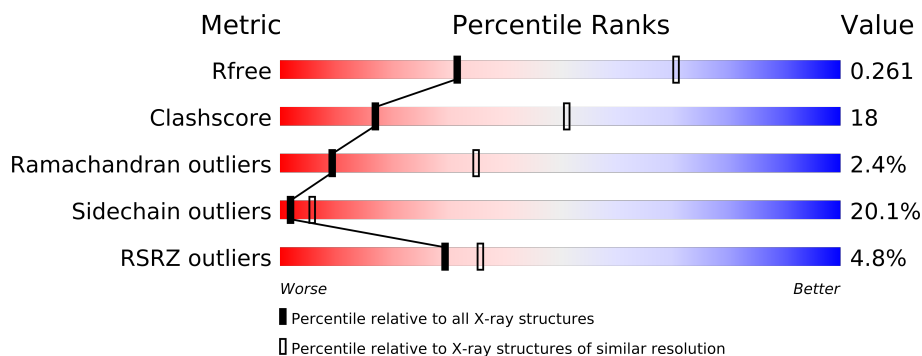
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.89 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	408	
1	B	408	
1	C	408	
1	D	408	
1	E	408	
1	F	408	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16587 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2776	1755	474	541	6			
1	B	383	Total	C	N	O	S	0	0	0
			2836	1796	485	549	6			
1	C	370	Total	C	N	O	S	0	0	0
			2744	1737	469	532	6			
1	D	369	Total	C	N	O	S	0	0	0
			2738	1734	468	530	6			
1	E	369	Total	C	N	O	S	0	0	0
			2738	1734	468	530	6			
1	F	372	Total	C	N	O	S	0	0	0
			2755	1744	471	534	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q50790
A	-4	HIS	-	EXPRESSION TAG	UNP Q50790
A	-3	HIS	-	EXPRESSION TAG	UNP Q50790
A	-2	HIS	-	EXPRESSION TAG	UNP Q50790
A	-1	HIS	-	EXPRESSION TAG	UNP Q50790
A	0	HIS	-	EXPRESSION TAG	UNP Q50790
B	-5	HIS	-	EXPRESSION TAG	UNP Q50790
B	-4	HIS	-	EXPRESSION TAG	UNP Q50790
B	-3	HIS	-	EXPRESSION TAG	UNP Q50790
B	-2	HIS	-	EXPRESSION TAG	UNP Q50790
B	-1	HIS	-	EXPRESSION TAG	UNP Q50790
B	0	HIS	-	EXPRESSION TAG	UNP Q50790
C	-5	HIS	-	EXPRESSION TAG	UNP Q50790
C	-4	HIS	-	EXPRESSION TAG	UNP Q50790
C	-3	HIS	-	EXPRESSION TAG	UNP Q50790
C	-2	HIS	-	EXPRESSION TAG	UNP Q50790
C	-1	HIS	-	EXPRESSION TAG	UNP Q50790

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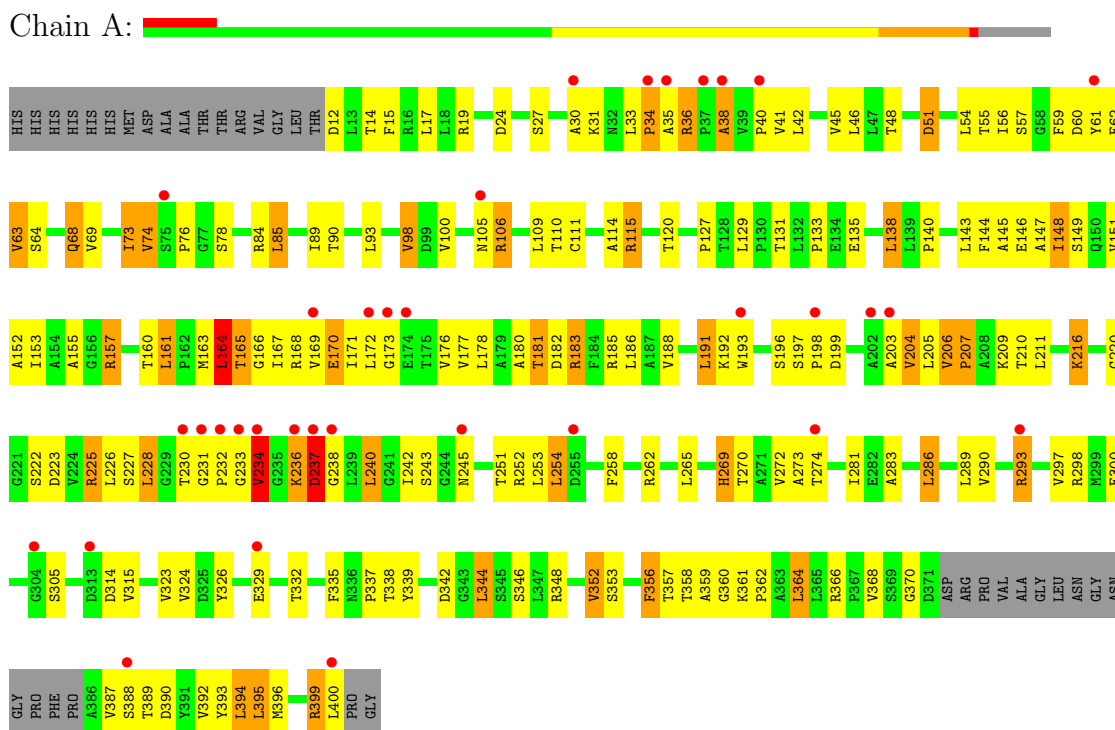
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q50790
D	-5	HIS	-	EXPRESSION TAG	UNP Q50790
D	-4	HIS	-	EXPRESSION TAG	UNP Q50790
D	-3	HIS	-	EXPRESSION TAG	UNP Q50790
D	-2	HIS	-	EXPRESSION TAG	UNP Q50790
D	-1	HIS	-	EXPRESSION TAG	UNP Q50790
D	0	HIS	-	EXPRESSION TAG	UNP Q50790
E	-5	HIS	-	EXPRESSION TAG	UNP Q50790
E	-4	HIS	-	EXPRESSION TAG	UNP Q50790
E	-3	HIS	-	EXPRESSION TAG	UNP Q50790
E	-2	HIS	-	EXPRESSION TAG	UNP Q50790
E	-1	HIS	-	EXPRESSION TAG	UNP Q50790
E	0	HIS	-	EXPRESSION TAG	UNP Q50790
F	-5	HIS	-	EXPRESSION TAG	UNP Q50790
F	-4	HIS	-	EXPRESSION TAG	UNP Q50790
F	-3	HIS	-	EXPRESSION TAG	UNP Q50790
F	-2	HIS	-	EXPRESSION TAG	UNP Q50790
F	-1	HIS	-	EXPRESSION TAG	UNP Q50790
F	0	HIS	-	EXPRESSION TAG	UNP Q50790

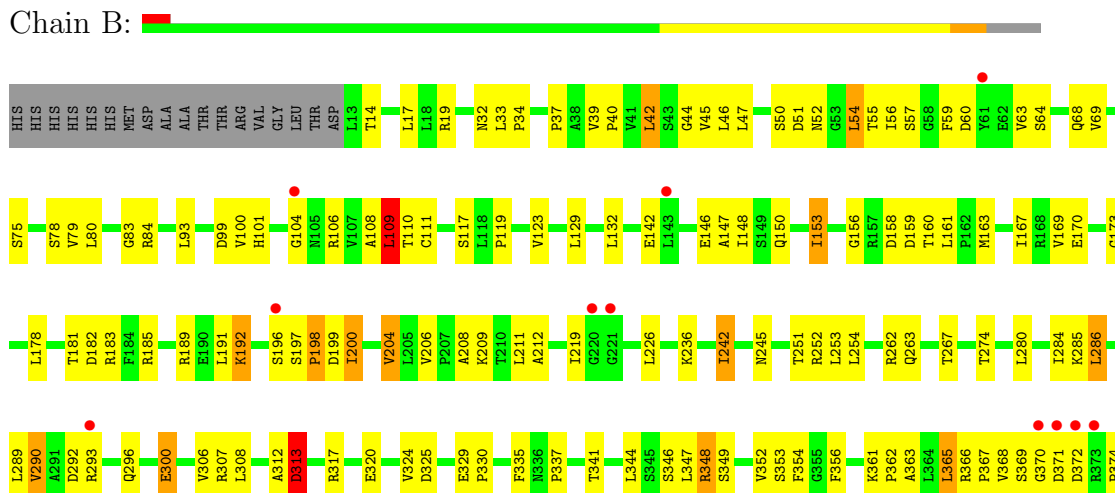
### 3 Residue-property plots

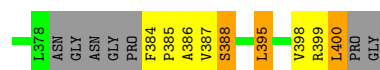
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: DNA polymerase III subunit beta



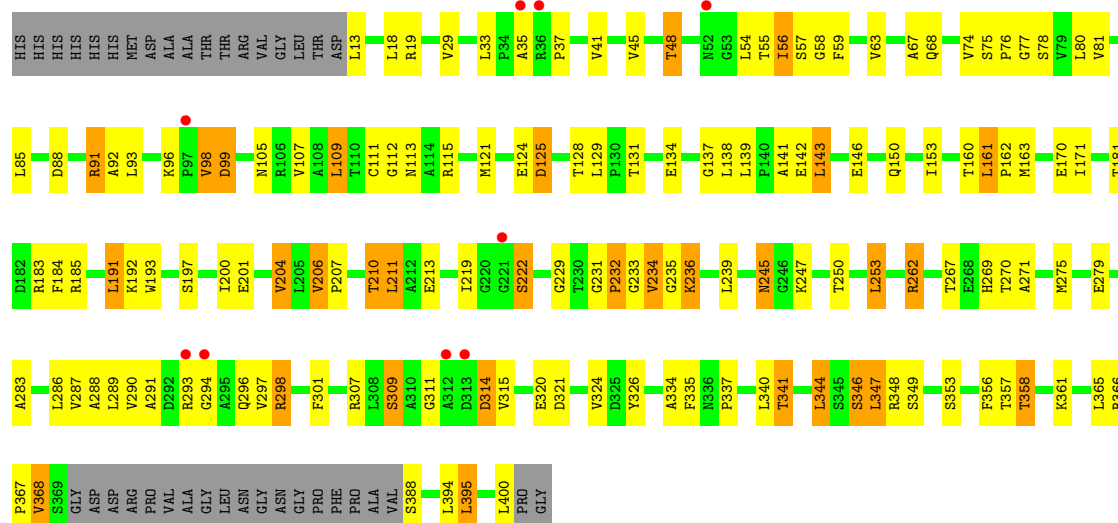
#### • Molecule 1: DNA polymerase III subunit beta





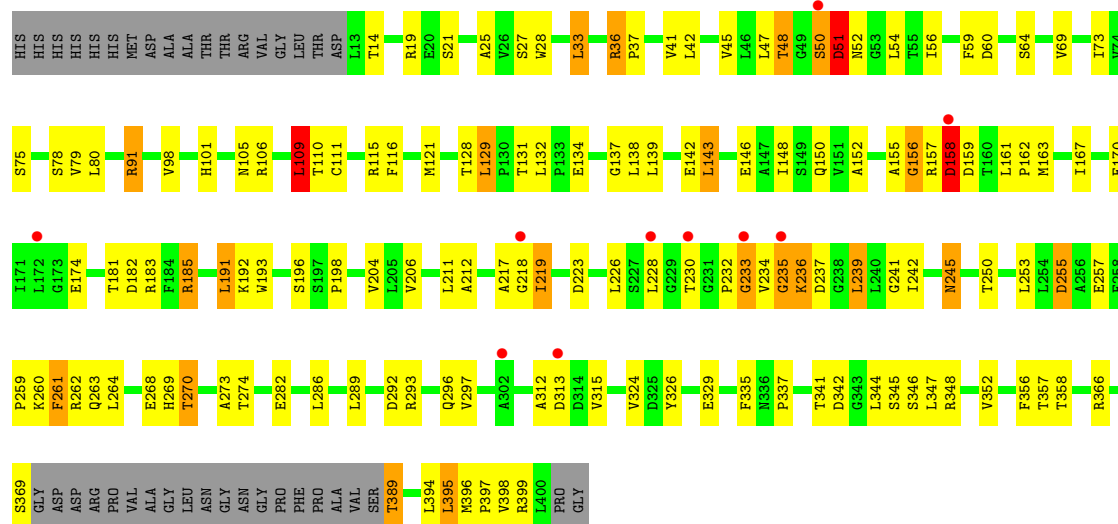
• Molecule 1: DNA polymerase III subunit beta

Chain C:



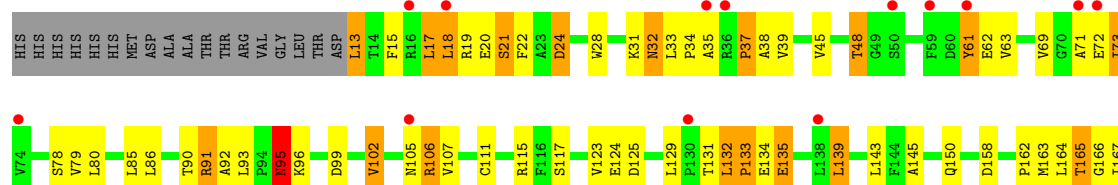
• Molecule 1: DNA polymerase III subunit beta

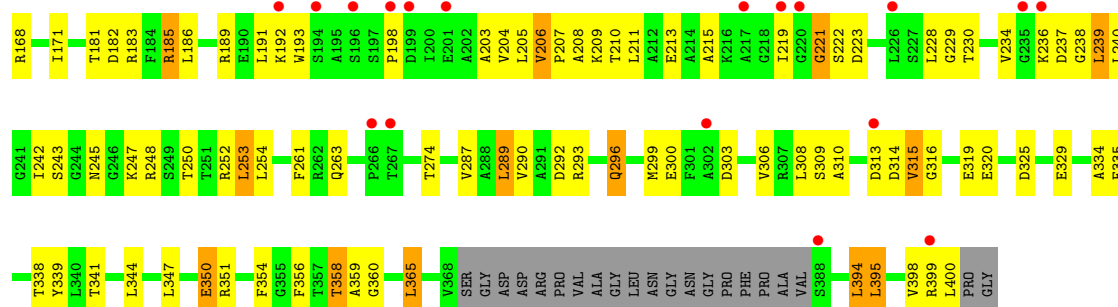
Chain D:



• Molecule 1: DNA polymerase III subunit beta

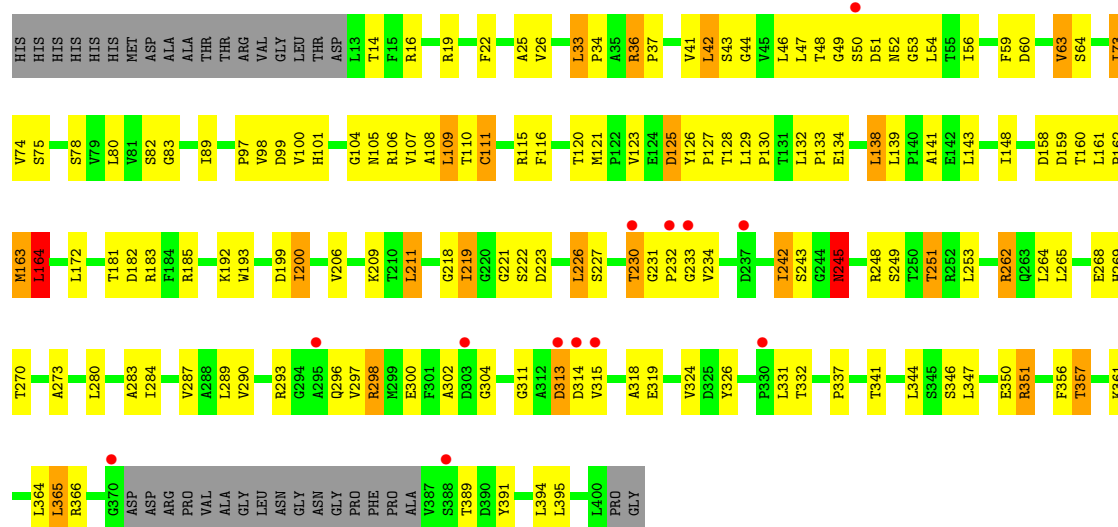
Chain E:





• Molecule 1: DNA polymerase III subunit beta

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.05Å 132.97Å 113.78Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	50.00 – 2.89 36.65 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.89) 97.8 (36.65-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.260 , 0.287 0.258 , 0.261	Depositor DCC
$R_{free}$ test set	2738 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54109 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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	0.53	0/2821	0.69	0/3845
1	B	0.46	0/2884	0.67	1/3932 (0.0%)
1	C	0.47	1/2789 (0.0%)	0.71	0/3801
1	D	0.47	0/2783	0.66	2/3793 (0.1%)
1	E	0.53	0/2783	0.69	2/3793 (0.1%)
1	F	0.48	0/2800	0.70	4/3816 (0.1%)
All	All	0.49	1/16860 (0.0%)	0.69	9/22980 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	368	VAL	CB-CG1	-5.60	1.41	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	33	LEU	CA-CB-CG	5.99	129.08	115.30
1	E	394	LEU	CA-CB-CG	5.80	128.65	115.30
1	F	365	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	109	LEU	CA-CB-CG	5.68	128.36	115.30
1	F	138	LEU	CA-CB-CG	5.57	128.12	115.30
1	F	164	LEU	CA-CB-CG	5.40	127.72	115.30
1	E	139	LEU	CA-CB-CG	5.23	127.33	115.30
1	D	109	LEU	CA-CB-CG	5.11	127.05	115.30
1	D	33	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2776	0	2826	156	0
1	B	2836	0	2890	90	0
1	C	2744	0	2801	78	0
1	D	2738	0	2796	86	0
1	E	2738	0	2796	116	0
1	F	2755	0	2813	95	0
All	All	16587	0	16922	594	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (594) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:234:VAL:HG11	1:E:236:LYS:NZ	1.48	1.28
1:A:30:ALA:HA	1:A:34:PRO:HG2	1.24	1.16
1:A:161:LEU:HD12	1:A:161:LEU:H	1.01	1.15
1:E:234:VAL:HG22	1:E:236:LYS:HG3	1.23	1.11
1:E:134:GLU:OE1	1:E:230:THR:HG22	1.49	1.08
1:E:234:VAL:HG11	1:E:236:LYS:CE	1.84	1.07
1:F:296:GLN:HB3	1:F:337:PRO:HD3	1.38	1.04
1:F:36:ARG:N	1:F:36:ARG:HD2	1.67	1.04
1:A:185:ARG:HD3	1:A:339:TYR:HB3	1.37	1.03
1:B:42:LEU:HD21	1:B:60:ASP:HA	1.41	1.02
1:E:234:VAL:HG21	1:E:236:LYS:HE3	1.37	1.01
1:E:234:VAL:CG2	1:E:236:LYS:HG3	1.91	1.00
1:E:206:VAL:HG23	1:E:207:PRO:HD2	1.44	1.00
1:B:280:LEU:O	1:B:284:ILE:HG12	1.61	0.99
1:C:298:ARG:HG2	1:C:298:ARG:HH11	1.27	0.97
1:D:59:PHE:CD1	1:D:64:SER:HB3	2.00	0.96
1:F:36:ARG:H	1:F:36:ARG:HD2	1.26	0.93
1:A:35:ALA:HA	1:A:84:ARG:HE	1.34	0.93
1:D:59:PHE:HD1	1:D:64:SER:HB3	1.28	0.92
1:E:145:ALA:HA	1:E:215:ALA:HB1	1.52	0.92
1:E:234:VAL:HG11	1:E:236:LYS:HZ2	1.35	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:387:VAL:HG22	1:A:388:SER:H	1.37	0.89
1:F:37:PRO:HG2	1:F:43:SER:HB3	1.55	0.88
1:B:349:SER:HB2	1:B:367:PRO:HB3	1.56	0.88
1:A:161:LEU:HD12	1:A:161:LEU:N	1.85	0.87
1:A:73:ILE:HD13	1:A:73:ILE:H	1.38	0.86
1:A:161:LEU:CD1	1:A:161:LEU:H	1.87	0.86
1:D:59:PHE:HD1	1:D:64:SER:CB	1.88	0.86
1:F:80:LEU:HD23	1:F:121:MET:HB2	1.58	0.85
1:A:204:VAL:HG22	1:A:253:LEU:HD13	1.59	0.85
1:A:155:ALA:O	1:A:157:ARG:HG3	1.76	0.84
1:E:48:THR:HG23	1:E:78:SER:HB3	1.58	0.84
1:E:354:PHE:HB3	1:E:356:PHE:CE2	2.13	0.84
1:A:161:LEU:HD11	1:C:183:ARG:C	1.99	0.83
1:A:59:PHE:HB3	1:A:64:SER:HA	1.59	0.83
1:A:100:VAL:HG22	1:A:109:LEU:HD13	1.59	0.82
1:B:354:PHE:HB3	1:B:356:PHE:CE2	2.14	0.82
1:A:27:SER:O	1:A:31:LYS:HG2	1.80	0.81
1:F:337:PRO:O	1:F:341:THR:HG22	1.80	0.81
1:B:335:PHE:HZ	1:B:356:PHE:HE1	1.27	0.81
1:A:161:LEU:CD1	1:C:183:ARG:O	2.29	0.80
1:F:164:LEU:HG	1:F:181:THR:O	1.81	0.80
1:E:20:GLU:H	1:E:20:GLU:CD	1.84	0.80
1:D:366:ARG:HD2	1:D:389:THR:HG21	1.64	0.80
1:A:157:ARG:O	1:A:157:ARG:HD2	1.81	0.79
1:E:234:VAL:HG13	1:E:236:LYS:HD2	1.63	0.78
1:E:61:TYR:HD1	1:E:62:GLU:HG2	1.48	0.78
1:E:132:LEU:N	1:E:133:PRO:HD3	1.99	0.77
1:D:19:ARG:HH21	1:D:91:ARG:HA	1.49	0.77
1:E:234:VAL:CG1	1:E:236:LYS:NZ	2.41	0.77
1:B:199:ASP:C	1:B:200:ILE:HG22	2.05	0.77
1:A:185:ARG:HD2	1:A:393:TYR:OH	1.83	0.77
1:D:366:ARG:CD	1:D:389:THR:HG21	2.15	0.76
1:E:234:VAL:CG1	1:E:236:LYS:HD2	2.16	0.76
1:E:234:VAL:HG11	1:E:236:LYS:HZ1	1.49	0.76
1:E:335:PHE:CD1	1:E:395:LEU:HD13	2.21	0.75
1:A:133:PRO:O	1:A:227:SER:HB3	1.86	0.75
1:E:204:VAL:CG2	1:E:253:LEU:HG	2.17	0.75
1:B:399:ARG:HG3	1:B:400:LEU:HG	1.68	0.75
1:F:181:THR:O	1:F:181:THR:HG23	1.86	0.74
1:F:218:GLY:HA2	1:F:245:ASN:HD21	1.51	0.74
1:D:234:VAL:O	1:D:236:LYS:N	2.21	0.74
1:A:161:LEU:HD12	1:C:183:ARG:O	1.87	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:GLU:HG3	1:A:332:THR:OG1	1.87	0.73
1:A:297:VAL:HG23	1:A:337:PRO:HG3	1.70	0.73
1:A:315:VAL:HA	1:B:119:PRO:HG2	1.70	0.73
1:D:268:GLU:HG3	1:D:269:HIS:H	1.54	0.73
1:D:270:THR:HB	1:D:357:THR:HA	1.68	0.73
1:F:218:GLY:CA	1:F:245:ASN:HD21	2.02	0.72
1:F:109:LEU:HB3	1:F:116:PHE:HB2	1.71	0.72
1:E:181:THR:OG1	1:E:182:ASP:O	2.07	0.72
1:B:40:PRO:HG3	1:D:36:ARG:HH11	1.53	0.72
1:A:144:PHE:O	1:A:148:ILE:HG13	1.89	0.72
1:E:73:ILE:O	1:E:73:ILE:HG13	1.89	0.72
1:C:233:GLY:O	1:C:236:LYS:HB2	1.90	0.72
1:B:354:PHE:HB3	1:B:356:PHE:HE2	1.53	0.72
1:D:260:LYS:HD3	1:D:263:GLN:HE22	1.55	0.72
1:E:234:VAL:CG2	1:E:236:LYS:CG	2.68	0.71
1:A:273:ALA:HB2	1:A:326:TYR:HD1	1.54	0.71
1:C:170:GLU:OE1	1:C:262:ARG:NH2	2.23	0.71
1:A:185:ARG:HD3	1:A:339:TYR:CB	2.15	0.71
1:E:134:GLU:HB3	1:E:229:GLY:HA2	1.72	0.70
1:B:198:PRO:O	1:B:200:ILE:HG22	1.91	0.70
1:A:389:THR:CG2	1:A:390:ASP:H	2.04	0.70
1:A:59:PHE:CZ	1:A:127:PRO:HB2	2.27	0.70
1:B:199:ASP:O	1:B:200:ILE:CG2	2.40	0.70
1:A:387:VAL:CG2	1:A:388:SER:H	2.05	0.70
1:A:387:VAL:HG22	1:A:388:SER:N	2.07	0.70
1:D:268:GLU:HG3	1:D:269:HIS:N	2.07	0.70
1:A:364:LEU:HD11	1:A:392:VAL:CG2	2.21	0.70
1:A:151:VAL:HG23	1:A:167:ILE:HD13	1.73	0.69
1:A:181:THR:HB	1:A:186:LEU:HA	1.74	0.69
1:A:161:LEU:CD1	1:C:183:ARG:C	2.60	0.69
1:F:25:ALA:HB1	1:F:56:ILE:HD12	1.73	0.69
1:A:238:GLY:O	1:A:252:ARG:HA	1.92	0.69
1:A:55:THR:HG22	1:A:68:GLN:HB2	1.73	0.69
1:E:234:VAL:HG22	1:E:236:LYS:CG	2.13	0.69
1:A:15:PHE:HB3	1:A:73:ILE:HG22	1.75	0.68
1:A:389:THR:HG22	1:A:390:ASP:H	1.58	0.68
1:E:234:VAL:CG1	1:E:236:LYS:CE	2.67	0.68
1:B:37:PRO:HB3	1:C:314:ASP:HB2	1.76	0.68
1:D:59:PHE:CD1	1:D:64:SER:CB	2.69	0.68
1:A:36:ARG:HH12	1:A:38:ALA:CB	2.07	0.68
1:A:140:PRO:HA	1:A:222:SER:HA	1.75	0.67
1:E:234:VAL:CG2	1:E:236:LYS:HE3	2.21	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293:ARG:O	1:B:293:ARG:CG	2.43	0.67
1:D:25:ALA:HB1	1:D:56:ILE:HD13	1.77	0.67
1:B:150:GLN:OE1	1:B:189:ARG:HD3	1.95	0.66
1:A:147:ALA:HB1	1:A:178:LEU:HD12	1.78	0.66
1:D:274:THR:O	1:D:324:VAL:HG23	1.95	0.66
1:C:57:SER:HB3	1:C:129:LEU:HD11	1.77	0.66
1:E:238:GLY:O	1:E:252:ARG:HA	1.95	0.66
1:F:46:LEU:HD11	1:F:123:VAL:HG13	1.76	0.66
1:E:61:TYR:CD1	1:E:62:GLU:HG2	2.31	0.65
1:A:206:VAL:HG21	1:A:240:LEU:HD12	1.79	0.65
1:C:197:SER:O	1:C:200:ILE:HG12	1.97	0.65
1:C:29:VAL:HG21	1:C:56:ILE:O	1.96	0.65
1:A:35:ALA:HA	1:A:84:ARG:NE	2.10	0.65
1:F:364:LEU:HD21	1:F:366:ARG:HH21	1.60	0.65
1:D:183:ARG:HB3	1:F:160:THR:HG23	1.78	0.65
1:B:54:LEU:HD12	1:B:69:VAL:HG12	1.79	0.64
1:E:234:VAL:HG21	1:E:236:LYS:CE	2.20	0.64
1:A:389:THR:HG22	1:A:390:ASP:N	2.12	0.64
1:A:36:ARG:NH1	1:A:38:ALA:HB3	2.12	0.64
1:D:293:ARG:HH22	1:F:293:ARG:NH1	1.96	0.64
1:F:49:GLY:O	1:F:73:ILE:HD13	1.98	0.64
1:B:54:LEU:HD11	1:B:56:ILE:HD11	1.80	0.63
1:E:86:LEU:O	1:E:90:THR:HG23	1.97	0.63
1:B:366:ARG:CZ	1:B:387:VAL:HG21	2.27	0.63
1:B:199:ASP:C	1:B:200:ILE:CG2	2.66	0.63
1:A:269:HIS:CD2	1:A:272:VAL:CG1	2.82	0.63
1:F:141:ALA:HB1	1:F:219:ILE:O	1.99	0.62
1:B:148:ILE:HG21	1:B:212:ALA:HA	1.80	0.62
1:E:354:PHE:CB	1:E:356:PHE:CE2	2.82	0.62
1:E:234:VAL:CG1	1:E:236:LYS:CD	2.77	0.62
1:B:386:ALA:O	1:B:387:VAL:HG13	1.99	0.62
1:F:231:GLY:O	1:F:234:VAL:HG13	1.98	0.62
1:A:114:ALA:HB2	1:B:320:GLU:HG2	1.81	0.62
1:A:164:LEU:H	1:A:164:LEU:HD23	1.65	0.62
1:D:129:LEU:HD22	1:D:129:LEU:H	1.65	0.62
1:F:16:ARG:HD2	1:F:97:PRO:HB2	1.81	0.62
1:D:36:ARG:N	1:D:37:PRO:HD2	2.15	0.62
1:A:135:GLU:OE1	1:A:225:ARG:HD3	2.00	0.61
1:B:356:PHE:CE1	1:B:363:ALA:CB	2.83	0.61
1:E:20:GLU:OE2	1:E:95:ASN:HB3	2.01	0.61
1:B:14:THR:HG23	1:B:101:HIS:HB3	1.83	0.61
1:C:298:ARG:CG	1:C:298:ARG:HH11	2.08	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:173:GLY:HA2	1:B:200:ILE:HG23	1.81	0.61
1:E:31:LYS:HD2	1:E:213:GLU:HG3	1.82	0.61
1:D:146:GLU:O	1:D:150:GLN:HG3	2.00	0.61
1:C:207:PRO:HB2	1:C:210:THR:HG23	1.83	0.61
1:A:205:LEU:O	1:A:253:LEU:HB2	2.01	0.60
1:E:204:VAL:HG22	1:E:253:LEU:HG	1.82	0.60
1:A:389:THR:CG2	1:A:390:ASP:N	2.65	0.60
1:B:293:ARG:O	1:B:293:ARG:HG3	2.01	0.60
1:B:54:LEU:HD13	1:B:54:LEU:C	2.21	0.60
1:D:312:ALA:HB3	1:D:315:VAL:HB	1.83	0.60
1:B:199:ASP:O	1:B:200:ILE:HG22	2.00	0.60
1:B:353:SER:HB3	1:B:366:ARG:HG3	1.82	0.59
1:B:156:GLY:HA2	1:B:182:ASP:HB3	1.83	0.59
1:D:293:ARG:HH22	1:F:293:ARG:HH11	1.49	0.59
1:A:12:ASP:O	1:A:76:PRO:O	2.20	0.59
1:F:41:VAL:HG13	1:F:126:TYR:HD1	1.67	0.59
1:B:55:THR:HG23	1:B:68:GLN:HG2	1.84	0.59
1:E:13:LEU:O	1:E:102:VAL:HG13	2.02	0.59
1:F:226:LEU:HD12	1:F:242:ILE:HG22	1.83	0.59
1:F:269:HIS:HB3	1:F:356:PHE:O	2.03	0.59
1:E:234:VAL:CG1	1:E:236:LYS:HZ2	2.08	0.59
1:F:51:ASP:C	1:F:53:GLY:H	2.06	0.59
1:A:42:LEU:HD21	1:A:60:ASP:HA	1.84	0.59
1:A:36:ARG:HH12	1:A:38:ALA:HB3	1.65	0.59
1:C:298:ARG:HG2	1:C:298:ARG:NH1	2.06	0.59
1:B:354:PHE:CD1	1:B:356:PHE:CZ	2.91	0.58
1:E:33:LEU:N	1:E:34:PRO:HD3	2.18	0.58
1:E:234:VAL:HG11	1:E:236:LYS:CD	2.32	0.58
1:D:132:LEU:HD13	1:D:241:GLY:HA3	1.84	0.58
1:A:106:ARG:CG	1:A:106:ARG:HH11	2.15	0.58
1:B:356:PHE:CE1	1:B:363:ALA:HB2	2.38	0.58
1:C:80:LEU:HD23	1:C:121:MET:HB2	1.85	0.58
1:A:33:LEU:HD23	1:A:63:VAL:HG13	1.86	0.58
1:C:181:THR:O	1:C:181:THR:HG23	2.03	0.58
1:A:144:PHE:O	1:A:148:ILE:CG1	2.52	0.58
1:E:315:VAL:HG13	1:F:106:ARG:HH12	1.68	0.58
1:C:201:GLU:O	1:C:234:VAL:HG13	2.04	0.57
1:E:228:LEU:O	1:E:234:VAL:O	2.21	0.57
1:A:73:ILE:HD13	1:A:73:ILE:N	2.15	0.57
1:A:181:THR:HG22	1:A:258:PHE:CZ	2.39	0.57
1:F:48:THR:HG22	1:F:50:SER:H	1.69	0.57
1:E:296:GLN:HE21	1:E:400:LEU:HD22	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:59:PHE:CD2	1:B:64:SER:HB3	2.40	0.57
1:C:269:HIS:HB3	1:C:356:PHE:O	2.05	0.57
1:C:141:ALA:H	1:C:222:SER:HA	1.69	0.56
1:A:62:GLU:HA	1:A:252:ARG:HG3	1.88	0.56
1:A:110:THR:HG22	1:A:115:ARG:HG3	1.87	0.56
1:D:268:GLU:CG	1:D:269:HIS:H	2.17	0.56
1:A:46:LEU:HB3	1:A:57:SER:HB2	1.87	0.56
1:D:219:ILE:HG12	1:D:219:ILE:O	2.04	0.56
1:C:81:VAL:HG11	1:C:107:VAL:HG11	1.87	0.56
1:B:59:PHE:HB2	1:B:129:LEU:HD22	1.87	0.56
1:A:170:GLU:HG3	1:A:177:VAL:HB	1.87	0.56
1:F:283:ALA:O	1:F:287:VAL:HG22	2.06	0.55
1:C:207:PRO:HB2	1:C:210:THR:CG2	2.37	0.55
1:B:374:PRO:HD2	1:B:388:SER:HB3	1.88	0.55
1:E:134:GLU:CD	1:E:230:THR:H	2.09	0.55
1:A:269:HIS:HD2	1:A:272:VAL:CG1	2.19	0.55
1:A:145:ALA:O	1:A:149:SER:HB2	2.07	0.55
1:C:48:THR:HG23	1:C:78:SER:HB3	1.88	0.55
1:A:197:SER:HB2	1:A:230:THR:HG22	1.88	0.55
1:A:364:LEU:HD11	1:A:392:VAL:HG22	1.87	0.55
1:F:49:GLY:O	1:F:73:ILE:CD1	2.55	0.55
1:C:161:LEU:HD23	1:C:162:PRO:HD2	1.88	0.55
1:B:335:PHE:CZ	1:B:356:PHE:HE1	2.16	0.54
1:B:398:VAL:HG12	1:B:399:ARG:N	2.22	0.54
1:C:337:PRO:O	1:C:341:THR:HB	2.07	0.54
1:D:185:ARG:HA	1:D:394:LEU:O	2.07	0.54
1:D:335:PHE:CD1	1:D:395:LEU:HD13	2.42	0.54
1:A:168:ARG:HH12	1:A:203:ALA:HB1	1.72	0.54
1:A:59:PHE:HB3	1:A:64:SER:CA	2.35	0.54
1:A:225:ARG:HB3	1:A:243:SER:HB2	1.90	0.54
1:B:192:LYS:H	1:B:192:LYS:HD3	1.73	0.54
1:C:335:PHE:CD1	1:C:395:LEU:HD13	2.42	0.54
1:C:35:ALA:O	1:C:37:PRO:HD3	2.07	0.54
1:B:361:LYS:HB3	1:B:362:PRO:HD2	1.88	0.54
1:B:199:ASP:O	1:B:200:ILE:HG23	2.07	0.54
1:A:161:LEU:HD11	1:C:184:PHE:N	2.23	0.54
1:F:181:THR:O	1:F:181:THR:CG2	2.56	0.54
1:A:314:ASP:OD2	1:A:315:VAL:N	2.40	0.54
1:A:335:PHE:CD1	1:A:395:LEU:HD13	2.42	0.54
1:B:39:VAL:HG23	1:B:42:LEU:HB2	1.89	0.53
1:A:399:ARG:HE	1:A:399:ARG:H	1.55	0.53
1:A:399:ARG:NE	1:A:399:ARG:H	2.06	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ARG:HA	1:A:205:LEU:HD12	1.89	0.53
1:B:356:PHE:CE1	1:B:363:ALA:HB1	2.43	0.53
1:A:163:MET:O	1:A:164:LEU:C	2.45	0.53
1:E:300:GLU:O	1:E:306:VAL:HA	2.09	0.53
1:E:132:LEU:N	1:E:133:PRO:CD	2.70	0.53
1:D:36:ARG:HG3	1:D:37:PRO:HD3	1.90	0.53
1:A:33:LEU:HD11	1:A:60:ASP:HB3	1.89	0.53
1:D:157:ARG:O	1:D:158:ASP:C	2.47	0.53
1:A:40:PRO:C	1:A:42:LEU:H	2.12	0.53
1:A:33:LEU:HG	1:A:63:VAL:O	2.08	0.53
1:C:143:LEU:HD13	1:C:191:LEU:CD2	2.39	0.53
1:E:21:SER:OG	1:E:69:VAL:HG21	2.09	0.53
1:A:42:LEU:O	1:A:42:LEU:HD23	2.09	0.53
1:A:170:GLU:CG	1:A:177:VAL:HB	2.39	0.53
1:B:169:VAL:HB	1:B:204:VAL:HG12	1.91	0.53
1:D:181:THR:OG1	1:D:182:ASP:O	2.17	0.53
1:A:85:LEU:O	1:A:89:ILE:HG13	2.09	0.53
1:B:267:THR:O	1:B:386:ALA:HB2	2.09	0.53
1:C:231:GLY:O	1:C:234:VAL:HG12	2.08	0.53
1:D:139:LEU:HD22	1:D:193:TRP:HE1	1.74	0.52
1:C:109:LEU:C	1:C:109:LEU:HD12	2.29	0.52
1:F:98:VAL:HG12	1:F:111:CYS:SG	2.49	0.52
1:C:88:ASP:HB3	1:D:289:LEU:HD22	1.91	0.52
1:E:338:THR:O	1:E:341:THR:HG22	2.09	0.52
1:E:91:ARG:HG2	1:E:92:ALA:N	2.22	0.52
1:C:245:ASN:H	1:C:245:ASN:ND2	2.06	0.52
1:F:231:GLY:H	1:F:234:VAL:HG12	1.75	0.52
1:F:44:GLY:HA2	1:F:83:GLY:H	1.74	0.52
1:B:93:LEU:HD22	1:B:111:CYS:HB3	1.92	0.52
1:B:99:ASP:O	1:B:109:LEU:HA	2.10	0.52
1:D:245:ASN:O	1:D:245:ASN:ND2	2.40	0.52
1:E:106:ARG:HD3	1:E:117:SER:OG	2.10	0.52
1:A:353:SER:HB2	1:A:368:VAL:CG2	2.40	0.52
1:F:243:SER:CB	1:F:248:ARG:HB3	2.39	0.52
1:C:55:THR:HG22	1:C:68:GLN:HG2	1.92	0.51
1:E:106:ARG:HH11	1:E:106:ARG:CG	2.23	0.51
1:D:98:VAL:HG12	1:D:111:CYS:HB2	1.91	0.51
1:E:134:GLU:OE2	1:E:229:GLY:HA2	2.10	0.51
1:A:146:GLU:HG3	1:A:348:ARG:NH1	2.26	0.51
1:F:200:ILE:HD11	1:F:230:THR:CG2	2.41	0.51
1:E:234:VAL:HG21	1:E:236:LYS:CG	2.40	0.51
1:E:131:THR:C	1:E:133:PRO:HD3	2.31	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:ARG:HH12	1:A:38:ALA:HB2	1.76	0.51
1:F:59:PHE:HB2	1:F:129:LEU:HD12	1.92	0.51
1:E:186:LEU:HD21	1:E:261:PHE:HB2	1.93	0.51
1:D:366:ARG:HD3	1:D:389:THR:HG21	1.91	0.51
1:D:159:ASP:C	1:D:161:LEU:H	2.13	0.50
1:D:36:ARG:N	1:D:37:PRO:CD	2.75	0.50
1:F:364:LEU:HD21	1:F:366:ARG:NH2	2.26	0.50
1:A:33:LEU:HD11	1:A:60:ASP:CB	2.42	0.50
1:A:387:VAL:CG2	1:A:388:SER:N	2.73	0.50
1:A:168:ARG:NH1	1:A:203:ALA:HB1	2.27	0.50
1:D:269:HIS:HB3	1:D:356:PHE:O	2.10	0.50
1:D:28:TRP:HE1	1:D:219:ILE:HG22	1.76	0.50
1:A:14:THR:HB	1:A:74:VAL:HG22	1.93	0.50
1:F:16:ARG:CD	1:F:97:PRO:HB2	2.42	0.50
1:D:139:LEU:HB3	1:D:193:TRP:CD1	2.47	0.50
1:A:176:VAL:HB	1:A:191:LEU:HB3	1.92	0.50
1:A:290:VAL:HG12	1:A:290:VAL:O	2.12	0.50
1:D:19:ARG:NH2	1:D:91:ARG:HA	2.23	0.50
1:F:22:PHE:O	1:F:26:VAL:HG23	2.12	0.50
1:A:169:VAL:HG12	1:A:178:LEU:HD22	1.93	0.50
1:F:219:ILE:C	1:F:219:ILE:HD13	2.31	0.49
1:C:347:LEU:HB3	1:C:367:PRO:HB3	1.93	0.49
1:E:359:ALA:HB3	1:E:399:ARG:HH21	1.76	0.49
1:B:372:ASP:O	1:B:374:PRO:HD3	2.13	0.49
1:E:206:VAL:CG2	1:E:207:PRO:HD2	2.31	0.49
1:A:59:PHE:CB	1:A:64:SER:HA	2.35	0.49
1:D:259:PRO:HB3	1:F:163:MET:HG2	1.94	0.49
1:A:274:THR:HA	1:A:352:VAL:O	2.12	0.49
1:A:357:THR:HG22	1:A:358:THR:HG23	1.95	0.49
1:A:36:ARG:NH1	1:A:38:ALA:CB	2.73	0.49
1:E:314:ASP:O	1:E:315:VAL:HG12	2.13	0.49
1:D:396:MET:HE3	1:D:397:PRO:HD2	1.95	0.49
1:A:151:VAL:CG2	1:A:167:ILE:HD13	2.42	0.49
1:F:41:VAL:HG21	1:F:125:ASP:HB3	1.95	0.49
1:D:228:LEU:O	1:D:235:GLY:HA2	2.13	0.49
1:A:33:LEU:HD21	1:A:60:ASP:OD1	2.12	0.49
1:F:63:VAL:HB	1:F:251:THR:HA	1.95	0.49
1:A:233:GLY:C	1:A:234:VAL:HG13	2.33	0.49
1:B:284:ILE:HD13	1:B:308:LEU:HD21	1.94	0.48
1:C:297:VAL:HG23	1:C:337:PRO:HG3	1.93	0.48
1:F:22:PHE:CD2	1:F:98:VAL:HG21	2.46	0.48
1:E:150:GLN:OE1	1:E:189:ARG:HD3	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:129:LEU:N	1:D:129:LEU:HD22	2.27	0.48
1:A:114:ALA:CB	1:B:320:GLU:HG2	2.43	0.48
1:F:59:PHE:HB2	1:F:129:LEU:CD1	2.43	0.48
1:E:289:LEU:HD23	1:F:89:ILE:HA	1.95	0.48
1:D:109:LEU:HB3	1:D:116:PHE:HB2	1.95	0.48
1:C:96:LYS:HD2	1:C:112:GLY:HA3	1.94	0.48
1:E:15:PHE:CD2	1:E:17:LEU:HD13	2.48	0.48
1:C:296:GLN:HG3	1:C:334:ALA:HB1	1.96	0.48
1:D:48:THR:HG23	1:D:78:SER:HB3	1.94	0.48
1:D:50:SER:O	1:D:51:ASP:C	2.52	0.48
1:A:315:VAL:HA	1:B:119:PRO:CG	2.42	0.48
1:B:181:THR:O	1:B:181:THR:HG23	2.12	0.48
1:E:35:ALA:HB1	1:E:39:VAL:HG23	1.94	0.48
1:D:296:GLN:HG2	1:D:398:VAL:HG21	1.94	0.48
1:E:236:LYS:O	1:E:237:ASP:HB2	2.13	0.48
1:A:166:GLY:HA2	1:A:207:PRO:HA	1.96	0.48
1:E:365:LEU:HD23	1:E:365:LEU:N	2.28	0.48
1:F:262:ARG:HA	1:F:265:LEU:HD12	1.95	0.48
1:F:232:PRO:HG2	1:F:233:GLY:H	1.79	0.48
1:E:206:VAL:HG23	1:E:207:PRO:CD	2.31	0.47
1:A:157:ARG:CD	1:A:157:ARG:O	2.57	0.47
1:C:13:LEU:HD13	1:C:77:GLY:O	2.14	0.47
1:C:340:LEU:O	1:C:344:LEU:HD22	2.15	0.47
1:F:59:PHE:CE2	1:F:130:PRO:HD3	2.48	0.47
1:D:80:LEU:HD23	1:D:121:MET:HB2	1.94	0.47
1:E:167:ILE:HG13	1:E:208:ALA:HA	1.96	0.47
1:A:161:LEU:N	1:A:161:LEU:CD1	2.61	0.47
1:E:19:ARG:C	1:E:19:ARG:HD3	2.35	0.47
1:A:90:THR:HA	1:A:93:LEU:HD12	1.97	0.47
1:C:98:VAL:HB	1:C:111:CYS:HB2	1.97	0.47
1:F:34:PRO:HB2	1:F:36:ARG:CZ	2.44	0.47
1:E:204:VAL:HG21	1:E:253:LEU:HG	1.94	0.47
1:C:298:ARG:HD2	1:C:309:SER:OG	2.15	0.47
1:F:37:PRO:CG	1:F:43:SER:HB3	2.35	0.47
1:B:146:GLU:HG3	1:B:348:ARG:HH11	1.79	0.47
1:F:298:ARG:HH22	1:F:311:GLY:N	2.12	0.47
1:F:148:ILE:HD12	1:F:211:LEU:HD13	1.95	0.47
1:A:233:GLY:O	1:A:234:VAL:HG22	2.14	0.47
1:A:236:LYS:O	1:A:236:LYS:HD2	2.14	0.47
1:E:168:ARG:NH1	1:E:203:ALA:HB1	2.29	0.47
1:A:33:LEU:HD21	1:A:60:ASP:CG	2.36	0.47
1:C:271:ALA:HB3	1:C:356:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:307:ARG:HG3	1:C:321:ASP:OD2	2.14	0.47
1:A:205:LEU:HD23	1:A:254:LEU:HD13	1.96	0.47
1:B:354:PHE:CE1	1:B:365:LEU:HD22	2.50	0.47
1:E:20:GLU:N	1:E:20:GLU:CD	2.60	0.47
1:B:159:ASP:C	1:B:161:LEU:H	2.17	0.47
1:B:306:VAL:HG12	1:B:324:VAL:HB	1.96	0.47
1:E:206:VAL:HB	1:E:253:LEU:CD1	2.45	0.47
1:E:17:LEU:C	1:E:18:LEU:HD13	2.35	0.47
1:A:181:THR:HG22	1:A:258:PHE:HZ	1.78	0.46
1:F:270:THR:HG23	1:F:357:THR:HG23	1.97	0.46
1:D:234:VAL:C	1:D:236:LYS:N	2.67	0.46
1:E:13:LEU:O	1:E:102:VAL:CG1	2.64	0.46
1:A:399:ARG:H	1:A:399:ARG:CD	2.28	0.46
1:D:148:ILE:CG2	1:D:212:ALA:HA	2.46	0.46
1:A:93:LEU:HD22	1:A:111:CYS:HB3	1.97	0.46
1:B:106:ARG:NH2	1:B:117:SER:O	2.48	0.46
1:D:273:ALA:HB2	1:D:326:TYR:HD1	1.80	0.46
1:E:334:ALA:HB3	1:E:398:VAL:O	2.15	0.46
1:F:296:GLN:CB	1:F:337:PRO:HD3	2.27	0.46
1:A:135:GLU:OE2	1:A:138:LEU:HD12	2.15	0.46
1:A:356:PHE:N	1:A:356:PHE:CD2	2.80	0.46
1:E:315:VAL:O	1:F:106:ARG:NH2	2.45	0.46
1:F:200:ILE:HD11	1:F:230:THR:HG22	1.97	0.46
1:D:161:LEU:O	1:D:162:PRO:C	2.54	0.46
1:A:358:THR:C	1:A:360:GLY:H	2.19	0.46
1:E:15:PHE:CE2	1:E:17:LEU:HD13	2.50	0.46
1:A:98:VAL:HG12	1:A:111:CYS:SG	2.55	0.46
1:F:14:THR:OG1	1:F:101:HIS:HD2	1.99	0.46
1:B:296:GLN:HA	1:B:337:PRO:HD3	1.96	0.46
1:F:100:VAL:HA	1:F:108:ALA:O	2.16	0.46
1:F:42:LEU:CD1	1:F:59:PHE:O	2.64	0.46
1:A:298:ARG:HH22	1:A:400:LEU:HA	1.81	0.45
1:B:312:ALA:O	1:B:313:ASP:C	2.54	0.45
1:D:236:LYS:HD2	1:D:236:LYS:HA	1.68	0.45
1:D:143:LEU:HD22	1:D:191:LEU:HD21	1.98	0.45
1:A:254:LEU:HD12	1:A:254:LEU:H	1.82	0.45
1:F:164:LEU:HD21	1:F:182:ASP:HA	1.98	0.45
1:D:217:ALA:O	1:D:219:ILE:HG23	2.16	0.45
1:B:384:PHE:N	1:B:385:PRO:CD	2.79	0.45
1:C:291:ALA:HA	1:C:311:GLY:O	2.17	0.45
1:B:170:GLU:OE1	1:B:262:ARG:NH2	2.50	0.45
1:E:79:VAL:HG21	1:E:107:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:364:LEU:HD12	1:A:366:ARG:HG3	1.99	0.45
1:A:149:SER:HB2	1:A:216:LYS:NZ	2.31	0.45
1:F:304:GLY:HA2	1:F:324:VAL:O	2.16	0.45
1:C:45:VAL:HG23	1:C:57:SER:O	2.16	0.45
1:F:74:VAL:HG12	1:F:75:SER:OG	2.16	0.45
1:D:155:ALA:O	1:D:156:GLY:O	2.35	0.45
1:F:222:SER:OG	1:F:223:ASP:N	2.50	0.45
1:D:219:ILE:O	1:D:219:ILE:CG1	2.65	0.45
1:D:148:ILE:HG21	1:D:212:ALA:HA	1.99	0.45
1:D:170:GLU:OE1	1:D:262:ARG:NH2	2.50	0.45
1:A:364:LEU:CD2	1:A:394:LEU:HD12	2.46	0.45
1:D:185:ARG:NH2	1:D:342:ASP:OD2	2.50	0.45
1:C:146:GLU:O	1:C:150:GLN:HG3	2.16	0.45
1:B:78:SER:OG	1:B:123:VAL:HG11	2.17	0.45
1:E:204:VAL:HG22	1:E:205:LEU:N	2.33	0.44
1:B:50:SER:HB3	1:B:51:ASP:H	1.64	0.44
1:C:206:VAL:HG21	1:C:211:LEU:HG	1.99	0.44
1:A:269:HIS:CD2	1:A:272:VAL:HG12	2.51	0.44
1:D:137:GLY:HA3	1:D:193:TRP:CH2	2.52	0.44
1:E:15:PHE:CE2	1:E:17:LEU:CD1	3.00	0.44
1:E:186:LEU:HB3	1:E:394:LEU:HB3	1.99	0.44
1:A:357:THR:CG2	1:A:361:LYS:HD2	2.48	0.44
1:C:315:VAL:HG13	1:D:106:ARG:HH22	1.81	0.44
1:A:283:ALA:HA	1:A:286:LEU:HB2	2.00	0.44
1:A:293:ARG:HA	1:A:293:ARG:HD2	1.81	0.44
1:A:167:ILE:HG12	1:A:180:ALA:HB2	1.99	0.44
1:A:148:ILE:HG12	1:A:148:ILE:H	1.47	0.44
1:E:17:LEU:HB3	1:E:71:ALA:HB1	2.00	0.44
1:F:280:LEU:HG	1:F:284:ILE:HD11	1.99	0.44
1:E:237:ASP:N	1:E:237:ASP:OD1	2.51	0.44
1:A:152:ALA:HB2	1:A:167:ILE:HD11	2.00	0.44
1:A:106:ARG:CG	1:A:106:ARG:NH1	2.78	0.44
1:C:171:ILE:HG21	1:C:193:TRP:HZ3	1.83	0.44
1:F:273:ALA:HB2	1:F:326:TYR:HD1	1.83	0.44
1:D:217:ALA:O	1:D:219:ILE:N	2.50	0.44
1:E:292:ASP:O	1:E:293:ARG:HG2	2.18	0.44
1:F:133:PRO:HG2	1:F:227:SER:O	2.17	0.44
1:D:366:ARG:HD2	1:D:389:THR:CG2	2.41	0.44
1:F:60:ASP:HB3	1:F:63:VAL:O	2.18	0.44
1:C:301:PHE:HB3	1:C:326:TYR:CE1	2.53	0.44
1:B:60:ASP:HB3	1:B:63:VAL:O	2.18	0.44
1:B:335:PHE:CD1	1:B:395:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ALA:HB2	1:A:326:TYR:CD1	2.44	0.44
1:E:63:VAL:HG23	1:E:250:THR:O	2.18	0.44
1:A:182:ASP:OD1	1:A:183:ARG:N	2.49	0.44
1:F:64:SER:O	1:F:249:SER:HB2	2.18	0.44
1:F:350:GLU:HG2	1:F:351:ARG:HG2	2.00	0.44
1:E:236:LYS:O	1:E:237:ASP:CB	2.65	0.43
1:A:45:VAL:HG23	1:A:57:SER:O	2.18	0.43
1:C:204:VAL:HG22	1:C:253:LEU:HG	2.00	0.43
1:B:33:LEU:HA	1:B:34:PRO:HD3	1.87	0.43
1:B:167:ILE:HG13	1:B:208:ALA:HB2	2.00	0.43
1:F:80:LEU:HD23	1:F:121:MET:CB	2.39	0.43
1:F:219:ILE:HG12	1:F:219:ILE:O	2.18	0.43
1:A:146:GLU:HG3	1:A:348:ARG:HH12	1.81	0.43
1:E:32:ASN:O	1:E:32:ASN:CG	2.56	0.43
1:E:131:THR:CA	1:E:133:PRO:HD3	2.48	0.43
1:A:188:VAL:HB	1:A:392:VAL:HG12	1.99	0.43
1:F:59:PHE:HD2	1:F:129:LEU:HA	1.83	0.43
1:D:163:MET:HE3	1:D:257:GLU:C	2.39	0.43
1:A:234:VAL:O	1:A:237:ASP:OD1	2.35	0.43
1:A:171:ILE:HG12	1:A:193:TRP:CZ3	2.54	0.43
1:C:99:ASP:N	1:C:99:ASP:OD2	2.51	0.43
1:F:25:ALA:CB	1:F:56:ILE:HD12	2.43	0.43
1:F:290:VAL:HG21	1:F:318:ALA:N	2.34	0.43
1:B:290:VAL:HG13	1:B:290:VAL:O	2.19	0.43
1:A:35:ALA:CA	1:A:84:ARG:HE	2.18	0.43
1:D:161:LEU:HD22	1:F:183:ARG:HD3	2.00	0.43
1:A:362:PRO:HG3	1:A:396:MET:SD	2.58	0.43
1:D:239:LEU:HD23	1:D:250:THR:HB	2.01	0.43
1:A:185:ARG:NH1	1:A:342:ASP:OD2	2.45	0.43
1:E:238:GLY:C	1:E:253:LEU:HD22	2.39	0.43
1:A:148:ILE:HD13	1:A:148:ILE:HG23	1.57	0.43
1:C:55:THR:HA	1:C:67:ALA:O	2.18	0.43
1:C:270:THR:HG23	1:C:357:THR:HA	2.00	0.43
1:F:300:GLU:HG3	1:F:332:THR:HG23	2.00	0.43
1:B:226:LEU:HD12	1:B:242:ILE:HG22	2.01	0.43
1:C:262:ARG:HB2	1:C:262:ARG:HE	1.69	0.43
1:B:192:LYS:CD	1:B:192:LYS:H	2.31	0.43
1:D:274:THR:HA	1:D:352:VAL:O	2.18	0.43
1:A:399:ARG:HG2	1:A:400:LEU:H	1.83	0.43
1:D:261:PHE:HA	1:D:264:LEU:HD12	2.00	0.43
1:C:29:VAL:HG13	1:C:58:GLY:HA3	2.01	0.42
1:F:364:LEU:HD13	1:F:394:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:16:ARG:NE	1:F:99:ASP:OD2	2.52	0.42
1:A:173:GLY:HA2	1:A:199:ASP:HA	2.00	0.42
1:E:132:LEU:HB2	1:E:239:LEU:HD22	2.02	0.42
1:B:80:LEU:HB2	1:B:123:VAL:HG22	2.01	0.42
1:E:28:TRP:CH2	1:E:247:LYS:HB3	2.54	0.42
1:F:42:LEU:HD11	1:F:59:PHE:O	2.18	0.42
1:B:46:LEU:HB3	1:B:57:SER:HB2	2.01	0.42
1:B:353:SER:O	1:B:365:LEU:HA	2.19	0.42
1:B:189:ARG:HD2	1:B:189:ARG:HA	1.87	0.42
1:B:54:LEU:HD13	1:B:54:LEU:O	2.19	0.42
1:C:91:ARG:NH1	1:C:91:ARG:HB3	2.33	0.42
1:D:42:LEU:HG	1:D:60:ASP:HA	2.02	0.42
1:C:290:VAL:O	1:C:290:VAL:HG12	2.20	0.42
1:E:171:ILE:HG23	1:E:193:TRP:HZ3	1.84	0.42
1:E:185:ARG:NH2	1:E:339:TYR:HD1	2.17	0.42
1:B:354:PHE:CD1	1:B:356:PHE:HZ	2.34	0.42
1:B:45:VAL:HG13	1:B:47:LEU:HD13	2.01	0.42
1:B:14:THR:HA	1:B:100:VAL:O	2.20	0.42
1:C:92:ALA:O	1:D:286:LEU:HD13	2.20	0.42
1:F:59:PHE:HE2	1:F:130:PRO:HD3	1.84	0.42
1:A:281:ILE:HD11	1:A:344:LEU:HB3	2.00	0.42
1:A:262:ARG:HA	1:A:265:LEU:HD12	2.01	0.42
1:F:139:LEU:HB3	1:F:193:TRP:CD1	2.54	0.42
1:A:48:THR:HB	1:A:55:THR:OG1	2.20	0.42
1:E:350:GLU:HB3	1:E:351:ARG:HG2	2.01	0.42
1:D:357:THR:HG22	1:D:358:THR:HG23	2.02	0.42
1:F:366:ARG:HB3	1:F:389:THR:HG21	2.01	0.42
1:C:234:VAL:CG2	1:C:235:GLY:N	2.82	0.42
1:D:232:PRO:HG2	1:D:233:GLY:H	1.84	0.42
1:C:353:SER:HB3	1:C:366:ARG:HG3	2.00	0.42
1:F:161:LEU:HA	1:F:162:PRO:HD3	1.81	0.42
1:E:206:VAL:HB	1:E:253:LEU:HD12	2.02	0.42
1:D:28:TRP:HE1	1:D:219:ILE:CG2	2.33	0.42
1:E:245:ASN:C	1:E:247:LYS:H	2.24	0.42
1:E:85:LEU:HD22	1:F:315:VAL:HG22	2.02	0.42
1:B:368:VAL:O	1:B:370:GLY:N	2.47	0.42
1:A:40:PRO:O	1:A:42:LEU:N	2.52	0.41
1:F:357:THR:HB	1:F:361:LYS:HE3	2.02	0.41
1:C:239:LEU:HG	1:C:250:THR:HB	2.01	0.41
1:C:358:THR:HG23	1:C:361:LYS:HE3	2.02	0.41
1:B:300:GLU:HB2	1:B:307:ARG:HB3	2.02	0.41
1:D:234:VAL:O	1:D:235:GLY:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:135:GLU:HG3	1:E:135:GLU:H	1.58	0.41
1:C:75:SER:HA	1:C:76:PRO:HD3	1.91	0.41
1:B:99:ASP:HB2	1:B:110:THR:HB	2.02	0.41
1:D:47:LEU:O	1:D:78:SER:HA	2.20	0.41
1:B:147:ALA:HB1	1:B:178:LEU:HD12	2.01	0.41
1:E:319:GLU:HB2	1:F:115:ARG:HB2	2.03	0.41
1:E:358:THR:C	1:E:360:GLY:H	2.24	0.41
1:C:59:PHE:HB2	1:C:129:LEU:CD2	2.50	0.41
1:F:268:GLU:HG3	1:F:269:HIS:H	1.85	0.41
1:A:93:LEU:HA	1:B:286:LEU:HD11	2.01	0.41
1:C:346:SER:O	1:C:348:ARG:HD2	2.20	0.41
1:E:221:GLY:C	1:E:223:ASP:H	2.24	0.41
1:E:37:PRO:HB2	1:E:38:ALA:H	1.62	0.41
1:D:150:GLN:HE21	1:D:348:ARG:HD2	1.86	0.41
1:F:98:VAL:HA	1:F:111:CYS:SG	2.61	0.41
1:B:153:ILE:HD11	1:B:346:SER:HB2	2.01	0.41
1:E:290:VAL:HG11	1:E:316:GLY:O	2.19	0.41
1:D:59:PHE:CD1	1:D:64:SER:HB2	2.55	0.41
1:B:386:ALA:O	1:B:387:VAL:CG1	2.68	0.41
1:F:218:GLY:CA	1:F:245:ASN:ND2	2.79	0.41
1:E:15:PHE:HE2	1:E:17:LEU:HD11	1.84	0.41
1:E:79:VAL:CG2	1:E:80:LEU:N	2.84	0.41
1:C:41:VAL:HG11	1:C:125:ASP:HB3	2.03	0.41
1:A:169:VAL:HG23	1:A:204:VAL:HG12	2.03	0.41
1:A:33:LEU:CD2	1:A:63:VAL:HG13	2.51	0.41
1:C:93:LEU:HD11	1:C:109:LEU:HD11	2.02	0.41
1:C:288:ALA:C	1:C:290:VAL:H	2.24	0.41
1:F:268:GLU:HG3	1:F:269:HIS:N	2.35	0.41
1:E:134:GLU:CD	1:E:229:GLY:HA2	2.41	0.41
1:A:152:ALA:O	1:A:157:ARG:NH2	2.54	0.41
1:A:269:HIS:HD2	1:A:272:VAL:HG13	1.85	0.41
1:B:100:VAL:HA	1:B:108:ALA:O	2.21	0.41
1:F:126:TYR:HA	1:F:127:PRO:HD3	1.94	0.41
1:E:313:ASP:C	1:E:315:VAL:H	2.24	0.41
1:C:294:GLY:O	1:C:337:PRO:HD2	2.21	0.41
1:C:93:LEU:HD23	1:D:286:LEU:HD21	2.03	0.41
1:E:106:ARG:NH1	1:E:106:ARG:CG	2.83	0.41
1:F:59:PHE:CD2	1:F:129:LEU:HA	2.56	0.41
1:E:79:VAL:HG22	1:E:80:LEU:N	2.35	0.41
1:E:299:MET:HG2	1:E:308:LEU:HD12	2.02	0.41
1:B:274:THR:HA	1:B:352:VAL:O	2.21	0.41
1:D:152:ALA:HB2	1:D:167:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:275:MET:HB3	1:C:324:VAL:HG12	2.03	0.41
1:E:164:LEU:C	1:E:166:GLY:H	2.23	0.41
1:E:205:LEU:HD23	1:E:254:LEU:HB2	2.03	0.41
1:C:33:LEU:HD11	1:C:45:VAL:HB	2.03	0.41
1:F:51:ASP:C	1:F:53:GLY:N	2.74	0.41
1:D:255:ASP:N	1:D:255:ASP:OD2	2.54	0.41
1:D:297:VAL:HG13	1:D:337:PRO:HG3	2.02	0.41
1:B:197:SER:HB2	1:B:200:ILE:HD13	2.02	0.40
1:B:54:LEU:HD12	1:B:69:VAL:CG1	2.50	0.40
1:A:42:LEU:HD11	1:A:60:ASP:HA	2.03	0.40
1:E:287:VAL:O	1:E:310:ALA:HB3	2.21	0.40
1:C:134:GLU:OE1	1:C:229:GLY:HA2	2.21	0.40
1:F:346:SER:HG	1:F:391:TYR:HH	1.68	0.40
1:A:228:LEU:O	1:A:234:VAL:HB	2.21	0.40
1:C:286:LEU:HG	1:D:116:PHE:HZ	1.86	0.40
1:A:198:PRO:O	1:A:199:ASP:C	2.59	0.40
1:C:283:ALA:O	1:C:287:VAL:HG22	2.22	0.40
1:C:275:MET:HE3	1:C:324:VAL:HG12	2.03	0.40
1:E:274:THR:OG1	1:E:325:ASP:HB2	2.21	0.40
1:B:44:GLY:HA2	1:B:83:GLY:H	1.87	0.40
1:A:157:ARG:HB3	1:A:165:THR:HG21	2.03	0.40
1:A:14:THR:HA	1:A:100:VAL:O	2.21	0.40
1:C:232:PRO:O	1:C:234:VAL:HG12	2.22	0.40
1:E:296:GLN:NE2	1:E:400:LEU:HD22	2.36	0.40
1:D:14:THR:HG23	1:D:101:HIS:HB3	2.03	0.40
1:E:162:PRO:HA	1:E:165:THR:OG1	2.21	0.40
1:E:24:ASP:OD1	1:E:24:ASP:C	2.59	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	371/408 (91%)	309 (83%)	47 (13%)	15 (4%)	5 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	379/408 (93%)	334 (88%)	36 (10%)	9 (2%)	9	35
1	C	366/408 (90%)	327 (89%)	36 (10%)	3 (1%)	27	68
1	D	365/408 (90%)	315 (86%)	41 (11%)	9 (2%)	9	32
1	E	365/408 (90%)	302 (83%)	51 (14%)	12 (3%)	6	24
1	F	368/408 (90%)	334 (91%)	28 (8%)	6 (2%)	14	47
All	All	2214/2448 (90%)	1921 (87%)	239 (11%)	54 (2%)	9	35

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	LYS
1	A	234	VAL
1	B	198	PRO
1	A	34	PRO
1	A	41	VAL
1	A	51	ASP
1	A	220	GLY
1	A	231	GLY
1	A	232	PRO
1	A	237	ASP
1	B	158	ASP
1	B	313	ASP
1	C	137	GLY
1	C	232	PRO
1	D	51	ASP
1	D	156	GLY
1	D	198	PRO
1	D	218	GLY
1	D	235	GLY
1	D	261	PHE
1	E	37	PRO
1	E	165	THR
1	E	222	SER
1	F	104	GLY
1	F	313	ASP
1	A	164	LEU
1	A	196	SER
1	A	270	THR
1	A	359	ALA
1	C	222	SER

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Mol	Chain	Res	Type
1	D	158	ASP
1	E	95	ASN
1	E	132	LEU
1	E	198	PRO
1	F	221	GLY
1	B	160	THR
1	B	369	SER
1	D	233	GLY
1	E	221	GLY
1	F	52	ASN
1	F	245	ASN
1	B	292	ASP
1	B	330	PRO
1	D	292	ASP
1	E	124	GLU
1	E	133	PRO
1	E	219	ILE
1	A	38	ALA
1	A	370	GLY
1	E	303	ASP
1	F	302	ALA
1	E	315	VAL
1	B	200	ILE
1	B	104	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/322 (92%)	225 (76%)	72 (24%)	1	3
1	B	303/322 (94%)	253 (84%)	50 (16%)	3	9
1	C	294/322 (91%)	232 (79%)	62 (21%)	1	5
1	D	293/322 (91%)	233 (80%)	60 (20%)	2	5
1	E	293/322 (91%)	237 (81%)	56 (19%)	2	6
1	F	295/322 (92%)	239 (81%)	56 (19%)	2	6
All	All	1775/1932 (92%)	1419 (80%)	356 (20%)	2	6

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	19	ARG
1	A	24	ASP
1	A	36	ARG
1	A	51	ASP
1	A	54	LEU
1	A	56	ILE
1	A	61	TYR
1	A	63	VAL
1	A	68	GLN
1	A	69	VAL
1	A	73	ILE
1	A	74	VAL
1	A	78	SER
1	A	85	LEU
1	A	98	VAL
1	A	105	ASN
1	A	106	ARG
1	A	115	ARG
1	A	120	THR
1	A	129	LEU
1	A	131	THR
1	A	138	LEU
1	A	143	LEU
1	A	148	ILE
1	A	153	ILE
1	A	157	ARG
1	A	160	THR
1	A	161	LEU
1	A	164	LEU
1	A	165	THR
1	A	170	GLU
1	A	172	LEU
1	A	181	THR
1	A	183	ARG
1	A	191	LEU
1	A	192	LYS
1	A	204	VAL
1	A	206	VAL
1	A	207	PRO
1	A	210	THR
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	216	LYS
1	A	223	ASP
1	A	225	ARG
1	A	226	LEU
1	A	228	LEU
1	A	234	VAL
1	A	236	LYS
1	A	237	ASP
1	A	240	LEU
1	A	242	ILE
1	A	245	ASN
1	A	251	THR
1	A	254	LEU
1	A	269	HIS
1	A	286	LEU
1	A	289	LEU
1	A	293	ARG
1	A	305	SER
1	A	323	VAL
1	A	324	VAL
1	A	329	GLU
1	A	338	THR
1	A	344	LEU
1	A	346	SER
1	A	352	VAL
1	A	356	PHE
1	A	364	LEU
1	A	394	LEU
1	A	395	LEU
1	A	399	ARG
1	B	17	LEU
1	B	19	ARG
1	B	32	ASN
1	B	42	LEU
1	B	52	ASN
1	B	54	LEU
1	B	75	SER
1	B	79	VAL
1	B	84	ARG
1	B	109	LEU
1	B	132	LEU
1	B	142	GLU

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Mol	Chain	Res	Type
1	B	153	ILE
1	B	163	MET
1	B	183	ARG
1	B	185	ARG
1	B	191	LEU
1	B	192	LYS
1	B	196	SER
1	B	204	VAL
1	B	206	VAL
1	B	209	LYS
1	B	211	LEU
1	B	219	ILE
1	B	236	LYS
1	B	242	ILE
1	B	245	ASN
1	B	251	THR
1	B	252	ARG
1	B	253	LEU
1	B	254	LEU
1	B	263	GLN
1	B	285	LYS
1	B	286	LEU
1	B	289	LEU
1	B	290	VAL
1	B	300	GLU
1	B	313	ASP
1	B	317	ARG
1	B	325	ASP
1	B	329	GLU
1	B	341	THR
1	B	344	LEU
1	B	347	LEU
1	B	348	ARG
1	B	365	LEU
1	B	371	ASP
1	B	388	SER
1	B	395	LEU
1	B	400	LEU
1	C	18	LEU
1	C	19	ARG
1	C	48	THR
1	C	54	LEU

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Mol	Chain	Res	Type
1	C	56	ILE
1	C	63	VAL
1	C	74	VAL
1	C	85	LEU
1	C	91	ARG
1	C	98	VAL
1	C	99	ASP
1	C	105	ASN
1	C	109	LEU
1	C	113	ASN
1	C	115	ARG
1	C	124	GLU
1	C	125	ASP
1	C	128	THR
1	C	131	THR
1	C	138	LEU
1	C	139	LEU
1	C	142	GLU
1	C	143	LEU
1	C	153	ILE
1	C	160	THR
1	C	161	LEU
1	C	163	MET
1	C	185	ARG
1	C	191	LEU
1	C	192	LYS
1	C	204	VAL
1	C	206	VAL
1	C	210	THR
1	C	211	LEU
1	C	213	GLU
1	C	219	ILE
1	C	234	VAL
1	C	236	LYS
1	C	245	ASN
1	C	247	LYS
1	C	253	LEU
1	C	262	ARG
1	C	267	THR
1	C	279	GLU
1	C	289	LEU
1	C	293	ARG

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Mol	Chain	Res	Type
1	C	298	ARG
1	C	309	SER
1	C	314	ASP
1	C	320	GLU
1	C	341	THR
1	C	344	LEU
1	C	346	SER
1	C	347	LEU
1	C	349	SER
1	C	358	THR
1	C	365	LEU
1	C	368	VAL
1	C	388	SER
1	C	394	LEU
1	C	395	LEU
1	C	400	LEU
1	D	21	SER
1	D	27	SER
1	D	33	LEU
1	D	36	ARG
1	D	41	VAL
1	D	45	VAL
1	D	48	THR
1	D	50	SER
1	D	51	ASP
1	D	52	ASN
1	D	54	LEU
1	D	69	VAL
1	D	73	ILE
1	D	75	SER
1	D	79	VAL
1	D	91	ARG
1	D	105	ASN
1	D	109	LEU
1	D	110	THR
1	D	115	ARG
1	D	128	THR
1	D	129	LEU
1	D	131	THR
1	D	134	GLU
1	D	138	LEU
1	D	142	GLU

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Mol	Chain	Res	Type
1	D	143	LEU
1	D	158	ASP
1	D	174	GLU
1	D	185	ARG
1	D	191	LEU
1	D	192	LYS
1	D	196	SER
1	D	204	VAL
1	D	206	VAL
1	D	211	LEU
1	D	219	ILE
1	D	223	ASP
1	D	226	LEU
1	D	230	THR
1	D	236	LYS
1	D	237	ASP
1	D	239	LEU
1	D	242	ILE
1	D	245	ASN
1	D	253	LEU
1	D	255	ASP
1	D	270	THR
1	D	282	GLU
1	D	313	ASP
1	D	329	GLU
1	D	341	THR
1	D	344	LEU
1	D	345	SER
1	D	346	SER
1	D	347	LEU
1	D	369	SER
1	D	389	THR
1	D	395	LEU
1	D	399	ARG
1	E	13	LEU
1	E	17	LEU
1	E	18	LEU
1	E	21	SER
1	E	22	PHE
1	E	24	ASP
1	E	32	ASN
1	E	45	VAL

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Mol	Chain	Res	Type
1	E	48	THR
1	E	61	TYR
1	E	72	GLU
1	E	73	ILE
1	E	91	ARG
1	E	93	LEU
1	E	95	ASN
1	E	96	LYS
1	E	99	ASP
1	E	102	VAL
1	E	105	ASN
1	E	106	ARG
1	E	111	CYS
1	E	115	ARG
1	E	123	VAL
1	E	125	ASP
1	E	129	LEU
1	E	135	GLU
1	E	139	LEU
1	E	143	LEU
1	E	158	ASP
1	E	163	MET
1	E	183	ARG
1	E	185	ARG
1	E	191	LEU
1	E	192	LYS
1	E	206	VAL
1	E	209	LYS
1	E	210	THR
1	E	211	LEU
1	E	239	LEU
1	E	240	LEU
1	E	242	ILE
1	E	243	SER
1	E	248	ARG
1	E	253	LEU
1	E	263	GLN
1	E	289	LEU
1	E	296	GLN
1	E	309	SER
1	E	320	GLU
1	E	329	GLU

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Mol	Chain	Res	Type
1	E	344	LEU
1	E	347	LEU
1	E	350	GLU
1	E	358	THR
1	E	365	LEU
1	E	395	LEU
1	F	19	ARG
1	F	33	LEU
1	F	36	ARG
1	F	42	LEU
1	F	47	LEU
1	F	54	LEU
1	F	63	VAL
1	F	73	ILE
1	F	78	SER
1	F	82	SER
1	F	105	ASN
1	F	107	VAL
1	F	109	LEU
1	F	110	THR
1	F	111	CYS
1	F	120	THR
1	F	125	ASP
1	F	128	THR
1	F	132	LEU
1	F	134	GLU
1	F	138	LEU
1	F	143	LEU
1	F	158	ASP
1	F	159	ASP
1	F	163	MET
1	F	164	LEU
1	F	172	LEU
1	F	185	ARG
1	F	192	LYS
1	F	199	ASP
1	F	200	ILE
1	F	206	VAL
1	F	209	LYS
1	F	211	LEU
1	F	219	ILE
1	F	226	LEU

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Mol	Chain	Res	Type
1	F	230	THR
1	F	242	ILE
1	F	245	ASN
1	F	251	THR
1	F	253	LEU
1	F	262	ARG
1	F	264	LEU
1	F	289	LEU
1	F	297	VAL
1	F	298	ARG
1	F	313	ASP
1	F	314	ASP
1	F	319	GLU
1	F	331	LEU
1	F	344	LEU
1	F	347	LEU
1	F	351	ARG
1	F	357	THR
1	F	365	LEU
1	F	395	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	269	HIS
1	B	263	GLN
1	C	245	ASN
1	D	263	GLN
1	E	32	ASN
1	E	263	GLN
1	F	101	HIS
1	F	105	ASN
1	F	245	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	375/408 (91%)	0.46	34 (9%) 9 12	24, 50, 81, 95	0
1	B	383/408 (93%)	0.19	11 (2%) 49 58	17, 49, 80, 100	0
1	C	370/408 (90%)	0.16	9 (2%) 56 65	19, 46, 79, 122	0
1	D	369/408 (90%)	0.15	10 (2%) 52 61	21, 47, 79, 103	0
1	E	369/408 (90%)	0.47	31 (8%) 11 14	24, 52, 85, 118	0
1	F	372/408 (91%)	0.18	13 (3%) 42 50	19, 49, 85, 102	0
All	All	2238/2448 (91%)	0.27	108 (4%) 29 36	17, 49, 83, 122	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	50	SER	7.9
1	F	50	SER	6.5
1	E	220	GLY	6.4
1	B	221	GLY	6.3
1	A	400	LEU	5.6
1	D	158	ASP	5.5
1	A	388	SER	5.4
1	A	40	PRO	5.3
1	F	295	ALA	5.3
1	B	370	GLY	4.7
1	A	233	GLY	4.7
1	E	267	THR	4.3
1	B	371	ASP	4.2
1	D	235	GLY	4.0
1	E	196	SER	3.9
1	E	236	LYS	3.9
1	A	232	PRO	3.9
1	E	105	ASN	3.7
1	A	236	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	59	PHE	3.5
1	E	61	TYR	3.5
1	B	372	ASP	3.4
1	E	266	PRO	3.4
1	C	36	ARG	3.4
1	A	234	VAL	3.4
1	B	104	GLY	3.3
1	F	303	ASP	3.3
1	A	313	ASP	3.3
1	C	313	ASP	3.3
1	B	143	LEU	3.3
1	A	231	GLY	3.3
1	C	294	GLY	3.2
1	F	230	THR	3.2
1	E	235	GLY	3.2
1	C	52	ASN	3.2
1	D	233	GLY	3.1
1	B	196	SER	3.0
1	A	203	ALA	3.0
1	B	373	ARG	2.9
1	D	172	LEU	2.9
1	E	71	ALA	2.9
1	A	230	THR	2.8
1	E	199	ASP	2.8
1	D	313	ASP	2.8
1	A	198	PRO	2.8
1	E	130	PRO	2.7
1	F	330	PRO	2.7
1	A	172	LEU	2.6
1	A	293	ARG	2.6
1	E	194	SER	2.6
1	E	18	LEU	2.6
1	E	226	LEU	2.6
1	E	217	ALA	2.6
1	A	245	ASN	2.6
1	F	370	GLY	2.6
1	F	315	VAL	2.6
1	A	255	ASP	2.5
1	F	314	ASP	2.5
1	E	192	LYS	2.5
1	E	16	ARG	2.5
1	C	35	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	230	THR	2.5
1	F	313	ASP	2.5
1	A	304	GLY	2.5
1	E	74	VAL	2.5
1	A	35	ALA	2.4
1	F	388	SER	2.4
1	A	38	ALA	2.4
1	C	312	ALA	2.4
1	F	233	GLY	2.4
1	C	293	ARG	2.4
1	A	173	GLY	2.4
1	A	329	GLU	2.4
1	E	302	ALA	2.4
1	A	34	PRO	2.3
1	A	37	PRO	2.3
1	C	221	GLY	2.3
1	A	237	ASP	2.3
1	E	313	ASP	2.3
1	F	232	PRO	2.2
1	A	169	VAL	2.2
1	E	201	GLU	2.2
1	A	75	SER	2.2
1	B	293	ARG	2.2
1	E	198	PRO	2.2
1	A	274	THR	2.2
1	E	36	ARG	2.2
1	C	97	PRO	2.2
1	A	238	GLY	2.2
1	B	220	GLY	2.2
1	E	399	ARG	2.2
1	D	218	GLY	2.2
1	E	219	ILE	2.1
1	A	61	TYR	2.1
1	A	105	ASN	2.1
1	A	193	TRP	2.1
1	B	61	TYR	2.1
1	F	237	ASP	2.1
1	D	302	ALA	2.1
1	E	35	ALA	2.1
1	A	30	ALA	2.1
1	E	138	LEU	2.1
1	E	388	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	ALA	2.0
1	E	72	GLU	2.0
1	D	228	LEU	2.0
1	D	50	SER	2.0
1	A	174	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.