Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 06:24 AM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

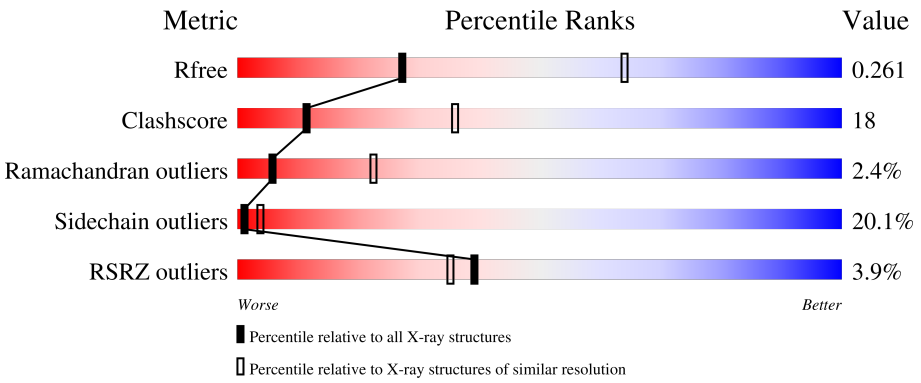
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	408	8% 45% 36% 10% • 8%
1	B	408	2% 57% 32% • 6%
1	C	408	% 55% 28% 8% 9%
1	D	408	2% 55% 29% 5% • 10%
1	E	408	7% 52% 30% 8% 10%

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Mol	Chain	Length	Quality of chain
1	F	408	2% 54% 31% 6% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16587 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 DNA polymerase III subunit beta.

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

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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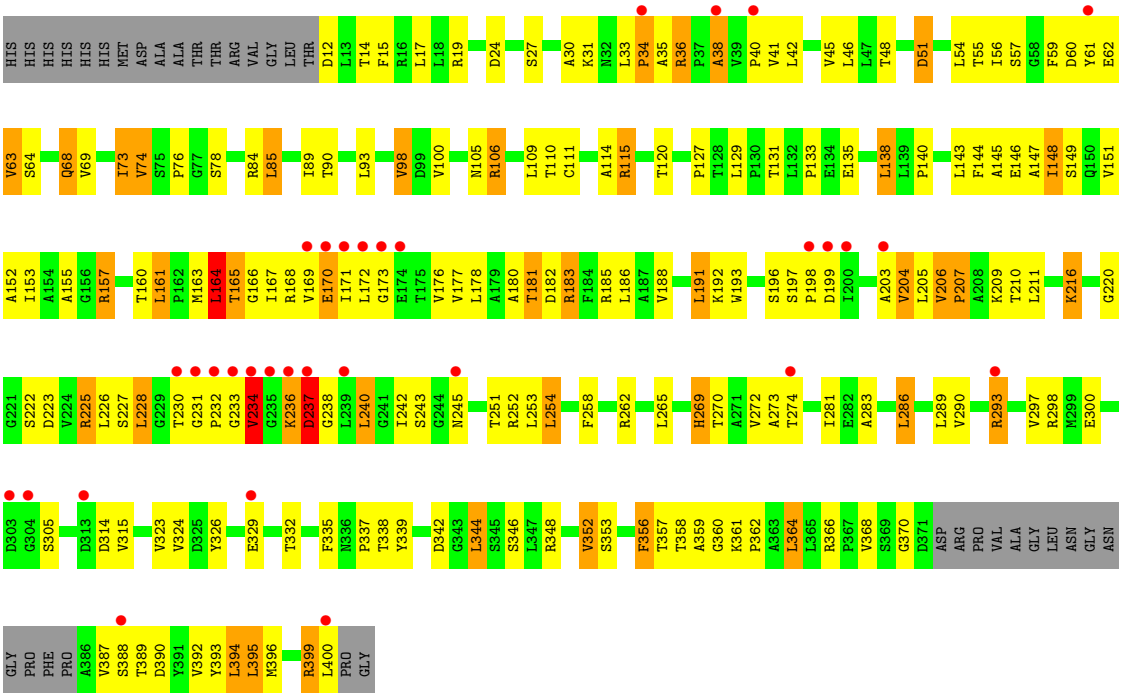
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q50790
D	-5	HIS	-	expression tag	UNP Q50790
D	-4	HIS	-	expression tag	UNP Q50790
D	-3	HIS	-	expression tag	UNP Q50790
D	-2	HIS	-	expression tag	UNP Q50790
D	-1	HIS	-	expression tag	UNP Q50790
D	0	HIS	-	expression tag	UNP Q50790
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 (i)

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

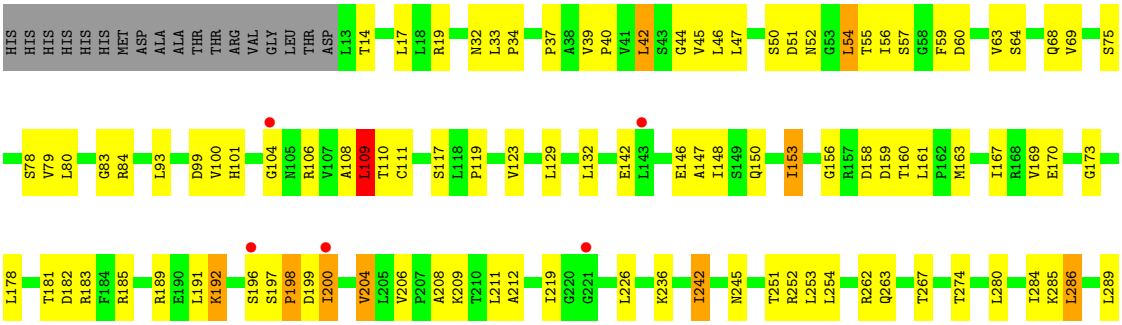
• Molecule 1: DNA polymerase III subunit beta

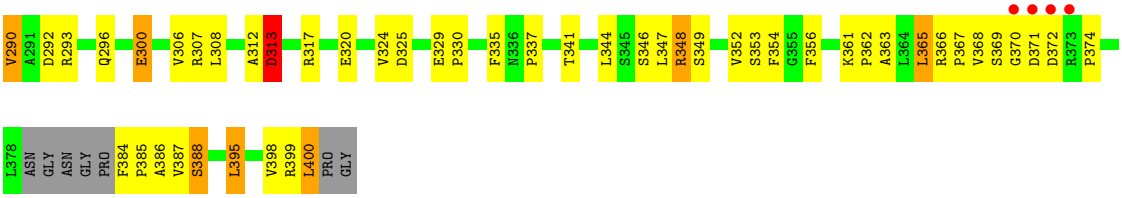
Chain A:



• Molecule 1: DNA polymerase III subunit beta

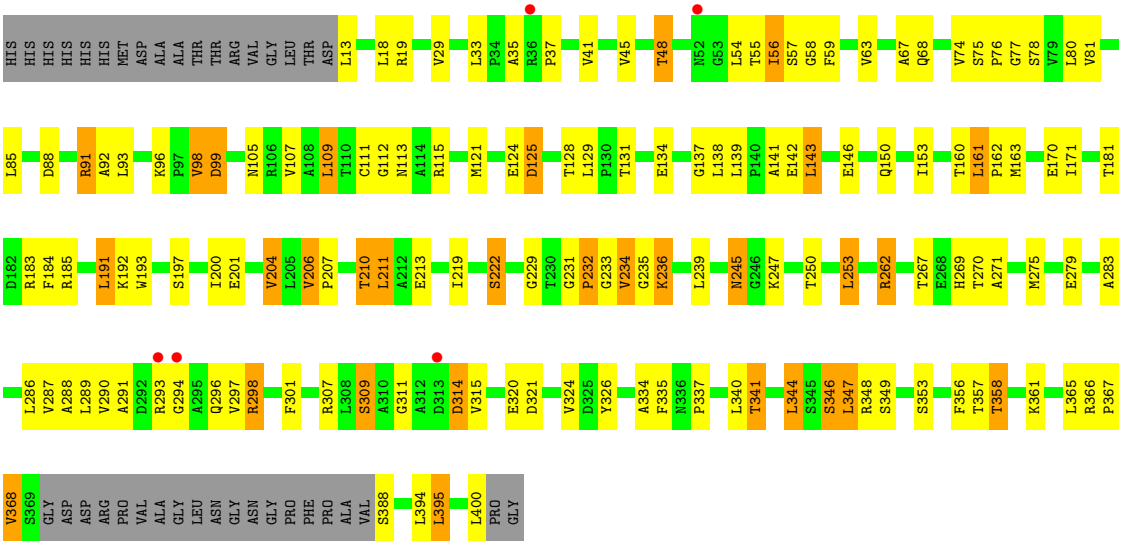
Chain B:





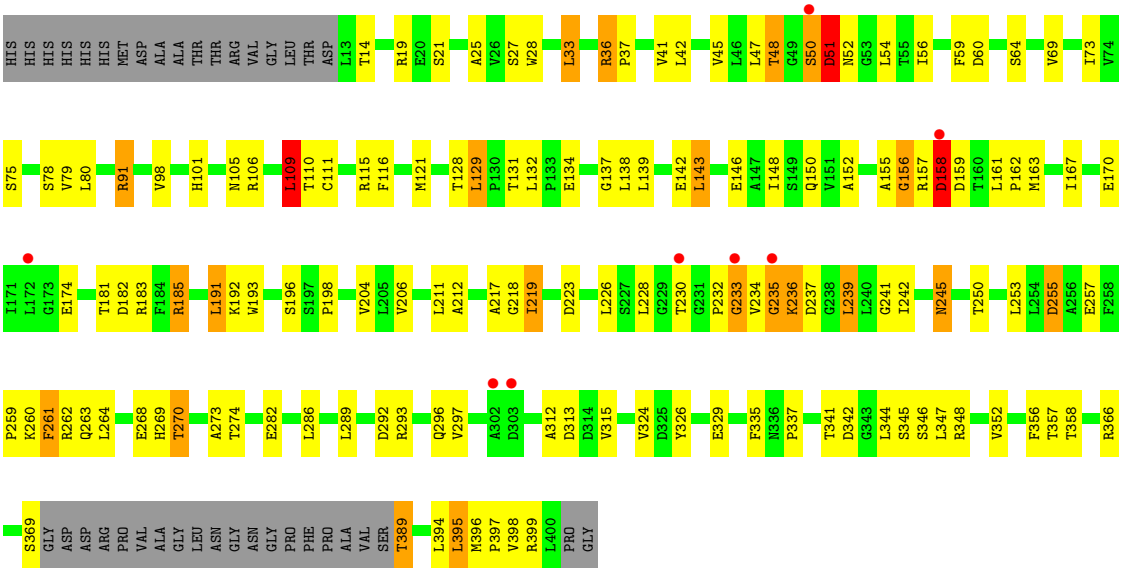
• Molecule 1: DNA polymerase III subunit beta

Chain C:



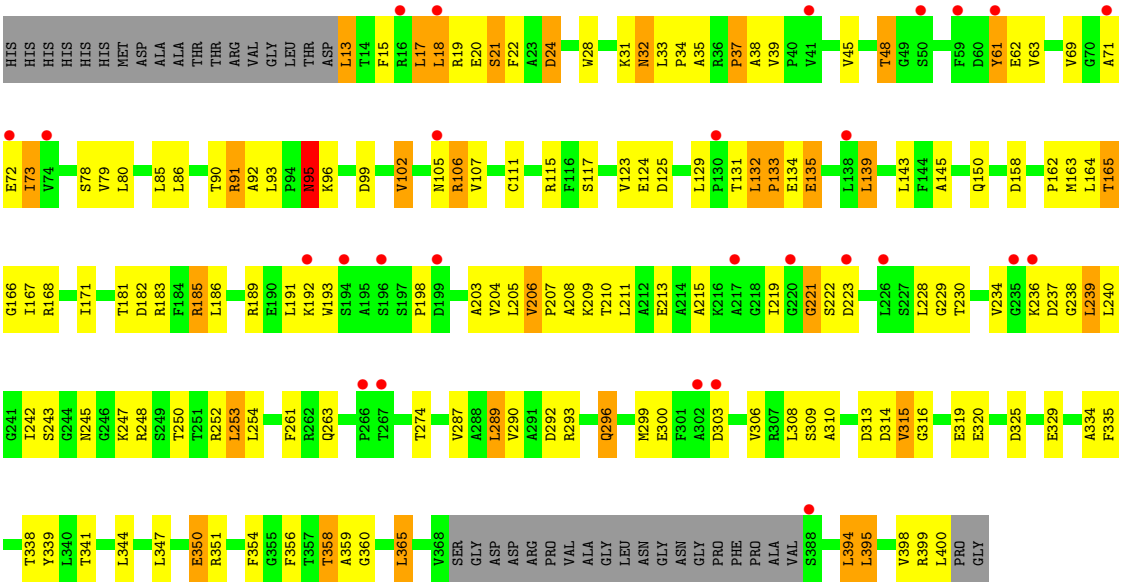
• Molecule 1: DNA polymerase III subunit beta

Chain D:



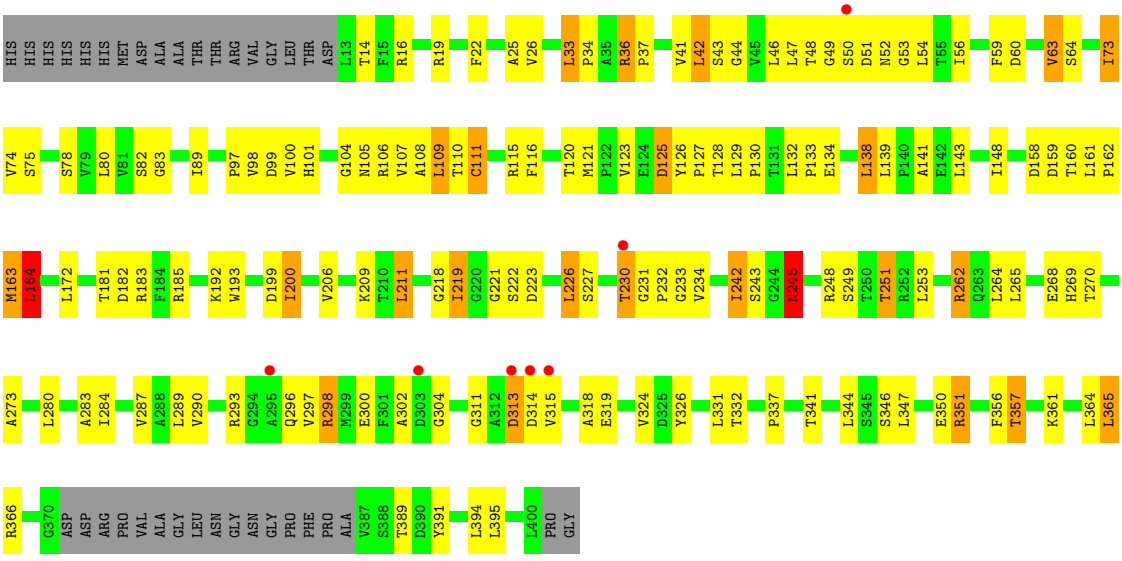
• Molecule 1: DNA polymerase III subunit beta

Chain E:



- Molecule 1: DNA polymerase III subunit beta

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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	2745 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	16587	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.53	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(^{o})	Ideal(^{o})
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 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	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (594) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E: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:36:ARG:HD2	1:F:36:ARG:N	1.67	1.04
1:F:296:GLN:HB3	1:F:337:PRO:HD3	1.38	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:A:35:ALA:HA	1:A:84:ARG:HE	1.34	0.93
1:F:36:ARG:HD2	1:F:36:ARG:H	1.26	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	Interatomic distance (Å)	Clash overlap (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:H	1:A:161:LEU:CD1	1.87	0.86
1:D:59:PHE:HD1	1:D:64:SER:CB	1.88	0.86
1:A:204:VAL:HG22	1:A:253:LEU:HD13	1.59	0.85
1:F:80:LEU:HD23	1:F:121:MET:HB2	1.58	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:HD2	1:A:157:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HD12	1:C:183:ARG:O	1.87	0.73
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:109:LEU:HB3	1:F:116:PHE:HB2	1.71	0.72
1:F:218:GLY:CA	1:F:245:ASN:HD21	2.02	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:B:198:PRO:O	1:B:200:ILE:HG22	1.91	0.70
1:E:134:GLU:HB3	1:E:229:GLY:HA2	1.72	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:364:LEU:HD11	1:A:392:VAL:CG2	2.21	0.70
1:A:387:VAL:HG22	1:A:388:SER:N	2.07	0.70
1:A:387:VAL:CG2	1:A:388:SER:H	2.05	0.70
1:D:268:GLU:HG3	1:D:269:HIS:N	2.07	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:A:238:GLY:O	1:A:252:ARG:HA	1.92	0.69
1:F:25:ALA:HB1	1:F:56:ILE:HD12	1.73	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:B:37:PRO:HB3	1:C:314:ASP:HB2	1.76	0.68
1:E:234:VAL:CG1	1:E:236:LYS:CE	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PRO:HA	1:A:222:SER:HA	1.75	0.67
1:B:293:ARG:CG	1:B:293:ARG:O	2.43	0.67
1:D:25:ALA:HB1	1:D:56:ILE:HD13	1.77	0.67
1:E:234:VAL:CG2	1:E:236:LYS:HE3	2.21	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:C:57:SER:HB3	1:C:129:LEU:HD11	1.77	0.66
1:D:274:THR:O	1:D:324:VAL:HG23	1.95	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:D:183:ARG:HB3	1:F:160:THR:HG23	1.78	0.65
1:F:364:LEU:HD21	1:F:366:ARG:HH21	1.60	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:A:269:HIS:CD2	1:A:272:VAL:CG1	2.82	0.63
1:B:199:ASP:C	1:B:200:ILE:CG2	2.66	0.63
1:B:148:ILE:HG21	1:B:212:ALA:HA	1.80	0.62
1:F:141:ALA:HB1	1:F:219:ILE:O	1.99	0.62
1:E:354:PHE:CB	1:E:356:PHE:CE2	2.82	0.62
1:A:114:ALA:HB2	1:B:320:GLU:HG2	1.81	0.62
1:B:386:ALA:O	1:B:387:VAL:HG13	1.99	0.62
1:E:234:VAL:CG1	1:E:236:LYS:CD	2.77	0.62
1:F:231:GLY:O	1:F:234:VAL:HG13	1.98	0.62
1:A:164:LEU:HD23	1:A:164:LEU:H	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:14:THR:HG23	1:B:101:HIS:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:298:ARG:HH11	1:C:298:ARG:CG	2.08	0.61
1:B:173:GLY:HA2	1:B:200:ILE:HG23	1.81	0.61
1:D:146:GLU:O	1:D:150:GLN:HG3	2.00	0.61
1:E:31:LYS:HD2	1:E:213:GLU:HG3	1.82	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:C	1:B:54:LEU:HD13	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:156:GLY:HA2	1:B:182:ASP:HB3	1.83	0.59
1:B:353:SER:HB3	1:B:366:ARG:HG3	1.82	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:A:42:LEU:HD21	1:A:60:ASP:HA	1.84	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: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:A:106:ARG:CG	1:A:106:ARG:HH11	2.15	0.58
1:D:132:LEU:HD13	1:D:241:GLY:HA3	1.84	0.58
1:E:234:VAL:HG11	1:E:236:LYS:CD	2.32	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:A:73:ILE:HD13	1:A:73:ILE:N	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:HG22	1:A:258:PHE:CZ	2.39	0.57
1:E:228:LEU:O	1:E:234:VAL:O	2.21	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
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:A:46:LEU:HB3	1:A:57:SER:HB2	1.87	0.56
1:D:268:GLU:CG	1:D:269:HIS:H	2.17	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:B:374:PRO:HD2	1:B:388:SER:HB3	1.88	0.55
1:C:207:PRO:HB2	1:C:210:THR:CG2	2.37	0.55
1:A:269:HIS:HD2	1:A:272:VAL:CG1	2.19	0.55
1:E:134:GLU:CD	1:E:230:THR:H	2.09	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:C:161:LEU:HD23	1:C:162:PRO:HD2	1.88	0.55
1:F:49:GLY:O	1:F:73:ILE:CD1	2.55	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:35:ALA:O	1:C:37:PRO:HD3	2.07	0.54
1:C:335:PHE:CD1	1:C:395:LEU:HD13	2.42	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:A:314:ASP:OD2	1:A:315:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:CD1	1:A:395:LEU:HD13	2.42	0.54
1:F:181:THR:O	1:F:181:THR:CG2	2.56	0.54
1:A:399:ARG:H	1:A:399:ARG:HE	1.55	0.53
1:A:399:ARG:H	1:A:399:ARG:NE	2.06	0.53
1:B:39:VAL:HG23	1:B:42:LEU:HB2	1.89	0.53
1:A:163:MET:O	1:A:164:LEU:C	2.45	0.53
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:E:300:GLU:O	1:E:306:VAL:HA	2.09	0.53
1:D:36:ARG:HG3	1:D:37:PRO:HD3	1.90	0.53
1:E:132:LEU:N	1:E:133:PRO:CD	2.70	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:33:LEU:HG	1:A:63:VAL:O	2.08	0.53
1:A:40:PRO:C	1:A:42:LEU:H	2.12	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:HD23	1:A:42:LEU:O	2.09	0.53
1:A:85:LEU:O	1:A:89:ILE:HG13	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: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:HD12	1:C:109:LEU:C	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:C:245:ASN:ND2	1:C:245:ASN:H	2.06	0.52
1:E:91:ARG:HG2	1:E:92:ALA:N	2.22	0.52
1:F:44:GLY:HA2	1:F:83:GLY:H	1.74	0.52
1:F:231:GLY:H	1:F:234:VAL:HG12	1.75	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:D:98:VAL:HG12	1:D:111:CYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ARG:HH11	1:E:106:ARG:CG	2.23	0.51
1:A:146:GLU:HG3	1:A:348:ARG:NH1	2.26	0.51
1:E:134:GLU:OE2	1:E:229:GLY:HA2	2.10	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
1:A:36:ARG:HH12	1:A:38:ALA:HB2	1.76	0.51
1:E:186:LEU:HD21	1:E:261:PHE:HB2	1.93	0.51
1:F:59:PHE:HB2	1:F:129:LEU:HD12	1.92	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:A:33:LEU:HD11	1:A:60:ASP:CB	2.42	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: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:28:TRP:HE1	1:D:219:ILE:HG22	1.76	0.50
1:D:269:HIS:HB3	1:D:356:PHE:O	2.10	0.50
1:A:14:THR:HB	1:A:74:VAL:HG22	1.93	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:139:LEU:HB3	1:D:193:TRP:CD1	2.47	0.50
1:F:16:ARG:CD	1:F:97:PRO:HB2	2.42	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: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:F:219:ILE:HD13	1:F:219:ILE:C	2.31	0.49
1:B:372:ASP:O	1:B:374:PRO:HD3	2.13	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:E:206:VAL:CG2	1:E:207:PRO:HD2	2.31	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:D:396:MET:HE3	1:D:397:PRO:HD2	1.95	0.49
1:E:314:ASP:O	1:E:315:VAL:HG12	2.13	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:A:33:LEU:HD21	1:A:60:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:LEU:O	1:D:235:GLY:HA2	2.13	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:E:150:GLN:OE1	1:E:189:ARG:HD3	2.12	0.48
1:F:22:PHE:CD2	1:F:98:VAL:HG21	2.46	0.48
1:D:129:LEU:HD22	1:D:129:LEU:N	2.27	0.48
1:A:114:ALA:CB	1:B:320:GLU:HG2	2.43	0.48
1:C:96:LYS:HD2	1:C:112:GLY:HA3	1.94	0.48
1:D:109:LEU:HB3	1:D:116:PHE:HB2	1.95	0.48
1:E:289:LEU:HD23	1:F:89:ILE:HA	1.95	0.48
1:F:59:PHE:HB2	1:F:129:LEU:CD1	2.43	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:E:15:PHE:CD2	1:E:17:LEU:HD13	2.48	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:HG23	1:B:181:THR:O	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:A:166:GLY:HA2	1:A:207:PRO:HA	1.96	0.48
1:E:236:LYS:O	1:E:237:ASP:HB2	2.13	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:A:157:ARG:O	1:A:157:ARG:CD	2.57	0.47
1:C:13:LEU:HD13	1:C:77:GLY:O	2.14	0.47
1:E:206:VAL:HG23	1:E:207:PRO:CD	2.31	0.47
1:C:340:LEU:O	1:C:344:LEU:HD22	2.15	0.47
1:D:80:LEU:HD23	1:D:121:MET:HB2	1.94	0.47
1:F:59:PHE:CE2	1:F:130:PRO:HD3	2.48	0.47
1:E:167:ILE:HG13	1:E:208:ALA:HA	1.96	0.47
1:A:90:THR:HA	1:A:93:LEU:HD12	1.97	0.47
1:A:161:LEU:N	1:A:161:LEU:CD1	2.61	0.47
1:C:98:VAL:HB	1:C:111:CYS:HB2	1.97	0.47
1:E:19:ARG:HD3	1:E:19:ARG:C	2.35	0.47
1:B:146:GLU:HG3	1:B:348:ARG:HH11	1.79	0.47
1:C:298:ARG:HD2	1:C:309:SER:OG	2.15	0.47
1:E:204:VAL:HG21	1:E:253:LEU:HG	1.94	0.47
1:F:34:PRO:HB2	1:F:36:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:PRO:CG	1:F:43:SER:HB3	2.35	0.47
1:F:148:ILE:HD12	1:F:211:LEU:HD13	1.95	0.47
1:F:298:ARG:HH22	1:F:311:GLY:N	2.12	0.47
1:A:233:GLY:O	1:A:234:VAL:HG22	2.14	0.47
1:A:236:LYS:HD2	1:A:236:LYS:O	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
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: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:B:354:PHE:CE1	1:B:365:LEU:HD22	2.50	0.47
1:E:20:GLU:CD	1:E:20:GLU:N	2.60	0.47
1:E:17:LEU:C	1:E:18:LEU:HD13	2.35	0.47
1:E:206:VAL:HB	1:E:253:LEU:CD1	2.45	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: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:E:13:LEU:O	1:E:102:VAL:CG1	2.64	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:CD2	1:A:356:PHE:N	2.80	0.46
1:D:161:LEU:O	1:D:162:PRO:C	2.54	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:A:98:VAL:HG12	1:A:111:CYS:SG	2.55	0.46
1:A:358:THR:C	1:A:360:GLY:H	2.19	0.46
1:B:296:GLN:HA	1:B:337:PRO:HD3	1.96	0.46
1:E:15:PHE:CE2	1:E:17:LEU:HD13	2.50	0.46
1:F:14:THR:OG1	1:F:101:HIS:HD2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD22	1:D:191:LEU:HD21	1.98	0.45
1:D:236:LYS:HD2	1:D:236:LYS:HA	1.68	0.45
1:A:254:LEU:H	1:A:254:LEU:HD12	1.82	0.45
1:B:384:PHE:N	1:B:385:PRO:CD	2.79	0.45
1:D:217:ALA:O	1:D:219:ILE:HG23	2.16	0.45
1:F:164:LEU:HD21	1:F:182:ASP:HA	1.98	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
1:A:149:SER:HB2	1:A:216:LYS:NZ	2.31	0.45
1:A:364:LEU:HD12	1:A:366:ARG:HG3	1.99	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:D:155:ALA:O	1:D:156:GLY:O	2.35	0.45
1:F:74:VAL:HG12	1:F:75:SER:OG	2.16	0.45
1:F:222:SER:OG	1:F:223:ASP:N	2.50	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:D:219:ILE:O	1:D:219:ILE:CG1	2.65	0.45
1:A:364:LEU:CD2	1:A:394:LEU:HD12	2.46	0.45
1:B:78:SER:OG	1:B:123:VAL:HG11	2.17	0.45
1:C:146:GLU:O	1:C:150:GLN:HG3	2.16	0.45
1:D:185:ARG:NH2	1:D:342:ASP:OD2	2.50	0.45
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:E:204:VAL:HG22	1:E:205:LEU:N	2.33	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: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:E:186:LEU:HB3	1:E:394:LEU:HB3	1.99	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:148:ILE:H	1:A:148:ILE:HG12	1.47	0.44
1:A:167:ILE:HG12	1:A:180:ALA:HB2	1.99	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:A:106:ARG:CG	1:A:106:ARG:NH1	2.78	0.44
1:A:152:ALA:HB2	1:A:167:ILE:HD11	2.00	0.44
1:C:171:ILE:HG21	1:C:193:TRP:HZ3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:ASP:N	1:E:237:ASP:OD1	2.51	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:C:301:PHE:HB3	1:C:326:TYR:CE1	2.53	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:A:182:ASP:OD1	1:A:183:ARG:N	2.49	0.44
1:A:273:ALA:HB2	1:A:326:TYR:CD1	2.44	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
1:E:63:VAL:HG23	1:E:250:THR:O	2.18	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:A:45:VAL:HG23	1:A:57:SER:O	2.18	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:C:204:VAL:HG22	1:C:253:LEU:HG	2.00	0.43
1:E:236:LYS:O	1:E:237:ASP:CB	2.65	0.43
1:A:146:GLU:HG3	1:A:348:ARG:HH12	1.81	0.43
1:E:32:ASN:CG	1:E:32:ASN:O	2.56	0.43
1:F:80:LEU:HD23	1:F:121:MET:CB	2.39	0.43
1:F:219:ILE:O	1:F:219:ILE:HG12	2.18	0.43
1:A:188:VAL:HB	1:A:392:VAL:HG12	1.99	0.43
1:D:163:MET:HE3	1:D:257:GLU:C	2.39	0.43
1:E:131:THR:CA	1:E:133:PRO:HD3	2.48	0.43
1:F:59:PHE:HD2	1:F:129:LEU:HA	1.83	0.43
1:A:171:ILE:HG12	1:A:193:TRP:CZ3	2.54	0.43
1:A:234:VAL:O	1:A:237:ASP:OD1	2.35	0.43
1:C:99:ASP:OD2	1:C:99:ASP:N	2.51	0.43
1:B:290:VAL:HG13	1:B:290:VAL:O	2.19	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:A:35:ALA:CA	1:A:84:ARG:HE	2.18	0.43
1:A:362:PRO:HG3	1:A:396:MET:SD	2.58	0.43
1:D:161:LEU:HD22	1:F:183:ARG:HD3	2.00	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:A:148:ILE:HG23	1:A:148:ILE:HD13	1.57	0.43
1:B:226:LEU:HD12	1:B:242:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:238:GLY:C	1:E:253:LEU:HD22	2.39	0.43
1:F:300:GLU:HG3	1:F:332:THR:HG23	2.00	0.43
1:B:192:LYS:H	1:B:192:LYS:CD	2.31	0.43
1:C:262:ARG:HE	1:C:262:ARG:HB2	1.69	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:D:274:THR:HA	1:D:352:VAL:O	2.18	0.43
1:A:173:GLY:HA2	1:A:199:ASP:HA	2.00	0.42
1:C:29:VAL:HG13	1:C:58:GLY:HA3	2.01	0.42
1:F:16:ARG:NE	1:F:99:ASP:OD2	2.52	0.42
1:F:364:LEU:HD13	1:F:394:LEU:HD23	2.00	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:E:132:LEU:HB2	1:E:239:LEU:HD22	2.02	0.42
1:B:46:LEU:HB3	1:B:57:SER:HB2	2.01	0.42
1:F:42:LEU:HD11	1:F:59:PHE:O	2.18	0.42
1:B:54:LEU:HD13	1:B:54:LEU:O	2.19	0.42
1:B:189:ARG:HA	1:B:189:ARG:HD2	1.87	0.42
1:B:353:SER:O	1:B:365:LEU:HA	2.19	0.42
1:C:91:ARG:HB3	1:C:91:ARG:NH1	2.33	0.42
1:D:42:LEU:HG	1:D:60:ASP:HA	2.02	0.42
1:C:290:VAL:HG12	1:C:290:VAL:O	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:45:VAL:HG13	1:B:47:LEU:HD13	2.01	0.42
1:B:354:PHE:CD1	1:B:356:PHE:HZ	2.34	0.42
1:A:262:ARG:HA	1:A:265:LEU:HD12	2.01	0.42
1:A:281:ILE:HD11	1:A:344:LEU:HB3	2.00	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: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:C:234:VAL:CG2	1:C:235:GLY:N	2.82	0.42
1:C:353:SER:HB3	1:C:366:ARG:HG3	2.00	0.42
1:D:232:PRO:HG2	1:D:233:GLY:H	1.84	0.42
1:D:357:THR:HG22	1:D:358:THR:HG23	2.02	0.42
1:F:161:LEU:HA	1:F:162:PRO:HD3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:ARG:HB3	1:F:389:THR:HG21	2.01	0.42
1:B:368:VAL:O	1:B:370:GLY:N	2.47	0.42
1:D:28:TRP:HE1	1:D:219:ILE:CG2	2.33	0.42
1:E:85:LEU:HD22	1:F:315:VAL:HG22	2.02	0.42
1:E:206:VAL:HB	1:E:253:LEU:HD12	2.02	0.42
1:E:245:ASN:C	1:E:247:LYS:H	2.24	0.42
1:A:40:PRO:O	1:A:42:LEU:N	2.52	0.41
1:B:300:GLU:HB2	1:B:307:ARG:HB3	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:F:357:THR:HB	1:F:361:LYS:HE3	2.02	0.41
1:C:75:SER:HA	1:C:76:PRO:HD3	1.91	0.41
1:D:234:VAL:O	1:D:235:GLY:C	2.59	0.41
1:E:135:GLU:H	1:E:135:GLU:HG3	1.58	0.41
1:B:99:ASP:HB2	1:B:110:THR:HB	2.02	0.41
1:B:147:ALA:HB1	1:B:178:LEU:HD12	2.01	0.41
1:D:47:LEU:O	1:D:78:SER:HA	2.20	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:A:93:LEU:HA	1:B:286:LEU:HD11	2.01	0.41
1:C:59:PHE:HB2	1:C:129:LEU:CD2	2.50	0.41
1:C:346:SER:O	1:C:348:ARG:HD2	2.20	0.41
1:E:37:PRO:HB2	1:E:38:ALA:H	1.62	0.41
1:E:221:GLY:C	1:E:223:ASP:H	2.24	0.41
1:F:268:GLU:HG3	1:F:269:HIS:H	1.85	0.41
1:B:153:ILE:HD11	1:B:346:SER:HB2	2.01	0.41
1:D:150:GLN:HE21	1:D:348:ARG:HD2	1.86	0.41
1:E:290:VAL:HG11	1:E:316:GLY:O	2.19	0.41
1:F:98:VAL:HA	1:F:111:CYS:SG	2.61	0.41
1:B:386:ALA:O	1:B:387:VAL:CG1	2.68	0.41
1:C:41:VAL:HG11	1:C:125:ASP:HB3	2.03	0.41
1:D:59:PHE:CD1	1:D:64:SER:HB2	2.55	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:F:218:GLY:CA	1:F:245:ASN:ND2	2.79	0.41
1:A:33:LEU:CD2	1:A:63:VAL:HG13	2.51	0.41
1:A:169:VAL:HG23	1:A:204:VAL:HG12	2.03	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:A:152:ALA:O	1:A:157:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:274:THR:HA	1:B:352:VAL:O	2.21	0.41
1:C:93:LEU:HD23	1:D:286:LEU:HD21	2.03	0.41
1:C:275:MET:HB3	1:C:324:VAL:HG12	2.03	0.41
1:C:294:GLY:O	1:C:337:PRO:HD2	2.21	0.41
1:D:152:ALA:HB2	1:D:167:ILE:HD11	2.03	0.41
1:E:79:VAL:HG22	1:E:80:LEU:N	2.35	0.41
1:E:106:ARG:CG	1:E:106:ARG:NH1	2.83	0.41
1:E:134:GLU:CD	1:E:229:GLY:HA2	2.41	0.41
1:E:164:LEU:C	1:E:166:GLY:H	2.23	0.41
1:E:299:MET:HG2	1:E:308:LEU:HD12	2.02	0.41
1:E:313:ASP:C	1:E:315:VAL:H	2.24	0.41
1:F:59:PHE:CD2	1:F:129:LEU:HA	2.56	0.41
1:F:126:TYR:HA	1:F:127:PRO:HD3	1.94	0.41
1:C:33:LEU:HD11	1:C:45:VAL:HB	2.03	0.41
1:D:255:ASP:OD2	1:D:255:ASP:N	2.54	0.41
1:D:297:VAL:HG13	1:D:337:PRO:HG3	2.02	0.41
1:E:205:LEU:HD23	1:E:254:LEU:HB2	2.03	0.41
1:F:51:ASP:C	1:F:53:GLY:N	2.74	0.41
1:A:42:LEU:HD11	1:A:60:ASP:HA	2.03	0.40
1:B:54:LEU:HD12	1:B:69:VAL:CG1	2.50	0.40
1:B:197:SER:HB2	1:B:200:ILE:HD13	2.02	0.40
1:C:134:GLU:OE1	1:C:229:GLY:HA2	2.21	0.40
1:E:287:VAL:O	1:E:310:ALA:HB3	2.21	0.40
1:F:346:SER:HG	1:F:391:TYR:HH	1.68	0.40
1:A:198:PRO:O	1:A:199:ASP:C	2.59	0.40
1:A:228:LEU:O	1:A:234:VAL:HB	2.21	0.40
1:C:283:ALA:O	1:C:287:VAL:HG22	2.22	0.40
1:C:286:LEU:HG	1:D:116:PHE:HZ	1.86	0.40
1:B:44:GLY:HA2	1:B:83:GLY:H	1.87	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:A:14:THR:HA	1:A:100:VAL:O	2.21	0.40
1:A:157:ARG:HB3	1:A:165:THR:HG21	2.03	0.40
1:C:232:PRO:O	1:C:234:VAL:HG12	2.22	0.40
1:D:14:THR:HG23	1:D:101:HIS:HB3	2.03	0.40
1:E:24:ASP:OD1	1:E:24:ASP:C	2.59	0.40
1:E:162:PRO:HA	1:E:165:THR:OG1	2.21	0.40
1:E:296:GLN:NE2	1:E:400:LEU:HD22	2.36	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	371/408 (91%)	309 (83%)	47 (13%)	15 (4%)	3 11
1	B	379/408 (93%)	334 (88%)	36 (10%)	9 (2%)	6 22
1	C	366/408 (90%)	327 (89%)	36 (10%)	3 (1%)	19 51
1	D	365/408 (90%)	315 (86%)	41 (11%)	9 (2%)	5 21
1	E	365/408 (90%)	302 (83%)	51 (14%)	12 (3%)	4 15
1	F	368/408 (90%)	334 (91%)	28 (8%)	6 (2%)	9 32
All	All	2214/2448 (90%)	1921 (87%)	239 (11%)	54 (2%)	6 22

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

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Mol	Chain	Res	Type
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
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 (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	297/322 (92%)	225 (76%)	72 (24%)	0 2
1	B	303/322 (94%)	253 (84%)	50 (16%)	2 7
1	C	294/322 (91%)	232 (79%)	62 (21%)	1 3
1	D	293/322 (91%)	233 (80%)	60 (20%)	1 3
1	E	293/322 (91%)	237 (81%)	56 (19%)	1 4
1	F	295/322 (92%)	239 (81%)	56 (19%)	1 4
All	All	1775/1932 (92%)	1419 (80%)	356 (20%)	1 4

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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

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Mol	Chain	Res	Type
1	E	263	GLN
1	F	101	HIS
1	F	105	ASN
1	F	245	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	375/408 (91%)	0.47	32 (8%)	10	8	24, 50, 81, 95	0
1	B	383/408 (93%)	0.14	9 (2%)	60	58	17, 49, 80, 100	0
1	C	370/408 (90%)	0.13	5 (1%)	75	75	19, 46, 79, 122	0
1	D	369/408 (90%)	0.12	8 (2%)	62	59	21, 47, 79, 103	0
1	E	369/408 (90%)	0.40	27 (7%)	15	11	24, 52, 85, 118	0
1	F	372/408 (91%)	0.16	7 (1%)	66	65	19, 49, 85, 102	0
All	All	2238/2448 (91%)	0.24	88 (3%)	39	35	17, 49, 83, 122	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	SER	6.7
1	E	50	SER	6.5
1	E	220	GLY	5.5
1	A	388	SER	5.3
1	F	295	ALA	5.2
1	A	40	PRO	4.4
1	D	158	ASP	4.3
1	B	371	ASP	4.2
1	A	233	GLY	4.1
1	D	235	GLY	4.1
1	A	400	LEU	4.1
1	B	370	GLY	3.9
1	B	221	GLY	3.9
1	E	196	SER	3.8
1	A	172	LEU	3.7
1	A	313	ASP	3.6
1	A	232	PRO	3.6
1	E	59	PHE	3.6
1	E	61	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	36	ARG	3.4
1	A	173	GLY	3.3
1	A	234	VAL	3.3
1	B	372	ASP	3.3
1	B	196	SER	3.3
1	A	231	GLY	3.3
1	A	230	THR	3.2
1	C	313	ASP	3.2
1	E	236	LYS	3.2
1	C	294	GLY	3.1
1	B	373	ARG	3.1
1	E	192	LYS	3.1
1	E	267	THR	3.1
1	F	313	ASP	3.0
1	A	236	LYS	3.0
1	C	52	ASN	3.0
1	E	226	LEU	2.9
1	E	130	PRO	2.9
1	A	245	ASN	2.9
1	F	303	ASP	2.9
1	E	235	GLY	2.9
1	D	302	ALA	2.9
1	F	230	THR	2.8
1	A	304	GLY	2.8
1	A	329	GLU	2.7
1	D	233	GLY	2.7
1	A	61	TYR	2.7
1	A	169	VAL	2.7
1	A	198	PRO	2.7
1	A	34	PRO	2.6
1	B	104	GLY	2.6
1	A	203	ALA	2.6
1	E	388	SER	2.6
1	B	143	LEU	2.5
1	E	302	ALA	2.5
1	A	293	ARG	2.5
1	E	74	VAL	2.5
1	E	199	ASP	2.5
1	E	194	SER	2.5
1	D	50	SER	2.4
1	E	71	ALA	2.4
1	A	200	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	171	ILE	2.3
1	A	235	GLY	2.3
1	E	16	ARG	2.3
1	D	230	THR	2.3
1	E	223	ASP	2.3
1	A	170	GLU	2.3
1	E	18	LEU	2.3
1	E	72	GLU	2.3
1	E	105	ASN	2.2
1	A	239	LEU	2.2
1	E	217	ALA	2.2
1	F	315	VAL	2.2
1	B	200	ILE	2.2
1	E	138	LEU	2.1
1	E	303	ASP	2.1
1	F	314	ASP	2.1
1	A	303	ASP	2.1
1	A	199	ASP	2.1
1	C	293	ARG	2.1
1	E	41	VAL	2.1
1	A	174	GLU	2.1
1	D	172	LEU	2.1
1	A	274	THR	2.0
1	A	237	ASP	2.0
1	A	38	ALA	2.0
1	E	266	PRO	2.0
1	D	303	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.