Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:36 PM EDT

PDB ID	:	3BGW
Title	:	The Structure Of A DnaB-Like Replicative Helicase And Its Interactions With Primase
Authors	:	Wang, G.; Klein, M.G.; Tokonzaba, E.; Zhang, Y.; Holden, L.G.; Chen, X.S.
Deposited on	:	2007-11-27
Resolution	:	3.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

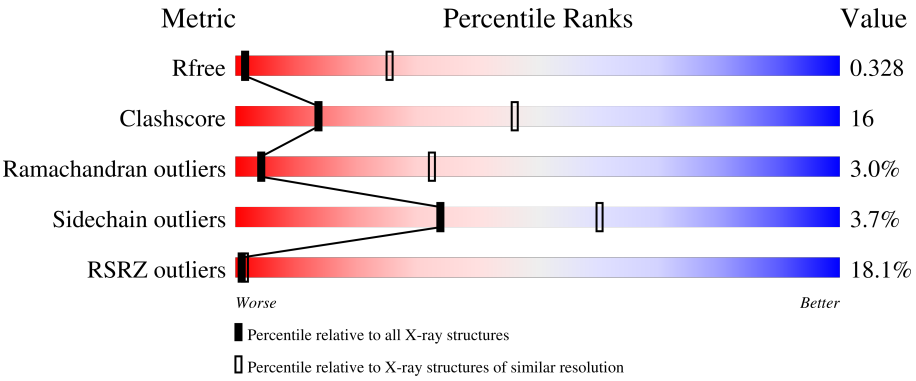
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.91 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	444	7% 63% 27% • • 6%
1	B	444	7% 67% 23% • • 6%
1	C	444	27% 67% 24% • 6%
1	D	444	21% 68% 21% • 8%
1	E	444	25% 68% 22% • • 6%

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Mol	Chain	Length	Quality of chain
1	F	444	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19724 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 DNAB-Like Replicative Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	B	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	C	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	D	409	Total	C	N	O	S	0	0	0
			3234	2029	561	632	12			
1	E	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	F	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			

There are 12 discrepancies between the modelled and reference sequences:

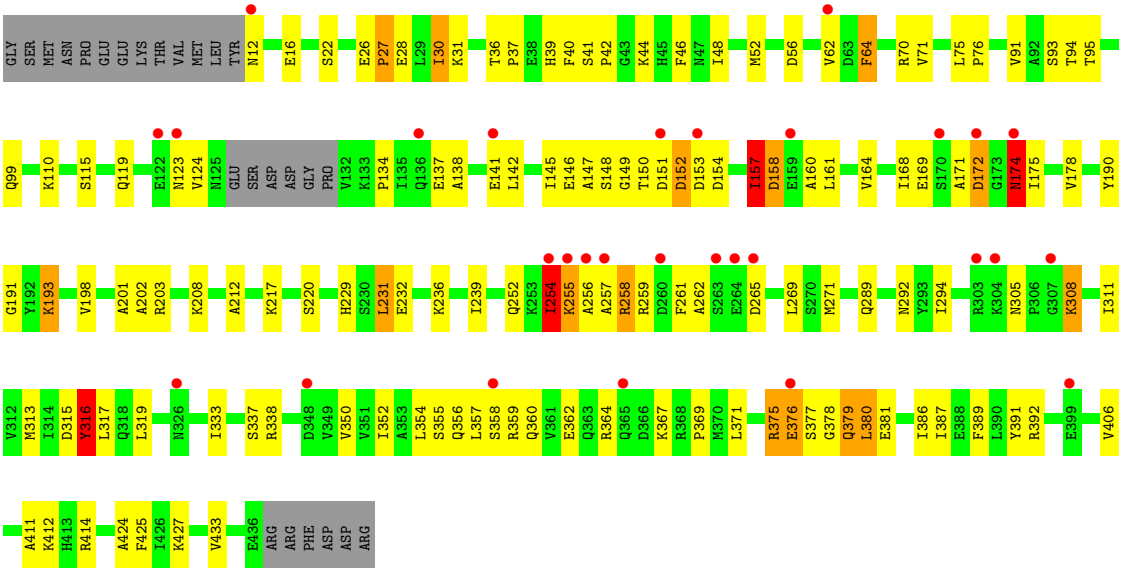
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q38152
A	0	SER	-	EXPRESSION TAG	UNP Q38152
B	-1	GLY	-	EXPRESSION TAG	UNP Q38152
B	0	SER	-	EXPRESSION TAG	UNP Q38152
C	-1	GLY	-	EXPRESSION TAG	UNP Q38152
C	0	SER	-	EXPRESSION TAG	UNP Q38152
D	-1	GLY	-	EXPRESSION TAG	UNP Q38152
D	0	SER	-	EXPRESSION TAG	UNP Q38152
E	-1	GLY	-	EXPRESSION TAG	UNP Q38152
E	0	SER	-	EXPRESSION TAG	UNP Q38152
F	-1	GLY	-	EXPRESSION TAG	UNP Q38152
F	0	SER	-	EXPRESSION TAG	UNP Q38152

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.

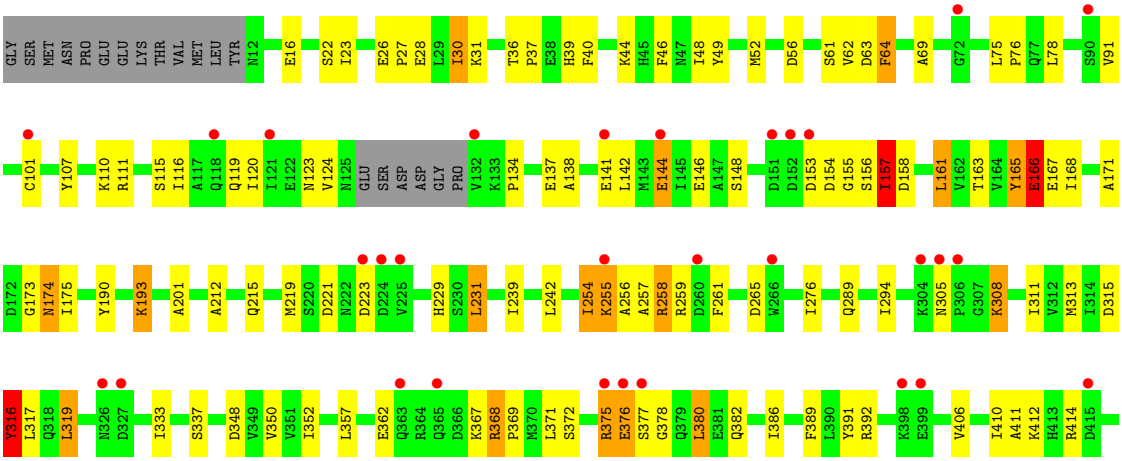
• Molecule 1: DNAB-Like Replicative Helicase

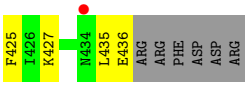
Chain A:



• Molecule 1: DNAB-Like Replicative Helicase

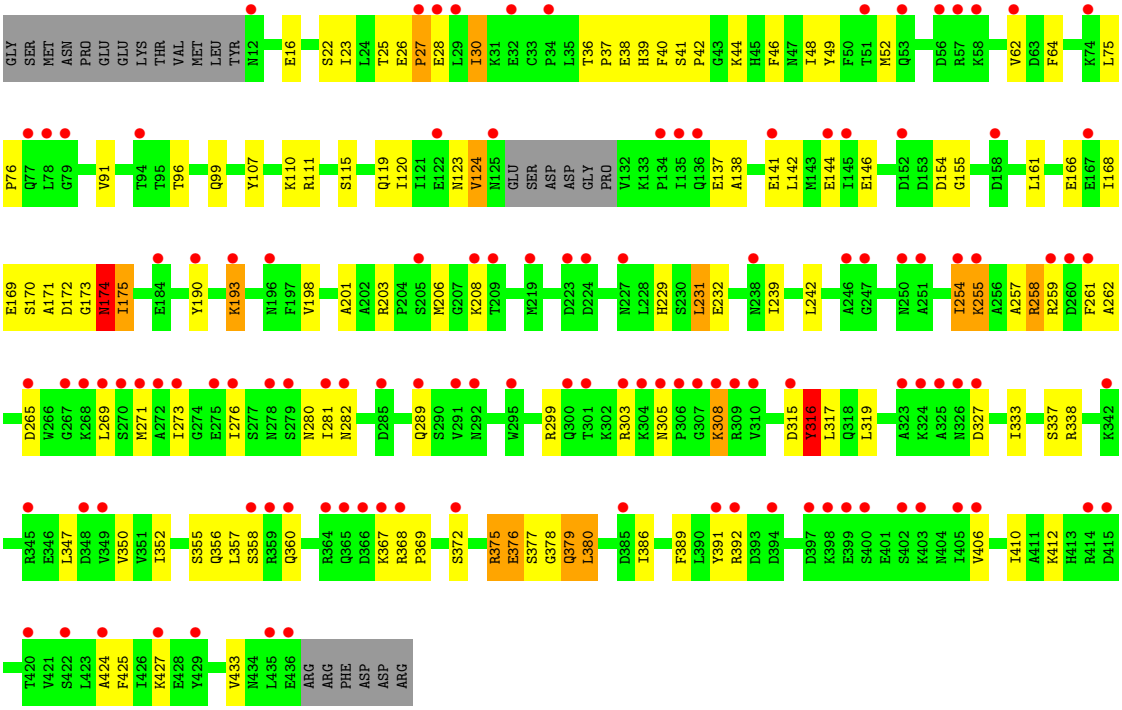
Chain B:





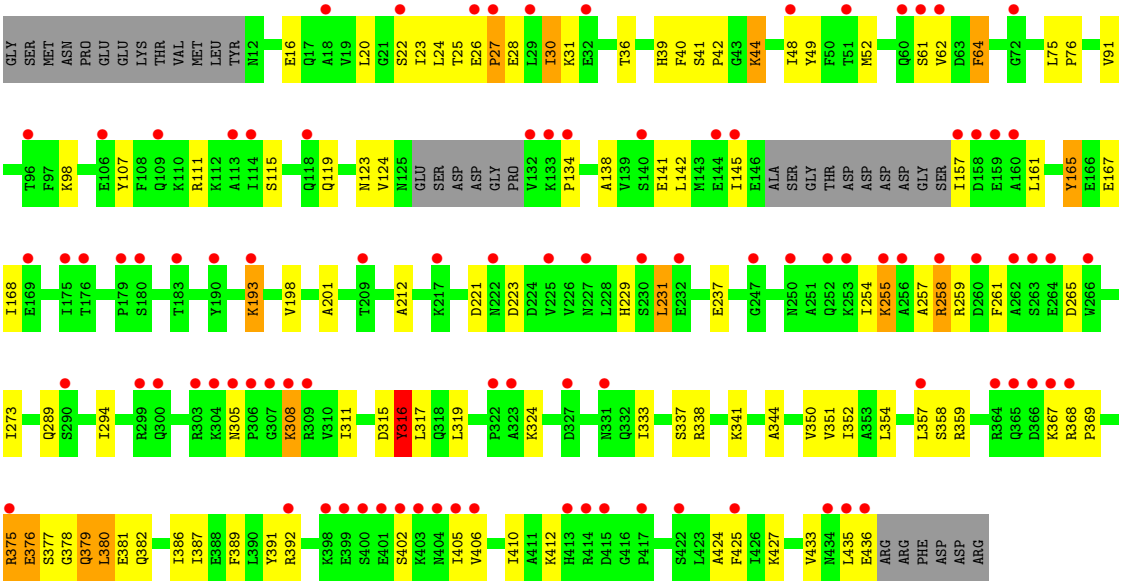
• Molecule 1: DNAB-Like Replicative Helicase

Chain C:



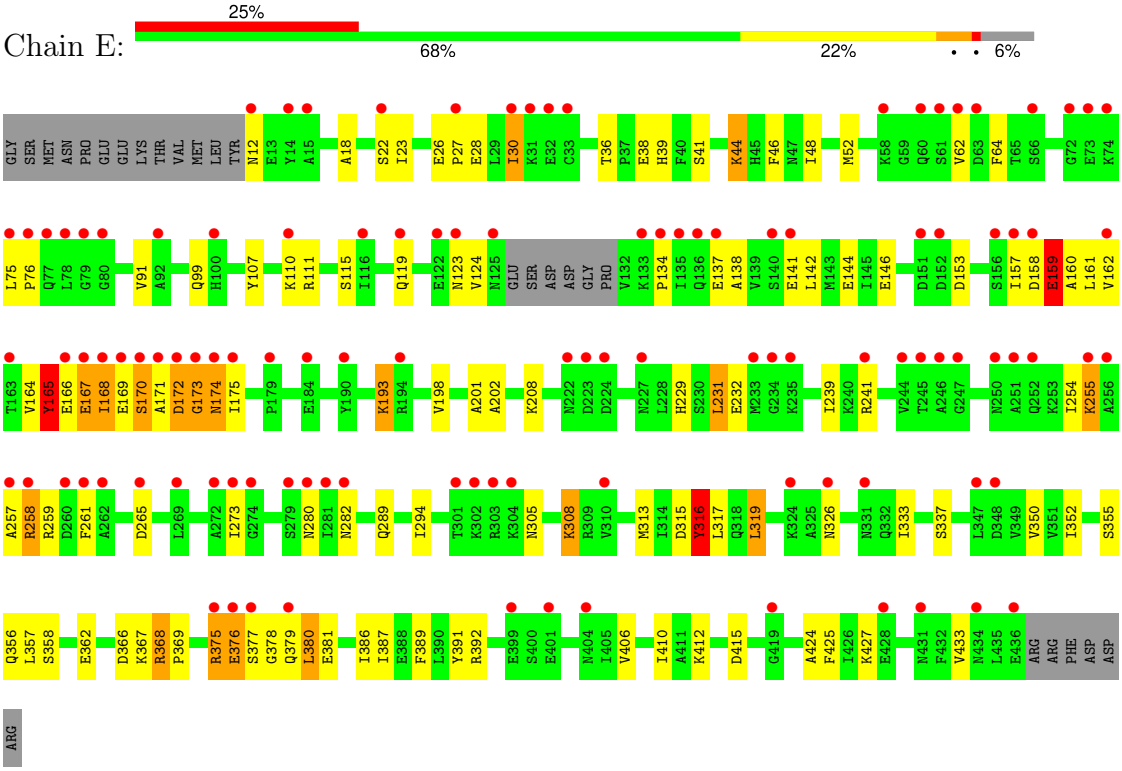
• Molecule 1: DNAB-Like Replicative Helicase

Chain D:



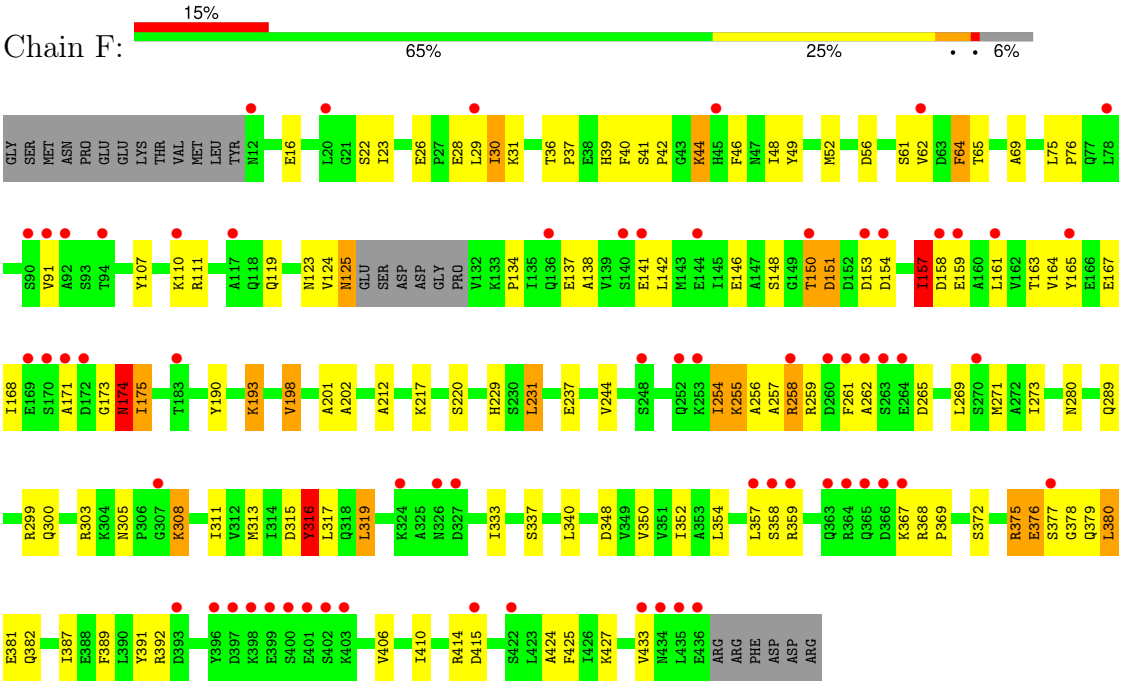
• Molecule 1: DNAB-Like Replicative Helicase

Chain E:



• Molecule 1: DNAB-Like Replicative Helicase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.63Å 184.41Å 184.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 3.91 38.80 – 3.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.81-3.91) 97.4 (38.80-3.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	12.68 (at 3.87Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.338 , 0.349 0.321 , 0.328	Depositor DCC
R_{free} test set	1750 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	65.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 139.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	19724	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

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	0.32	1/3345 (0.0%)	0.41	0/4507
1	B	0.26	0/3345	0.40	0/4507
1	C	0.30	2/3345 (0.1%)	0.39	0/4507
1	D	0.27	0/3280	0.39	0/4417
1	E	0.32	2/3345 (0.1%)	0.41	0/4507
1	F	0.34	4/3345 (0.1%)	0.42	1/4507 (0.0%)
All	All	0.30	9/20005 (0.0%)	0.40	1/26952 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	GLY	C-O	-8.20	1.10	1.23
1	F	174	ASN	CB-CG	-7.97	1.32	1.51
1	E	159	GLU	CD-OE2	6.62	1.32	1.25
1	A	174	ASN	CB-CG	-6.20	1.36	1.51
1	C	174	ASN	CB-CG	-6.08	1.37	1.51
1	C	174	ASN	CG-OD1	-5.54	1.11	1.24
1	F	174	ASN	C-O	-5.23	1.13	1.23
1	F	174	ASN	CA-C	-5.16	1.39	1.52
1	F	174	ASN	CA-CB	-5.13	1.39	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	174	ASN	N-CA-C	6.07	127.39	111.00

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	3298	0	3279	138	0
1	B	3298	0	3279	119	0
1	C	3298	0	3279	121	0
1	D	3234	0	3234	107	0
1	E	3298	0	3279	114	0
1	F	3298	0	3277	127	0
All	All	19724	0	19627	626	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 16.

All (626) 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:D:52:MET:HG3	1:D:62:VAL:HG11	1.28	1.08
1:E:232:GLU:OE2	1:F:414:ARG:NH1	1.87	1.07
1:D:259:ARG:HB2	1:E:170:SER:O	1.52	1.07
1:E:168:ILE:HG13	1:E:169:GLU:H	1.10	1.06
1:A:174:ASN:N	1:A:174:ASN:OD1	1.63	1.05
1:F:52:MET:HG3	1:F:62:VAL:HG11	1.37	1.05
1:A:315:ASP:O	1:A:316:TYR:HB2	1.54	1.05
1:C:299:ARG:NH2	1:D:31:LYS:HB3	1.73	1.03
1:F:315:ASP:O	1:F:316:TYR:HB2	1.58	1.02
1:C:315:ASP:O	1:C:316:TYR:HB2	1.57	1.02
1:D:315:ASP:O	1:D:316:TYR:HB2	1.59	1.02
1:A:190:TYR:OH	1:F:256:ALA:HB2	1.58	1.02
1:B:315:ASP:O	1:B:316:TYR:HB2	1.57	1.01
1:E:52:MET:HG3	1:E:62:VAL:HG11	1.43	1.00
1:C:52:MET:HG3	1:C:62:VAL:HG11	1.44	0.99
1:C:258:ARG:HG2	1:D:168:ILE:CG2	1.91	0.99
1:E:315:ASP:O	1:E:316:TYR:HB2	1.58	0.99
1:A:232:GLU:OE2	1:B:414:ARG:NH1	1.97	0.97
1:E:239:ILE:CD1	1:F:161:LEU:HG	1.94	0.96
1:E:157:ILE:HG13	1:E:158:ASP:H	1.31	0.95
1:C:299:ARG:HH22	1:D:31:LYS:HB3	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ILE:HD13	1:F:161:LEU:HG	1.46	0.94
1:A:157:ILE:HG23	1:A:158:ASP:H	1.29	0.94
1:E:377:SER:HB2	1:E:380:LEU:HB2	1.48	0.94
1:B:52:MET:HG3	1:B:62:VAL:HG11	1.46	0.94
1:D:377:SER:HB2	1:D:380:LEU:HB2	1.50	0.93
1:A:257:ALA:HA	1:B:173:GLY:HA2	1.51	0.93
1:C:377:SER:HB2	1:C:380:LEU:HB2	1.50	0.93
1:A:377:SER:HB2	1:A:380:LEU:HB2	1.50	0.92
1:B:377:SER:HB2	1:B:380:LEU:HB2	1.51	0.91
1:F:377:SER:HB2	1:F:380:LEU:HB2	1.53	0.90
1:C:258:ARG:HH22	1:C:265:ASP:HB2	1.39	0.88
1:E:168:ILE:HG13	1:E:169:GLU:N	1.89	0.87
1:F:317:LEU:HD21	1:F:380:LEU:HD21	1.56	0.87
1:A:258:ARG:HG2	1:B:168:ILE:HG23	1.54	0.87
1:E:18:ALA:HB2	1:F:65:THR:HG21	1.59	0.84
1:A:258:ARG:HH22	1:A:265:ASP:HB2	1.43	0.84
1:A:157:ILE:HG23	1:A:158:ASP:N	1.93	0.83
1:E:317:LEU:HD21	1:E:380:LEU:HD21	1.59	0.83
1:A:52:MET:HG3	1:A:62:VAL:HG11	1.60	0.82
1:D:273:ILE:HG23	1:E:161:LEU:HD11	1.61	0.82
1:E:157:ILE:HG13	1:E:158:ASP:N	1.95	0.82
1:D:317:LEU:HD21	1:D:380:LEU:HD21	1.62	0.82
1:F:258:ARG:HH22	1:F:265:ASP:HB2	1.44	0.82
1:C:317:LEU:HD21	1:C:380:LEU:HD21	1.60	0.81
1:D:52:MET:HG3	1:D:62:VAL:CG1	2.10	0.81
1:E:52:MET:HG3	1:E:62:VAL:CG1	2.10	0.81
1:B:258:ARG:HH22	1:B:265:ASP:HB2	1.46	0.81
1:B:317:LEU:HD21	1:B:380:LEU:HD21	1.63	0.80
1:D:258:ARG:HH22	1:D:265:ASP:HB2	1.43	0.80
1:A:75:LEU:N	1:A:76:PRO:HD2	1.97	0.79
1:E:75:LEU:N	1:E:76:PRO:HD2	1.98	0.79
1:E:258:ARG:HH22	1:E:265:ASP:HB2	1.48	0.78
1:B:174:ASN:OD1	1:B:174:ASN:N	2.17	0.78
1:A:317:LEU:HD21	1:A:380:LEU:HD21	1.66	0.77
1:F:157:ILE:HG13	1:F:158:ASP:N	1.99	0.77
1:C:356:GLN:NE2	1:D:379:GLN:OE1	2.16	0.77
1:F:193:LYS:O	1:F:350:VAL:HG22	1.84	0.77
1:B:52:MET:HG3	1:B:62:VAL:CG1	2.15	0.77
1:D:124:VAL:HG12	1:E:110:LYS:HG3	1.67	0.76
1:C:229:HIS:HD2	1:C:289:GLN:OE1	1.67	0.75
1:A:190:TYR:OH	1:F:256:ALA:CB	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:HG3	1:A:62:VAL:CG1	2.15	0.75
1:E:229:HIS:HD2	1:E:289:GLN:OE1	1.70	0.74
1:B:392:ARG:HG3	1:B:406:VAL:HG22	1.67	0.74
1:B:36:THR:H	1:B:39:HIS:CD2	2.06	0.74
1:F:229:HIS:HD2	1:F:289:GLN:OE1	1.70	0.73
1:C:175:ILE:H	1:C:175:ILE:HD12	1.51	0.73
1:E:168:ILE:CG1	1:E:169:GLU:H	1.95	0.73
1:D:75:LEU:N	1:D:76:PRO:HD2	2.03	0.73
1:F:52:MET:HG3	1:F:62:VAL:CG1	2.18	0.73
1:B:256:ALA:O	1:C:171:ALA:HB1	1.89	0.72
1:E:273:ILE:HG23	1:F:165:TYR:CE2	2.24	0.72
1:B:193:LYS:O	1:B:350:VAL:HG22	1.89	0.72
1:F:75:LEU:N	1:F:76:PRO:HD2	2.05	0.72
1:F:158:ASP:OD1	1:F:161:LEU:HD13	1.89	0.72
1:F:406:VAL:HG23	1:F:425:PHE:HB2	1.72	0.72
1:A:392:ARG:HG3	1:A:406:VAL:HG22	1.69	0.72
1:D:259:ARG:HG2	1:E:171:ALA:HB2	1.71	0.72
1:E:52:MET:CG	1:E:62:VAL:HG11	2.19	0.72
1:D:107:TYR:O	1:D:111:ARG:HG3	1.90	0.72
1:E:392:ARG:HG3	1:E:406:VAL:HG22	1.71	0.72
1:A:22:SER:N	1:A:91:VAL:HG21	2.05	0.72
1:A:229:HIS:HD2	1:A:289:GLN:OE1	1.73	0.71
1:A:52:MET:CG	1:A:62:VAL:HG11	2.20	0.71
1:A:193:LYS:O	1:A:350:VAL:HG22	1.89	0.71
1:D:193:LYS:O	1:D:350:VAL:HG22	1.90	0.71
1:B:231:LEU:HD12	1:B:231:LEU:H	1.56	0.71
1:E:193:LYS:O	1:E:350:VAL:HG22	1.91	0.71
1:A:333:ILE:HG21	1:A:377:SER:HB3	1.73	0.71
1:B:110:LYS:HG3	1:C:124:VAL:HG11	1.71	0.71
1:C:75:LEU:N	1:C:76:PRO:HD2	2.05	0.70
1:C:193:LYS:O	1:C:350:VAL:HG22	1.92	0.70
1:C:52:MET:HG3	1:C:62:VAL:CG1	2.19	0.70
1:A:254:ILE:HG13	1:B:168:ILE:HD12	1.73	0.70
1:C:281:ILE:O	1:D:157:ILE:HG23	1.91	0.69
1:C:392:ARG:HG3	1:C:406:VAL:HG22	1.73	0.69
1:B:75:LEU:N	1:B:76:PRO:HD2	2.08	0.69
1:E:232:GLU:CD	1:F:414:ARG:HD3	2.11	0.69
1:D:229:HIS:HD2	1:D:289:GLN:OE1	1.75	0.69
1:A:231:LEU:H	1:A:231:LEU:HD12	1.58	0.68
1:F:107:TYR:O	1:F:111:ARG:HG3	1.93	0.68
1:E:239:ILE:HD11	1:F:161:LEU:HG	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:O	1:A:28:GLU:N	2.26	0.68
1:B:124:VAL:HG11	1:C:110:LYS:HG3	1.74	0.68
1:D:124:VAL:CG1	1:E:110:LYS:HG3	2.23	0.68
1:B:362:GLU:HB2	1:C:372:SER:HB3	1.76	0.68
1:E:158:ASP:O	1:E:160:ALA:N	2.24	0.67
1:E:377:SER:HB2	1:E:380:LEU:CB	2.24	0.67
1:C:119:GLN:HG3	1:C:123:ASN:ND2	2.10	0.67
1:D:392:ARG:HG3	1:D:406:VAL:HG22	1.74	0.67
1:A:157:ILE:CG2	1:A:158:ASP:H	2.07	0.67
1:E:231:LEU:HD12	1:E:231:LEU:H	1.60	0.67
1:F:315:ASP:O	1:F:316:TYR:CB	2.41	0.67
1:E:392:ARG:CG	1:E:406:VAL:HG22	2.25	0.66
1:A:377:SER:HB2	1:A:380:LEU:CB	2.25	0.66
1:A:406:VAL:HG23	1:A:425:PHE:HB2	1.76	0.66
1:C:231:LEU:HD12	1:C:231:LEU:H	1.60	0.66
1:D:377:SER:HB2	1:D:380:LEU:CB	2.26	0.66
1:F:231:LEU:H	1:F:231:LEU:HD12	1.61	0.66
1:C:315:ASP:O	1:C:316:TYR:CB	2.41	0.66
1:B:406:VAL:HG23	1:B:425:PHE:HB2	1.78	0.66
1:C:258:ARG:HG2	1:D:168:ILE:HG22	1.78	0.65
1:B:48:ILE:O	1:B:52:MET:HB2	1.97	0.65
1:D:406:VAL:HG23	1:D:425:PHE:HB2	1.77	0.65
1:A:124:VAL:HG11	1:F:110:LYS:HG3	1.79	0.65
1:D:52:MET:CG	1:D:62:VAL:HG11	2.17	0.65
1:E:48:ILE:O	1:E:52:MET:HB2	1.96	0.65
1:A:161:LEU:HD11	1:F:273:ILE:HG23	1.78	0.65
1:F:124:VAL:HG13	1:F:134:PRO:HB3	1.78	0.65
1:E:23:ILE:HG21	1:E:30:ILE:HG23	1.79	0.65
1:B:119:GLN:HG3	1:B:123:ASN:ND2	2.11	0.64
1:A:36:THR:H	1:A:39:HIS:CD2	2.14	0.64
1:E:273:ILE:HG23	1:F:165:TYR:HE2	1.60	0.64
1:E:315:ASP:O	1:E:316:TYR:CB	2.41	0.64
1:F:392:ARG:HG3	1:F:406:VAL:HG22	1.79	0.64
1:C:392:ARG:CG	1:C:406:VAL:HG22	2.28	0.64
1:B:167:GLU:O	1:B:171:ALA:HB2	1.96	0.64
1:C:406:VAL:HG23	1:C:425:PHE:HB2	1.77	0.64
1:F:257:ALA:HB1	1:F:261:PHE:CB	2.27	0.64
1:F:377:SER:HB2	1:F:380:LEU:CB	2.27	0.64
1:E:406:VAL:HG23	1:E:425:PHE:HB2	1.79	0.64
1:D:273:ILE:CG2	1:E:161:LEU:HD11	2.27	0.64
1:D:392:ARG:CG	1:D:406:VAL:HG22	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:GLN:HG3	1:F:123:ASN:ND2	2.12	0.64
1:A:137:GLU:O	1:A:141:GLU:HG2	1.98	0.63
1:F:36:THR:H	1:F:39:HIS:CD2	2.15	0.63
1:A:315:ASP:O	1:A:316:TYR:CB	2.40	0.62
1:B:175:ILE:HD12	1:B:175:ILE:H	1.64	0.62
1:B:107:TYR:O	1:B:111:ARG:HG3	2.00	0.62
1:D:119:GLN:HG3	1:D:123:ASN:ND2	2.15	0.62
1:B:124:VAL:HG13	1:B:134:PRO:HB3	1.82	0.62
1:C:356:GLN:HE22	1:D:379:GLN:CD	2.02	0.62
1:A:154:ASP:HB3	1:F:300:GLN:HE22	1.65	0.61
1:D:333:ILE:HG21	1:D:377:SER:HB3	1.82	0.61
1:F:316:TYR:HB3	1:F:319:LEU:HB2	1.81	0.61
1:C:258:ARG:HG2	1:D:168:ILE:HG23	1.81	0.61
1:E:333:ILE:HG21	1:E:377:SER:HB3	1.81	0.61
1:C:137:GLU:O	1:C:141:GLU:HG2	2.00	0.61
1:B:229:HIS:HD2	1:B:289:GLN:OE1	1.83	0.61
1:C:174:ASN:O	1:C:175:ILE:C	2.39	0.61
1:A:110:LYS:HG3	1:F:124:VAL:HG11	1.82	0.61
1:C:36:THR:H	1:C:39:HIS:CD2	2.18	0.61
1:F:333:ILE:HG21	1:F:377:SER:HB3	1.83	0.61
1:F:157:ILE:CG1	1:F:158:ASP:N	2.63	0.61
1:A:37:PRO:HB2	1:A:46:PHE:CE1	2.36	0.60
1:D:375:ARG:HE	1:D:376:GLU:HG3	1.65	0.60
1:D:36:THR:H	1:D:39:HIS:CD2	2.18	0.60
1:D:231:LEU:HD12	1:D:231:LEU:H	1.65	0.60
1:C:107:TYR:O	1:C:111:ARG:HG3	2.01	0.60
1:D:257:ALA:HB1	1:D:261:PHE:CB	2.31	0.60
1:B:259:ARG:H	1:C:171:ALA:HB3	1.66	0.60
1:C:203:ARG:NH2	1:D:381:GLU:OE1	2.32	0.60
1:C:317:LEU:CD2	1:C:380:LEU:HD21	2.29	0.60
1:E:255:LYS:HG2	1:F:190:TYR:CD1	2.37	0.60
1:A:26:GLU:C	1:A:28:GLU:H	2.04	0.60
1:A:190:TYR:HH	1:F:256:ALA:HB2	1.67	0.59
1:A:124:VAL:HG13	1:A:134:PRO:HB3	1.83	0.59
1:A:157:ILE:CG2	1:A:158:ASP:N	2.65	0.59
1:A:48:ILE:O	1:A:52:MET:HB2	2.02	0.59
1:B:52:MET:CG	1:B:62:VAL:HG11	2.27	0.59
1:B:392:ARG:CG	1:B:406:VAL:HG22	2.33	0.59
1:D:357:LEU:HD13	1:D:369:PRO:HB3	1.85	0.59
1:B:154:ASP:OD1	1:B:155:GLY:N	2.34	0.59
1:A:164:VAL:O	1:A:168:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:HB2	1:B:380:LEU:CB	2.30	0.59
1:C:48:ILE:O	1:C:52:MET:HB2	2.03	0.59
1:F:41:SER:HB3	1:F:42:PRO:HD2	1.84	0.59
1:C:172:ASP:O	1:C:174:ASN:N	2.35	0.59
1:A:119:GLN:HG3	1:A:123:ASN:ND2	2.18	0.58
1:A:357:LEU:HD13	1:A:369:PRO:HB3	1.85	0.58
1:B:333:ILE:HG21	1:B:377:SER:HB3	1.84	0.58
1:C:356:GLN:CD	1:D:382:GLN:OE1	2.42	0.58
1:D:98:LYS:HE2	1:D:98:LYS:HA	1.84	0.58
1:E:317:LEU:CD2	1:E:380:LEU:HD21	2.32	0.58
1:B:316:TYR:HB3	1:B:319:LEU:HB2	1.85	0.58
1:C:377:SER:HB2	1:C:380:LEU:CB	2.28	0.58
1:C:257:ALA:HB1	1:C:261:PHE:CB	2.34	0.57
1:A:75:LEU:N	1:A:76:PRO:CD	2.67	0.57
1:E:12:ASN:HD21	1:F:69:ALA:HA	1.69	0.57
1:C:254:ILE:HA	1:C:258:ARG:HB2	1.86	0.57
1:B:305:ASN:HB3	1:B:308:LYS:HD2	1.85	0.57
1:C:333:ILE:HG21	1:C:377:SER:HB3	1.85	0.57
1:F:317:LEU:CD2	1:F:380:LEU:HD21	2.30	0.57
1:A:316:TYR:HB3	1:A:319:LEU:HB2	1.87	0.57
1:F:392:ARG:CG	1:F:406:VAL:HG22	2.33	0.57
1:B:22:SER:N	1:B:91:VAL:HG21	2.19	0.57
1:E:36:THR:H	1:E:39:HIS:CD2	2.22	0.57
1:C:16:GLU:OE2	1:C:40:PHE:HA	2.05	0.57
1:C:316:TYR:HB3	1:C:319:LEU:HB2	1.87	0.57
1:D:22:SER:N	1:D:91:VAL:HG21	2.19	0.57
1:D:316:TYR:HB3	1:D:319:LEU:HB2	1.87	0.57
1:A:258:ARG:CG	1:B:168:ILE:HG23	2.32	0.57
1:B:37:PRO:HB2	1:B:46:PHE:CE1	2.39	0.57
1:E:254:ILE:HA	1:E:258:ARG:HB2	1.85	0.57
1:B:124:VAL:CG1	1:C:110:LYS:HG3	2.35	0.56
1:D:48:ILE:O	1:D:52:MET:HB2	2.04	0.56
1:F:375:ARG:HE	1:F:376:GLU:HG3	1.70	0.56
1:A:236:LYS:NZ	1:B:163:THR:HG21	2.20	0.56
1:B:375:ARG:HE	1:B:376:GLU:HG3	1.71	0.56
1:D:305:ASN:HB3	1:D:308:LYS:HD2	1.88	0.56
1:C:22:SER:N	1:C:91:VAL:HG21	2.20	0.56
1:F:254:ILE:HG23	1:F:255:LYS:H	1.71	0.56
1:A:254:ILE:HG13	1:B:168:ILE:CD1	2.34	0.56
1:A:254:ILE:HA	1:A:258:ARG:HB2	1.88	0.56
1:C:299:ARG:HB3	1:C:299:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLN:HG3	1:E:123:ASN:ND2	2.20	0.56
1:C:299:ARG:NH1	1:D:31:LYS:O	2.39	0.56
1:F:378:GLY:C	1:F:380:LEU:H	2.09	0.56
1:C:375:ARG:HE	1:C:376:GLU:HG3	1.71	0.56
1:E:357:LEU:HD13	1:E:369:PRO:HB3	1.87	0.56
1:A:364:ARG:HD2	1:F:359:ARG:CZ	2.35	0.55
1:E:316:TYR:HB3	1:E:319:LEU:HB2	1.87	0.55
1:B:157:ILE:O	1:B:161:LEU:N	2.34	0.55
1:E:158:ASP:C	1:E:160:ALA:H	2.08	0.55
1:E:305:ASN:HB3	1:E:308:LYS:HD2	1.89	0.55
1:B:315:ASP:O	1:B:316:TYR:CB	2.41	0.55
1:B:257:ALA:HB1	1:B:261:PHE:CB	2.36	0.55
1:C:282:ASN:HA	1:D:157:ILE:HG23	1.89	0.55
1:F:254:ILE:O	1:F:255:LYS:C	2.44	0.55
1:B:254:ILE:HA	1:B:258:ARG:HB2	1.89	0.55
1:D:317:LEU:CD2	1:D:380:LEU:HD21	2.35	0.55
1:B:165:TYR:O	1:B:168:ILE:N	2.36	0.55
1:B:254:ILE:HG13	1:C:168:ILE:HG23	1.89	0.55
1:C:357:LEU:HD13	1:C:369:PRO:HB3	1.88	0.55
1:D:424:ALA:HB3	1:D:433:VAL:HB	1.89	0.54
1:A:392:ARG:CG	1:A:406:VAL:HG22	2.36	0.54
1:A:254:ILE:HG23	1:A:255:LYS:H	1.72	0.54
1:A:254:ILE:O	1:A:255:LYS:C	2.46	0.54
1:B:317:LEU:CD2	1:B:380:LEU:HD21	2.35	0.54
1:A:375:ARG:HE	1:A:376:GLU:HG3	1.72	0.54
1:A:392:ARG:HH21	1:A:427:LYS:HE2	1.73	0.54
1:D:254:ILE:HG23	1:D:255:LYS:H	1.73	0.54
1:B:165:TYR:O	1:B:168:ILE:HG12	2.08	0.54
1:D:315:ASP:O	1:D:316:TYR:CB	2.42	0.54
1:E:99:GLN:HE22	1:F:61:SER:H	1.54	0.54
1:F:23:ILE:HG21	1:F:30:ILE:HG23	1.89	0.54
1:E:75:LEU:N	1:E:76:PRO:CD	2.69	0.54
1:F:37:PRO:HB2	1:F:46:PHE:CE1	2.42	0.54
1:F:357:LEU:HD13	1:F:369:PRO:HB3	1.90	0.54
1:C:172:ASP:C	1:C:174:ASN:H	2.09	0.54
1:B:229:HIS:CD2	1:B:294:ILE:HG12	2.43	0.54
1:F:48:ILE:O	1:F:52:MET:HB2	2.08	0.54
1:D:201:ALA:O	1:D:389:PHE:HA	2.07	0.54
1:E:162:VAL:O	1:E:165:TYR:HB2	2.08	0.53
1:E:424:ALA:HB3	1:E:433:VAL:HB	1.90	0.53
1:C:52:MET:CG	1:C:62:VAL:HG11	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HG21	1:D:30:ILE:HG23	1.89	0.53
1:B:357:LEU:HD13	1:B:369:PRO:HB3	1.90	0.53
1:C:392:ARG:HH21	1:C:427:LYS:HE2	1.72	0.53
1:A:138:ALA:O	1:A:142:LEU:HB2	2.08	0.53
1:C:96:THR:HG22	1:D:61:SER:OG	2.09	0.53
1:A:317:LEU:CD2	1:A:380:LEU:HD21	2.36	0.53
1:F:137:GLU:O	1:F:141:GLU:HG2	2.09	0.53
1:F:316:TYR:HD2	1:F:319:LEU:HD13	1.73	0.53
1:A:27:PRO:HB3	1:A:62:VAL:O	2.08	0.53
1:A:424:ALA:HB3	1:A:433:VAL:HB	1.91	0.53
1:C:378:GLY:C	1:C:380:LEU:H	2.12	0.53
1:E:107:TYR:O	1:E:111:ARG:HG3	2.08	0.53
1:A:378:GLY:C	1:A:380:LEU:H	2.11	0.53
1:A:257:ALA:HB1	1:A:261:PHE:CB	2.39	0.53
1:D:161:LEU:HD23	1:D:161:LEU:O	2.08	0.53
1:B:392:ARG:HH21	1:B:427:LYS:HE2	1.72	0.53
1:E:257:ALA:HB1	1:E:261:PHE:CB	2.39	0.53
1:C:305:ASN:HB3	1:C:308:LYS:HD2	1.90	0.53
1:D:254:ILE:O	1:D:255:LYS:C	2.47	0.53
1:F:305:ASN:HB3	1:F:308:LYS:HD2	1.91	0.53
1:B:316:TYR:HD2	1:B:319:LEU:HD13	1.74	0.52
1:D:378:GLY:C	1:D:380:LEU:H	2.12	0.52
1:E:282:ASN:HA	1:F:157:ILE:HB	1.89	0.52
1:A:99:GLN:HE22	1:B:61:SER:H	1.57	0.52
1:B:165:TYR:O	1:B:166:GLU:C	2.47	0.52
1:F:52:MET:CG	1:F:62:VAL:HG11	2.24	0.52
1:B:156:SER:C	1:B:157:ILE:HG13	2.29	0.52
1:C:115:SER:O	1:C:119:GLN:HB2	2.09	0.52
1:F:150:THR:O	1:F:151:ASP:HB3	2.09	0.52
1:A:41:SER:HB3	1:A:42:PRO:HD2	1.91	0.52
1:A:160:ALA:O	1:A:164:VAL:HG23	2.10	0.52
1:B:201:ALA:O	1:B:389:PHE:HA	2.10	0.52
1:B:259:ARG:NH1	1:C:169:GLU:HG2	2.24	0.52
1:D:157:ILE:HG13	1:D:157:ILE:O	2.09	0.52
1:E:392:ARG:HH21	1:E:427:LYS:HE2	1.74	0.52
1:F:123:ASN:HB3	1:F:137:GLU:OE1	2.09	0.52
1:A:362:GLU:HB2	1:B:372:SER:HB3	1.91	0.52
1:B:254:ILE:O	1:B:255:LYS:C	2.48	0.52
1:C:41:SER:HB3	1:C:42:PRO:HD2	1.91	0.52
1:F:392:ARG:HH21	1:F:427:LYS:HE2	1.73	0.52
1:C:232:GLU:HG3	1:D:341:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:SER:O	1:E:119:GLN:HB2	2.09	0.52
1:F:16:GLU:OE2	1:F:40:PHE:HA	2.10	0.52
1:A:93:SER:C	1:A:95:THR:H	2.14	0.51
1:C:175:ILE:HD12	1:C:175:ILE:N	2.21	0.51
1:C:254:ILE:O	1:C:255:LYS:C	2.48	0.51
1:D:392:ARG:HH21	1:D:427:LYS:HE2	1.75	0.51
1:E:316:TYR:HD2	1:E:319:LEU:HD13	1.75	0.51
1:B:64:PHE:CD1	1:B:64:PHE:N	2.78	0.51
1:E:254:ILE:O	1:E:255:LYS:C	2.49	0.51
1:A:305:ASN:HB3	1:A:308:LYS:HD2	1.93	0.51
1:B:26:GLU:C	1:B:28:GLU:H	2.14	0.51
1:B:134:PRO:HG3	1:C:110:LYS:HB2	1.92	0.51
1:E:386:ILE:HA	1:E:412:LYS:O	2.10	0.51
1:A:16:GLU:OE2	1:A:40:PHE:HA	2.11	0.51
1:C:23:ILE:HG21	1:C:30:ILE:HG23	1.92	0.51
1:D:254:ILE:HA	1:D:258:ARG:HB2	1.93	0.51
1:B:254:ILE:HG23	1:B:255:LYS:H	1.76	0.51
1:C:356:GLN:OE1	1:D:382:GLN:OE1	2.29	0.51
1:D:141:GLU:O	1:D:145:ILE:HG13	2.11	0.51
1:A:198:VAL:HG22	1:A:352:ILE:HG12	1.92	0.51
1:A:123:ASN:HB3	1:A:137:GLU:OE1	2.11	0.51
1:A:169:GLU:HB2	1:F:259:ARG:NH1	2.26	0.50
1:A:316:TYR:HD2	1:A:319:LEU:HD13	1.76	0.50
1:B:378:GLY:C	1:B:380:LEU:H	2.14	0.50
1:D:16:GLU:OE2	1:D:40:PHE:HA	2.11	0.50
1:D:75:LEU:N	1:D:76:PRO:CD	2.73	0.50
1:F:167:GLU:OE1	1:F:167:GLU:N	2.40	0.50
1:F:198:VAL:HG22	1:F:352:ILE:HG12	1.93	0.50
1:A:371:LEU:HD11	1:A:411:ALA:HB1	1.94	0.50
1:B:435:LEU:O	1:B:436:GLU:HB2	2.11	0.50
1:E:375:ARG:HE	1:E:376:GLU:HG3	1.75	0.50
1:A:146:GLU:C	1:A:148:SER:H	2.14	0.50
1:A:175:ILE:HD12	1:A:175:ILE:N	2.26	0.50
1:E:208:LYS:HD2	1:E:355:SER:O	2.11	0.50
1:E:254:ILE:HD11	1:F:168:ILE:HD12	1.94	0.50
1:B:110:LYS:HG3	1:C:124:VAL:CG1	2.41	0.50
1:A:115:SER:O	1:A:119:GLN:HB2	2.11	0.50
1:A:256:ALA:O	1:B:171:ALA:HB1	2.11	0.50
1:B:23:ILE:HG21	1:B:30:ILE:HG23	1.93	0.50
1:A:157:ILE:HD13	1:A:158:ASP:N	2.27	0.50
1:C:75:LEU:N	1:C:76:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ALA:HB3	1:C:433:VAL:HB	1.93	0.50
1:D:157:ILE:O	1:D:157:ILE:CG1	2.59	0.50
1:E:22:SER:N	1:E:91:VAL:HG21	2.26	0.49
1:E:378:GLY:C	1:E:380:LEU:H	2.14	0.49
1:A:364:ARG:HD2	1:F:359:ARG:NH2	2.27	0.49
1:B:115:SER:O	1:B:119:GLN:HB2	2.12	0.49
1:B:137:GLU:O	1:B:141:GLU:HG2	2.13	0.49
1:D:358:SER:HB2	1:D:375:ARG:HB2	1.94	0.49
1:C:303:ARG:NH1	1:D:98:LYS:HD2	2.27	0.49
1:D:316:TYR:HD2	1:D:319:LEU:HD13	1.78	0.49
1:F:75:LEU:N	1:F:76:PRO:CD	2.75	0.49
1:C:198:VAL:HG22	1:C:352:ILE:HG12	1.94	0.49
1:F:138:ALA:O	1:F:142:LEU:HB2	2.13	0.49
1:E:167:GLU:HA	1:E:170:SER:HB2	1.94	0.49
1:B:120:ILE:HG23	1:B:141:GLU:HG3	1.95	0.49
1:F:161:LEU:O	1:F:164:VAL:HG22	2.13	0.49
1:B:16:GLU:OE2	1:B:40:PHE:HA	2.12	0.48
1:F:41:SER:O	1:F:46:PHE:HB2	2.12	0.48
1:A:141:GLU:O	1:A:145:ILE:HG13	2.12	0.48
1:B:119:GLN:HG3	1:B:123:ASN:HD22	1.77	0.48
1:D:20:LEU:O	1:D:24:LEU:HG	2.14	0.48
1:F:22:SER:N	1:F:91:VAL:HG21	2.28	0.48
1:F:64:PHE:CD1	1:F:64:PHE:N	2.82	0.48
1:F:280:ASN:N	1:F:280:ASN:HD22	2.11	0.48
1:B:239:ILE:HG21	1:C:161:LEU:HG	1.96	0.48
1:D:338:ARG:HG3	1:D:379:GLN:HG2	1.95	0.48
1:F:217:LYS:O	1:F:220:SER:N	2.47	0.48
1:C:120:ILE:O	1:C:124:VAL:HG23	2.14	0.48
1:B:258:ARG:HB3	1:C:171:ALA:CB	2.44	0.48
1:B:386:ILE:HA	1:B:412:LYS:O	2.14	0.48
1:E:142:LEU:O	1:E:146:GLU:HG3	2.14	0.48
1:E:337:SER:HB2	1:E:380:LEU:HD22	1.95	0.48
1:D:359:ARG:NH1	1:E:366:ASP:HB3	2.29	0.48
1:F:406:VAL:HG23	1:F:425:PHE:CB	2.42	0.48
1:A:356:GLN:HE22	1:B:382:GLN:CD	2.17	0.48
1:B:362:GLU:HB2	1:C:372:SER:CB	2.41	0.48
1:F:125:ASN:OD1	1:F:125:ASN:N	2.46	0.48
1:F:337:SER:HB2	1:F:380:LEU:HD22	1.96	0.48
1:B:116:ILE:HG12	1:B:144:GLU:HB3	1.95	0.47
1:E:282:ASN:ND2	1:F:157:ILE:HD13	2.29	0.47
1:A:157:ILE:HD13	1:A:158:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:O	1:C:146:GLU:HG3	2.14	0.47
1:A:414:ARG:O	1:F:237:GLU:OE1	2.32	0.47
1:D:26:GLU:C	1:D:28:GLU:H	2.17	0.47
1:E:239:ILE:HD11	1:F:161:LEU:CG	2.43	0.47
1:A:31:LYS:HE3	1:A:56:ASP:OD1	2.14	0.47
1:B:175:ILE:HD12	1:B:175:ILE:N	2.28	0.47
1:E:241:ARG:HH21	1:F:415:ASP:HA	1.79	0.47
1:F:424:ALA:HB3	1:F:433:VAL:HB	1.95	0.47
1:A:313:MET:HA	1:A:352:ILE:O	2.14	0.47
1:A:386:ILE:HA	1:A:412:LYS:O	2.15	0.47
1:B:337:SER:HB2	1:B:380:LEU:HD22	1.95	0.47
1:C:26:GLU:C	1:C:28:GLU:H	2.18	0.47
1:F:257:ALA:O	1:F:259:ARG:N	2.48	0.47
1:E:316:TYR:CD2	1:E:319:LEU:HD13	2.49	0.47
1:F:358:SER:HB2	1:F:375:ARG:HB2	1.95	0.47
1:A:229:HIS:CD2	1:A:294:ILE:HG12	2.50	0.47
1:E:282:ASN:ND2	1:F:157:ILE:CD1	2.78	0.47
1:D:316:TYR:CD2	1:D:319:LEU:HD13	2.49	0.47
1:A:269:LEU:C	1:A:271:MET:H	2.17	0.47
1:F:254:ILE:HA	1:F:258:ARG:HB2	1.97	0.47
1:A:152:ASP:N	1:A:152:ASP:OD1	2.48	0.46
1:B:316:TYR:CD2	1:B:319:LEU:HD13	2.50	0.46
1:A:142:LEU:O	1:A:146:GLU:HG3	2.14	0.46
1:B:138:ALA:O	1:B:142:LEU:HB2	2.15	0.46
1:E:160:ALA:O	1:E:164:VAL:N	2.42	0.46
1:C:201:ALA:O	1:C:389:PHE:HA	2.16	0.46
1:C:410:ILE:HD12	1:C:410:ILE:N	2.31	0.46
1:B:75:LEU:N	1:B:76:PRO:CD	2.76	0.46
1:C:358:SER:HB2	1:C:375:ARG:HB2	1.98	0.46
1:E:44:LYS:O	1:E:48:ILE:HG12	2.15	0.46
1:B:368:ARG:HA	1:B:369:PRO:HD3	1.77	0.46
1:C:99:GLN:HE22	1:D:61:SER:H	1.64	0.46
1:E:157:ILE:CG1	1:E:158:ASP:N	2.70	0.46
1:F:174:ASN:O	1:F:175:ILE:O	2.34	0.46
1:A:217:LYS:O	1:A:220:SER:N	2.49	0.46
1:A:259:ARG:HB3	1:B:171:ALA:O	2.16	0.46
1:F:254:ILE:O	1:F:258:ARG:HB2	2.16	0.46
1:F:316:TYR:CD2	1:F:319:LEU:HD13	2.50	0.46
1:A:64:PHE:CD1	1:A:64:PHE:N	2.84	0.46
1:C:41:SER:O	1:C:46:PHE:HB2	2.16	0.46
1:D:406:VAL:HG23	1:D:425:PHE:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:GLU:HB2	1:F:372:SER:HB3	1.97	0.46
1:E:406:VAL:HG23	1:E:425:PHE:CB	2.45	0.46
1:A:239:ILE:HD13	1:B:161:LEU:HD22	1.97	0.46
1:E:137:GLU:O	1:E:141:GLU:HG2	2.16	0.45
1:E:368:ARG:HA	1:E:369:PRO:HD3	1.79	0.45
1:F:257:ALA:HB1	1:F:261:PHE:HB2	1.98	0.45
1:A:12:ASN:HD21	1:B:69:ALA:HA	1.81	0.45
1:E:229:HIS:CD2	1:E:294:ILE:HG12	2.52	0.45
1:B:258:ARG:HB3	1:C:171:ALA:HB2	1.97	0.45
1:C:254:ILE:HG23	1:C:255:LYS:H	1.81	0.45
1:E:254:ILE:HG23	1:E:255:LYS:H	1.81	0.45
1:A:203:ARG:NH1	1:A:359:ARG:HA	2.31	0.45
1:C:208:LYS:HD2	1:C:355:SER:O	2.17	0.45
1:D:41:SER:HB3	1:D:42:PRO:HD2	1.98	0.45
1:B:175:ILE:H	1:B:175:ILE:CD1	2.29	0.45
1:B:406:VAL:HG23	1:B:425:PHE:CB	2.45	0.45
1:E:169:GLU:O	1:E:170:SER:O	2.35	0.45
1:E:172:ASP:OD2	1:E:172:ASP:N	2.50	0.45
1:E:381:GLU:HA	1:E:387:ILE:HD11	1.98	0.45
1:C:299:ARG:HB3	1:C:299:ARG:HH11	1.82	0.45
1:D:435:LEU:O	1:D:436:GLU:C	2.55	0.45
1:E:356:GLN:OE1	1:F:382:GLN:HG2	2.17	0.45
1:C:406:VAL:HG23	1:C:425:PHE:CB	2.45	0.45
1:E:26:GLU:C	1:E:28:GLU:H	2.20	0.45
1:E:175:ILE:N	1:E:175:ILE:HD12	2.31	0.45
1:E:254:ILE:O	1:E:258:ARG:HB2	2.16	0.45
1:F:254:ILE:HA	1:F:258:ARG:HD2	1.99	0.45
1:F:406:VAL:CG2	1:F:425:PHE:HB2	2.44	0.45
1:C:367:LYS:HB2	1:C:391:TYR:HE1	1.82	0.44
1:F:212:ALA:HB1	1:F:313:MET:CE	2.46	0.44
1:F:257:ALA:O	1:F:258:ARG:C	2.55	0.44
1:D:119:GLN:HG3	1:D:123:ASN:HD22	1.81	0.44
1:E:138:ALA:O	1:E:142:LEU:HB2	2.17	0.44
1:A:39:HIS:HE1	1:A:151:ASP:OD2	2.01	0.44
1:A:152:ASP:HB2	1:A:153:ASP:H	1.52	0.44
1:A:236:LYS:HZ1	1:B:163:THR:HG21	1.82	0.44
1:A:357:LEU:CD1	1:A:369:PRO:HB3	2.46	0.44
1:D:237:GLU:CD	1:E:415:ASP:HA	2.37	0.44
1:D:386:ILE:HA	1:D:412:LYS:O	2.18	0.44
1:A:316:TYR:CD2	1:A:319:LEU:HD13	2.53	0.44
1:E:280:ASN:N	1:E:280:ASN:HD22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ALA:O	1:F:202:ALA:HB2	2.17	0.44
1:B:258:ARG:HG2	1:C:168:ILE:O	2.16	0.44
1:B:371:LEU:HD11	1:B:411:ALA:HB1	2.00	0.44
1:C:37:PRO:HB2	1:C:46:PHE:CE1	2.52	0.44
1:D:44:LYS:O	1:D:48:ILE:HG12	2.17	0.44
1:D:368:ARG:HA	1:D:369:PRO:HD3	1.81	0.44
1:A:201:ALA:O	1:A:389:PHE:HA	2.17	0.44
1:A:212:ALA:HB2	1:A:354:LEU:HD11	2.00	0.44
1:A:337:SER:HB2	1:A:380:LEU:HD22	1.99	0.44
1:E:282:ASN:HD21	1:F:157:ILE:HD13	1.82	0.44
1:F:44:LYS:O	1:F:48:ILE:HG12	2.18	0.44
1:F:410:ILE:N	1:F:410:ILE:HD12	2.33	0.44
1:D:410:ILE:N	1:D:410:ILE:HD12	2.33	0.44
1:A:212:ALA:HB1	1:A:313:MET:CE	2.48	0.44
1:E:171:ALA:O	1:E:172:ASP:HB3	2.17	0.44
1:A:154:ASP:CB	1:F:300:GLN:HE22	2.30	0.43
1:C:280:ASN:N	1:C:280:ASN:HD22	2.16	0.43
1:D:124:VAL:HG13	1:D:134:PRO:HB3	2.00	0.43
1:E:201:ALA:O	1:E:389:PHE:HA	2.17	0.43
1:F:201:ALA:O	1:F:389:PHE:HA	2.19	0.43
1:A:30:ILE:HD12	1:A:31:LYS:H	1.83	0.43
1:A:178:VAL:O	1:A:191:GLY:HA2	2.18	0.43
1:A:406:VAL:CG2	1:A:425:PHE:HB2	2.47	0.43
1:F:161:LEU:O	1:F:161:LEU:HD23	2.18	0.43
1:A:259:ARG:CB	1:B:171:ALA:O	2.67	0.43
1:C:254:ILE:HA	1:C:258:ARG:HD2	2.00	0.43
1:F:146:GLU:C	1:F:148:SER:H	2.22	0.43
1:B:259:ARG:HB2	1:C:171:ALA:H	1.83	0.43
1:A:406:VAL:HG23	1:A:425:PHE:CB	2.44	0.43
1:B:165:TYR:O	1:B:167:GLU:N	2.52	0.43
1:E:410:ILE:HD12	1:E:410:ILE:N	2.33	0.43
1:D:254:ILE:O	1:D:258:ARG:HB2	2.19	0.43
1:F:158:ASP:HA	1:F:161:LEU:HB3	2.00	0.43
1:C:368:ARG:HA	1:C:369:PRO:HD3	1.79	0.43
1:D:311:ILE:HG13	1:D:350:VAL:HB	2.00	0.43
1:F:157:ILE:HG13	1:F:158:ASP:OD1	2.18	0.43
1:A:338:ARG:HG3	1:A:379:GLN:HG2	2.00	0.43
1:B:256:ALA:HB3	1:C:190:TYR:CE2	2.53	0.43
1:C:254:ILE:O	1:C:258:ARG:HB2	2.19	0.43
1:C:355:SER:OG	1:C:356:GLN:N	2.52	0.43
1:D:64:PHE:CD1	1:D:64:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ALA:HB1	1:B:313:MET:HE2	2.00	0.42
1:A:26:GLU:C	1:A:28:GLU:N	2.71	0.42
1:A:198:VAL:CG2	1:A:352:ILE:HG12	2.49	0.42
1:A:254:ILE:O	1:A:258:ARG:HB2	2.19	0.42
1:A:358:SER:HB2	1:A:375:ARG:HB2	2.00	0.42
1:C:172:ASP:C	1:C:174:ASN:N	2.72	0.42
1:C:316:TYR:OH	1:D:382:GLN:HB3	2.18	0.42
1:E:161:LEU:O	1:E:164:VAL:HB	2.20	0.42
1:C:262:ALA:HB1	1:C:265:ASP:OD2	2.19	0.42
1:C:337:SER:HB2	1:C:380:LEU:HD22	2.00	0.42
1:D:254:ILE:HA	1:D:258:ARG:HD2	2.00	0.42
1:B:367:LYS:HB2	1:B:391:TYR:HE1	1.85	0.42
1:D:402:SER:HB3	1:D:405:ILE:HB	2.02	0.42
1:E:119:GLN:HG3	1:E:123:ASN:HD22	1.84	0.42
1:E:367:LYS:HB2	1:E:391:TYR:HE1	1.85	0.42
1:F:119:GLN:HG3	1:F:123:ASN:HD22	1.84	0.42
1:A:208:LYS:HD2	1:A:355:SER:O	2.19	0.42
1:C:25:THR:O	1:C:27:PRO:HD3	2.19	0.42
1:D:367:LYS:HB2	1:D:391:TYR:HE1	1.84	0.42
1:A:52:MET:HG3	1:A:62:VAL:HG13	1.97	0.42
1:A:311:ILE:HD12	1:A:311:ILE:N	2.35	0.42
1:E:358:SER:HB2	1:E:375:ARG:HB2	2.01	0.42
1:B:31:LYS:HE3	1:B:56:ASP:OD1	2.20	0.42
1:C:154:ASP:CG	1:C:155:GLY:N	2.72	0.42
1:C:257:ALA:O	1:C:259:ARG:N	2.53	0.42
1:D:145:ILE:O	1:D:145:ILE:HG22	2.20	0.42
1:D:229:HIS:CD2	1:D:294:ILE:HG12	2.54	0.42
1:E:257:ALA:O	1:E:259:ARG:N	2.53	0.42
1:A:171:ALA:O	1:A:172:ASP:C	2.59	0.42
1:A:252:GLN:HG2	1:B:190:TYR:OH	2.19	0.42
1:E:173:GLY:O	1:E:174:ASN:CB	2.66	0.42
1:C:242:LEU:HB3	1:C:276:ILE:HD12	2.01	0.41
1:F:31:LYS:HE3	1:F:56:ASP:OD1	2.20	0.41
1:A:254:ILE:HA	1:A:258:ARG:HD2	2.02	0.41
1:A:292:ASN:HD22	1:B:31:LYS:HD3	1.85	0.41
1:A:381:GLU:HA	1:A:387:ILE:HD11	2.02	0.41
1:D:49:TYR:HA	1:D:52:MET:HB3	2.02	0.41
1:D:138:ALA:O	1:D:142:LEU:HB2	2.21	0.41
1:E:41:SER:O	1:E:46:PHE:HB2	2.20	0.41
1:F:26:GLU:C	1:F:28:GLU:H	2.23	0.41
1:A:212:ALA:HB1	1:A:313:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ILE:HA	1:C:412:LYS:O	2.20	0.41
1:D:406:VAL:CG2	1:D:425:PHE:HB2	2.46	0.41
1:A:269:LEU:C	1:A:271:MET:N	2.74	0.41
1:B:49:TYR:HA	1:B:52:MET:HB3	2.02	0.41
1:C:358:SER:C	1:C:360:GLN:H	2.24	0.41
1:D:115:SER:O	1:D:119:GLN:HB2	2.19	0.41
1:D:198:VAL:HG22	1:D:352:ILE:HG12	2.02	0.41
1:E:198:VAL:HG22	1:E:352:ILE:HG12	2.01	0.41
1:F:269:LEU:C	1:F:271:MET:H	2.23	0.41
1:F:368:ARG:HA	1:F:369:PRO:HD3	1.79	0.41
1:A:311:ILE:HG13	1:A:350:VAL:HB	2.02	0.41
1:C:38:GLU:H	1:C:38:GLU:HG2	1.67	0.41
1:E:167:GLU:O	1:E:170:SER:HB2	2.20	0.41
1:F:26:GLU:HB2	1:F:29:LEU:HD22	2.02	0.41
1:A:150:THR:HG21	1:F:303:ARG:NH2	2.35	0.41
1:C:138:ALA:O	1:C:142:LEU:HB2	2.20	0.41
1:D:25:THR:O	1:D:27:PRO:HD3	2.21	0.41
1:D:221:ASP:C	1:D:223:ASP:H	2.24	0.41
1:F:163:THR:O	1:F:167:GLU:OE1	2.39	0.41
1:A:262:ALA:HB1	1:A:265:ASP:OD2	2.19	0.41
1:A:358:SER:C	1:A:360:GLN:H	2.23	0.41
1:C:49:TYR:HA	1:C:52:MET:HB3	2.03	0.41
1:E:259:ARG:HB2	1:F:171:ALA:O	2.21	0.41
1:C:269:LEU:C	1:C:271:MET:H	2.22	0.41
1:E:201:ALA:O	1:E:202:ALA:HB2	2.20	0.41
1:F:262:ALA:HB1	1:F:265:ASP:OD2	2.20	0.41
1:F:381:GLU:HA	1:F:387:ILE:HD11	2.02	0.41
1:A:12:ASN:O	1:A:16:GLU:HB2	2.21	0.41
1:A:158:ASP:HA	1:A:161:LEU:HB2	2.03	0.41
1:A:178:VAL:HG21	1:A:311:ILE:HD11	2.03	0.41
1:A:201:ALA:O	1:A:202:ALA:HB2	2.20	0.41
1:B:63:ASP:O	1:B:64:PHE:C	2.58	0.41
1:B:146:GLU:C	1:B:148:SER:H	2.23	0.41
1:B:215:GLN:O	1:B:219:MET:HG3	2.20	0.41
1:B:221:ASP:C	1:B:223:ASP:H	2.24	0.41
1:B:242:LEU:HB3	1:B:276:ILE:HD12	2.03	0.41
1:B:311:ILE:N	1:B:311:ILE:HD12	2.36	0.41
1:B:410:ILE:HD12	1:B:410:ILE:N	2.36	0.41
1:E:124:VAL:HG13	1:E:134:PRO:HB3	2.02	0.41
1:E:326:ASN:HD22	1:E:326:ASN:HA	1.67	0.41
1:F:311:ILE:HD12	1:F:311:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:NZ	1:A:308:LYS:HB3	2.36	0.41
1:B:259:ARG:HD3	1:C:169:GLU:O	2.21	0.41
1:C:239:ILE:HD11	1:D:157:ILE:HD12	2.03	0.41
1:C:327:ASP:O	1:D:324:LYS:NZ	2.54	0.41
1:C:338:ARG:HG3	1:C:379:GLN:HG2	2.02	0.41
1:D:344:ALA:HB2	1:D:351:VAL:CG2	2.51	0.41
1:E:38:GLU:H	1:E:38:GLU:HG2	1.65	0.41
1:E:313:MET:HA	1:E:352:ILE:O	2.21	0.41
1:F:212:ALA:HB2	1:F:354:LEU:HD11	2.02	0.41
1:A:158:ASP:C	1:A:160:ALA:N	2.74	0.40
1:A:367:LYS:HB2	1:A:391:TYR:HE1	1.86	0.40
1:C:406:VAL:CG2	1:C:425:PHE:HB2	2.47	0.40
1:D:381:GLU:HA	1:D:387:ILE:HD11	2.03	0.40
1:F:257:ALA:HB1	1:F:261:PHE:HB3	2.02	0.40
1:F:340:LEU:HD23	1:F:340:LEU:HA	1.93	0.40
1:B:48:ILE:CD1	1:B:78:LEU:HB3	2.52	0.40
1:B:313:MET:HA	1:B:352:ILE:O	2.21	0.40
1:D:337:SER:HB2	1:D:380:LEU:HD22	2.03	0.40
1:C:273:ILE:HD13	1:D:165:TYR:CD2	2.57	0.40
1:F:49:TYR:HA	1:F:52:MET:HB3	2.02	0.40
1:C:206:MET:CE	1:C:391:TYR:HA	2.52	0.40
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.89	0.40
1:D:212:ALA:HB2	1:D:354:LEU:HD11	2.04	0.40
1:E:254:ILE:HA	1:E:258:ARG:HD2	2.03	0.40
1:F:244:VAL:O	1:F:244:VAL:HG12	2.20	0.40
1:F:299:ARG:HB3	1:F:299:ARG:NH1	2.37	0.40
1:A:30:ILE:HD12	1:A:31:LYS:N	2.36	0.40
1:B:26:GLU:O	1:B:28:GLU:N	2.50	0.40
1:B:154:ASP:CG	1:B:155:GLY:N	2.75	0.40
1:C:282:ASN:HA	1:D:157:ILE:CG2	2.52	0.40
1:F:367:LYS:HB2	1:F:391:TYR:HE1	1.86	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	415/444 (94%)	359 (86%)	41 (10%)	15 (4%)	3	29
1	B	415/444 (94%)	357 (86%)	47 (11%)	11 (3%)	5	34
1	C	415/444 (94%)	365 (88%)	38 (9%)	12 (3%)	4	33
1	D	403/444 (91%)	355 (88%)	40 (10%)	8 (2%)	7	40
1	E	415/444 (94%)	358 (86%)	43 (10%)	14 (3%)	3	30
1	F	415/444 (94%)	354 (85%)	46 (11%)	15 (4%)	3	29
All	All	2478/2664 (93%)	2148 (87%)	255 (10%)	75 (3%)	4	32

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	157	ILE
1	A	255	LYS
1	A	258	ARG
1	A	316	TYR
1	A	375	ARG
1	B	44	LYS
1	B	166	GLU
1	B	255	LYS
1	B	258	ARG
1	B	316	TYR
1	B	375	ARG
1	C	44	LYS
1	C	175	ILE
1	C	255	LYS
1	C	258	ARG
1	C	316	TYR
1	C	375	ARG
1	D	44	LYS
1	D	255	LYS
1	D	258	ARG
1	D	316	TYR
1	D	375	ARG
1	E	165	TYR
1	E	168	ILE
1	E	170	SER
1	E	255	LYS

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Mol	Chain	Res	Type
1	E	258	ARG
1	E	316	TYR
1	E	375	ARG
1	F	151	ASP
1	F	175	ILE
1	F	255	LYS
1	F	258	ARG
1	F	316	TYR
1	F	375	ARG
1	B	157	ILE
1	B	193	LYS
1	C	173	GLY
1	C	193	LYS
1	D	193	LYS
1	E	44	LYS
1	E	159	GLU
1	E	166	GLU
1	E	172	ASP
1	E	193	LYS
1	F	44	LYS
1	F	154	ASP
1	F	173	GLY
1	A	70	ARG
1	A	94	THR
1	A	172	ASP
1	A	193	LYS
1	B	158	ASP
1	F	193	LYS
1	A	27	PRO
1	F	379	GLN
1	A	147	ALA
1	A	149	GLY
1	A	254	ILE
1	B	27	PRO
1	C	170	SER
1	C	379	GLN
1	D	379	GLN
1	F	153	ASP
1	F	159	GLU
1	A	379	GLN
1	B	153	ASP
1	C	27	PRO

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Mol	Chain	Res	Type
1	E	379	GLN
1	F	254	ILE
1	C	124	VAL
1	F	157	ILE
1	D	27	PRO
1	E	27	PRO

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	361/386 (94%)	348 (96%)	13 (4%)	35	61
1	B	361/386 (94%)	343 (95%)	18 (5%)	24	53
1	C	361/386 (94%)	350 (97%)	11 (3%)	41	64
1	D	354/386 (92%)	345 (98%)	9 (2%)	47	69
1	E	361/386 (94%)	346 (96%)	15 (4%)	30	57
1	F	361/386 (94%)	347 (96%)	14 (4%)	32	59
All	All	2159/2316 (93%)	2079 (96%)	80 (4%)	34	60

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	64	PHE
1	A	71	VAL
1	A	152	ASP
1	A	157	ILE
1	A	158	ASP
1	A	174	ASN
1	A	231	LEU
1	A	254	ILE
1	A	308	LYS
1	A	316	TYR
1	A	376	GLU

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Mol	Chain	Res	Type
1	A	380	LEU
1	B	30	ILE
1	B	64	PHE
1	B	101	CYS
1	B	144	GLU
1	B	157	ILE
1	B	161	LEU
1	B	165	TYR
1	B	166	GLU
1	B	174	ASN
1	B	231	LEU
1	B	254	ILE
1	B	308	LYS
1	B	316	TYR
1	B	319	LEU
1	B	348	ASP
1	B	368	ARG
1	B	376	GLU
1	B	380	LEU
1	C	30	ILE
1	C	64	PHE
1	C	144	GLU
1	C	166	GLU
1	C	174	ASN
1	C	231	LEU
1	C	254	ILE
1	C	308	LYS
1	C	316	TYR
1	C	376	GLU
1	C	380	LEU
1	D	30	ILE
1	D	64	PHE
1	D	165	TYR
1	D	167	GLU
1	D	231	LEU
1	D	308	LYS
1	D	316	TYR
1	D	376	GLU
1	D	380	LEU
1	E	30	ILE
1	E	64	PHE
1	E	144	GLU

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Mol	Chain	Res	Type
1	E	153	ASP
1	E	159	GLU
1	E	165	TYR
1	E	167	GLU
1	E	174	ASN
1	E	231	LEU
1	E	308	LYS
1	E	316	TYR
1	E	319	LEU
1	E	368	ARG
1	E	376	GLU
1	E	380	LEU
1	F	30	ILE
1	F	64	PHE
1	F	125	ASN
1	F	150	THR
1	F	157	ILE
1	F	174	ASN
1	F	198	VAL
1	F	231	LEU
1	F	308	LYS
1	F	316	TYR
1	F	319	LEU
1	F	348	ASP
1	F	376	GLU
1	F	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	45	HIS
1	A	77	GLN
1	A	100	HIS
1	A	102	GLN
1	A	109	GLN
1	A	119	GLN
1	A	123	ASN
1	A	196	ASN
1	A	215	GLN
1	A	229	HIS
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	292	ASN
1	A	305	ASN
1	A	326	ASN
1	A	331	ASN
1	A	356	GLN
1	A	365	GLN
1	A	404	ASN
1	B	39	HIS
1	B	45	HIS
1	B	77	GLN
1	B	99	GLN
1	B	102	GLN
1	B	109	GLN
1	B	119	GLN
1	B	123	ASN
1	B	125	ASN
1	B	196	ASN
1	B	215	GLN
1	B	229	HIS
1	B	280	ASN
1	B	282	ASN
1	B	305	ASN
1	B	326	ASN
1	B	331	ASN
1	B	365	GLN
1	B	382	GLN
1	B	404	ASN
1	C	39	HIS
1	C	77	GLN
1	C	100	HIS
1	C	102	GLN
1	C	109	GLN
1	C	119	GLN
1	C	123	ASN
1	C	174	ASN
1	C	196	ASN
1	C	215	GLN
1	C	222	ASN
1	C	229	HIS
1	C	280	ASN
1	C	282	ASN

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Mol	Chain	Res	Type
1	C	305	ASN
1	C	326	ASN
1	C	331	ASN
1	C	356	GLN
1	C	365	GLN
1	C	404	ASN
1	D	39	HIS
1	D	45	HIS
1	D	77	GLN
1	D	99	GLN
1	D	102	GLN
1	D	109	GLN
1	D	119	GLN
1	D	123	ASN
1	D	196	ASN
1	D	215	GLN
1	D	222	ASN
1	D	229	HIS
1	D	280	ASN
1	D	282	ASN
1	D	305	ASN
1	D	326	ASN
1	D	331	ASN
1	D	365	GLN
1	D	379	GLN
1	D	404	ASN
1	E	39	HIS
1	E	77	GLN
1	E	100	HIS
1	E	102	GLN
1	E	109	GLN
1	E	119	GLN
1	E	123	ASN
1	E	196	ASN
1	E	215	GLN
1	E	222	ASN
1	E	229	HIS
1	E	252	GLN
1	E	280	ASN
1	E	282	ASN
1	E	305	ASN
1	E	326	ASN

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Mol	Chain	Res	Type
1	E	331	ASN
1	E	365	GLN
1	E	404	ASN
1	F	39	HIS
1	F	77	GLN
1	F	99	GLN
1	F	102	GLN
1	F	109	GLN
1	F	119	GLN
1	F	123	ASN
1	F	196	ASN
1	F	215	GLN
1	F	222	ASN
1	F	229	HIS
1	F	280	ASN
1	F	282	ASN
1	F	300	GLN
1	F	305	ASN
1	F	326	ASN
1	F	331	ASN
1	F	365	GLN
1	F	404	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	419/444 (94%)	0.58	29 (6%) 16 13	103, 118, 142, 151	0
1	B	419/444 (94%)	0.63	31 (7%) 14 12	103, 117, 142, 151	0
1	C	419/444 (94%)	1.39	118 (28%) 0 0	103, 117, 142, 150	0
1	D	409/444 (92%)	1.39	95 (23%) 0 0	103, 117, 142, 150	0
1	E	419/444 (94%)	1.39	113 (26%) 0 0	103, 117, 142, 150	0
1	F	419/444 (94%)	0.94	66 (15%) 2 2	103, 117, 142, 151	0
All	All	2504/2664 (93%)	1.05	452 (18%) 1 1	103, 117, 142, 151	0

All (452) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	263	SER	8.9
1	D	434	ASN	8.8
1	C	365	GLN	8.5
1	A	256	ALA	8.1
1	C	402	SER	8.0
1	F	365	GLN	7.4
1	D	435	LEU	7.2
1	E	79	GLY	6.7
1	C	358	SER	6.5
1	C	271	MET	6.5
1	B	399	GLU	6.5
1	F	363	GLN	6.3
1	A	255	LYS	5.8
1	D	158	ASP	5.7
1	E	32	GLU	5.7
1	E	376	GLU	5.7
1	B	152	ASP	5.6
1	D	250	ASN	5.6
1	F	159	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	260	ASP	5.6
1	D	262	ALA	5.5
1	C	400	SER	5.5
1	E	171	ALA	5.4
1	E	174	ASN	5.4
1	C	272	ALA	5.4
1	A	260	ASP	5.3
1	E	134	PRO	5.3
1	C	397	ASP	5.3
1	C	260	ASP	5.2
1	D	32	GLU	5.1
1	E	61	SER	5.1
1	E	77	GLN	5.0
1	F	252	GLN	4.9
1	E	223	ASP	4.8
1	C	279	SER	4.8
1	D	308	LYS	4.8
1	F	364	ARG	4.8
1	D	366	ASP	4.7
1	C	267	GLY	4.5
1	E	280	ASN	4.5
1	E	375	ARG	4.5
1	E	401	GLU	4.4
1	C	58	LYS	4.4
1	F	260	ASP	4.4
1	E	377	SER	4.4
1	E	78	LEU	4.4
1	F	12	ASN	4.4
1	E	119	GLN	4.4
1	D	306	PRO	4.3
1	E	72	GLY	4.3
1	F	90	SER	4.3
1	D	399	GLU	4.2
1	E	260	ASP	4.2
1	C	398	LYS	4.2
1	C	141	GLU	4.2
1	D	179	PRO	4.1
1	D	157	ILE	4.1
1	C	326	ASN	4.1
1	E	252	GLN	4.1
1	E	100	HIS	4.1
1	E	251	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	158	ASP	4.1
1	E	133	LYS	4.1
1	C	134	PRO	4.0
1	D	252	GLN	4.0
1	F	170	SER	4.0
1	C	403	LYS	4.0
1	E	141	GLU	4.0
1	D	404	ASN	3.9
1	D	113	ALA	3.9
1	C	57	ARG	3.9
1	F	358	SER	3.9
1	D	303	ARG	3.9
1	E	75	LEU	3.9
1	E	166	GLU	3.9
1	E	172	ASP	3.9
1	F	415	ASP	3.9
1	E	250	ASN	3.9
1	D	307	GLY	3.9
1	F	398	LYS	3.8
1	C	259	ARG	3.8
1	A	151	ASP	3.8
1	E	27	PRO	3.8
1	B	306	PRO	3.8
1	E	303	ARG	3.8
1	D	417	PRO	3.8
1	E	123	ASN	3.8
1	C	307	GLY	3.7
1	E	73	GLU	3.7
1	F	434	ASN	3.7
1	C	367	LYS	3.7
1	E	436	GLU	3.7
1	B	132	VAL	3.7
1	B	304	LYS	3.6
1	C	360	GLN	3.6
1	D	180	SER	3.6
1	E	62	VAL	3.6
1	D	405	ILE	3.6
1	C	32	GLU	3.6
1	C	427	LYS	3.6
1	C	391	TYR	3.6
1	D	436	GLU	3.6
1	F	154	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	179	PRO	3.5
1	C	366	ASP	3.5
1	E	326	ASN	3.5
1	D	190	TYR	3.5
1	F	91	VAL	3.5
1	F	366	ASP	3.5
1	E	33	CYS	3.5
1	E	256	ALA	3.5
1	C	323	ALA	3.5
1	D	159	GLU	3.5
1	C	406	VAL	3.4
1	F	436	GLU	3.4
1	D	61	SER	3.4
1	C	324	LYS	3.4
1	D	114	ILE	3.4
1	A	257	ALA	3.4
1	C	308	LYS	3.4
1	C	145	ILE	3.4
1	B	153	ASP	3.4
1	C	224	ASP	3.4
1	C	29	LEU	3.4
1	D	422	SER	3.4
1	C	359	ARG	3.4
1	E	157	ILE	3.3
1	E	282	ASN	3.3
1	D	258	ARG	3.3
1	C	372	SER	3.3
1	E	272	ALA	3.3
1	B	398	LYS	3.3
1	E	162	VAL	3.3
1	A	141	GLU	3.3
1	E	136	GLN	3.3
1	D	402	SER	3.3
1	D	209	THR	3.3
1	E	151	ASP	3.3
1	D	323	ALA	3.3
1	F	140	SER	3.2
1	E	302	LYS	3.2
1	A	174	ASN	3.2
1	F	263	SER	3.2
1	E	246	ALA	3.2
1	F	258	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	376	GLU	3.2
1	F	327	ASP	3.2
1	C	325	ALA	3.2
1	E	122	GLU	3.2
1	E	163	THR	3.1
1	C	348	ASP	3.1
1	F	402	SER	3.1
1	C	305	ASN	3.1
1	C	144	GLU	3.1
1	E	235	LYS	3.1
1	E	137	GLU	3.1
1	E	304	LYS	3.1
1	E	273	ILE	3.1
1	F	397	ASP	3.1
1	E	125	ASN	3.1
1	E	173	GLY	3.1
1	F	158	ASP	3.0
1	C	289	GLN	3.0
1	D	29	LEU	3.0
1	E	233	MET	3.0
1	B	225	VAL	3.0
1	C	303	ARG	3.0
1	C	399	GLU	3.0
1	D	134	PRO	3.0
1	E	14	TYR	3.0
1	D	253	LYS	3.0
1	D	305	ASN	3.0
1	E	347	LEU	3.0
1	E	310	VAL	3.0
1	F	307	GLY	3.0
1	D	247	GLY	3.0
1	A	159	GLU	3.0
1	F	78	LEU	3.0
1	F	172	ASP	3.0
1	C	53	GLN	3.0
1	A	172	ASP	3.0
1	E	227	ASN	3.0
1	D	414	ARG	3.0
1	A	263	SER	2.9
1	D	169	GLU	2.9
1	A	123	ASN	2.9
1	E	258	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	310	VAL	2.9
1	D	222	ASN	2.9
1	E	152	ASP	2.9
1	E	80	GLY	2.9
1	D	227	ASN	2.9
1	C	209	THR	2.9
1	D	140	SER	2.9
1	E	348	ASP	2.9
1	F	400	SER	2.9
1	C	136	GLN	2.9
1	C	436	GLU	2.9
1	E	169	GLU	2.9
1	D	118	GLN	2.9
1	E	281	ILE	2.9
1	B	141	GLU	2.9
1	B	327	ASP	2.8
1	C	304	LYS	2.8
1	F	253	LYS	2.8
1	B	305	ASN	2.8
1	F	359	ARG	2.8
1	A	170	SER	2.8
1	F	248	SER	2.8
1	C	193	LYS	2.8
1	B	326	ASN	2.8
1	D	368	ARG	2.8
1	D	183	THR	2.8
1	C	349	VAL	2.8
1	C	94	THR	2.8
1	D	401	GLU	2.8
1	C	368	ARG	2.8
1	E	140	SER	2.8
1	D	48	ILE	2.8
1	B	415	ASP	2.8
1	C	273	ILE	2.7
1	D	109	GLN	2.7
1	E	74	LYS	2.7
1	F	401	GLU	2.7
1	D	176	THR	2.7
1	C	435	LEU	2.7
1	E	245	THR	2.7
1	E	247	GLY	2.7
1	B	151	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	406	VAL	2.7
1	C	158	ASP	2.7
1	C	292	ASN	2.7
1	F	264	GLU	2.7
1	D	365	GLN	2.7
1	D	27	PRO	2.7
1	D	60	GLN	2.7
1	E	301	THR	2.7
1	F	324	LYS	2.7
1	E	170	SER	2.7
1	C	306	PRO	2.7
1	C	205	SER	2.7
1	D	322	PRO	2.6
1	F	399	GLU	2.6
1	A	62	VAL	2.6
1	E	30	ILE	2.6
1	D	62	VAL	2.6
1	C	208	LYS	2.6
1	A	307	GLY	2.6
1	D	299	ARG	2.6
1	E	58	LYS	2.6
1	C	122	GLU	2.6
1	C	278	ASN	2.6
1	C	269	LEU	2.6
1	C	394	ASP	2.6
1	C	261	PHE	2.6
1	B	223	ASP	2.6
1	C	364	ARG	2.6
1	D	255	LYS	2.6
1	C	250	ASN	2.6
1	C	27	PRO	2.6
1	D	26	GLU	2.6
1	A	365	GLN	2.6
1	D	392	ARG	2.6
1	F	92	ALA	2.6
1	C	315	ASP	2.5
1	A	304	LYS	2.5
1	F	94	THR	2.5
1	C	223	ASP	2.5
1	E	434	ASN	2.5
1	B	376	GLU	2.5
1	E	156	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	12	ASN	2.5
1	F	45	HIS	2.5
1	C	270	SER	2.5
1	F	136	GLN	2.5
1	E	184	GLU	2.5
1	D	304	LYS	2.5
1	F	435	LEU	2.5
1	E	194	ARG	2.5
1	A	348	ASP	2.5
1	E	399	GLU	2.5
1	F	169	GLU	2.5
1	D	144	GLU	2.5
1	C	34	PRO	2.5
1	F	422	SER	2.5
1	E	431	ASN	2.5
1	E	31	LYS	2.5
1	B	144	GLU	2.5
1	C	77	GLN	2.5
1	C	251	ALA	2.5
1	D	175	ILE	2.5
1	E	175	ILE	2.5
1	C	238	ASN	2.5
1	C	135	ILE	2.5
1	C	282	ASN	2.4
1	D	264	GLU	2.4
1	F	433	VAL	2.4
1	C	56	ASP	2.4
1	C	275	GLU	2.4
1	F	183	THR	2.4
1	D	256	ALA	2.4
1	B	375	ARG	2.4
1	C	309	ARG	2.4
1	E	255	LYS	2.4
1	E	269	LEU	2.4
1	C	79	GLY	2.4
1	C	285	ASP	2.4
1	D	132	VAL	2.4
1	E	257	ALA	2.4
1	B	90	SER	2.4
1	D	72	GLY	2.4
1	E	428	GLU	2.4
1	E	76	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	2.4
1	D	193	LYS	2.4
1	C	190	TYR	2.4
1	C	276	ILE	2.4
1	E	222	ASN	2.4
1	F	393	ASP	2.4
1	A	326	ASN	2.4
1	C	265	ASP	2.4
1	B	121	ILE	2.3
1	C	420	THR	2.4
1	D	364	ARG	2.3
1	E	404	ASN	2.3
1	E	419	GLY	2.3
1	C	300	GLN	2.3
1	D	398	LYS	2.3
1	A	254	ILE	2.3
1	E	15	ALA	2.3
1	B	266	TRP	2.3
1	C	291	VAL	2.3
1	E	241	ARG	2.3
1	F	20	LEU	2.3
1	D	375	ARG	2.3
1	C	301	THR	2.3
1	E	116	ILE	2.3
1	E	135	ILE	2.3
1	F	29	LEU	2.3
1	C	255	LYS	2.3
1	A	303	ARG	2.3
1	C	405	ILE	2.3
1	D	403	LYS	2.3
1	B	377	SER	2.3
1	F	377	SER	2.3
1	E	279	SER	2.3
1	F	150	THR	2.3
1	C	125	ASN	2.3
1	F	262	ALA	2.3
1	F	62	VAL	2.3
1	D	22	SER	2.2
1	C	422	SER	2.2
1	F	171	ALA	2.2
1	C	12	ASN	2.2
1	B	101	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	281	ILE	2.2
1	C	246	ALA	2.2
1	D	290	SER	2.2
1	F	261	PHE	2.2
1	B	363	GLN	2.2
1	D	96	THR	2.2
1	E	60	GLN	2.2
1	E	168	ILE	2.2
1	E	110	LYS	2.2
1	C	184	GLU	2.2
1	B	365	GLN	2.2
1	E	224	ASP	2.2
1	C	429	TYR	2.2
1	D	133	LYS	2.2
1	D	106	GLU	2.2
1	E	234	GLY	2.2
1	E	379	GLN	2.2
1	D	415	ASP	2.2
1	E	167	GLU	2.2
1	F	153	ASP	2.2
1	A	358	SER	2.2
1	C	254	ILE	2.2
1	E	244	VAL	2.2
1	F	165	TYR	2.2
1	E	63	ASP	2.2
1	D	400	SER	2.2
1	D	413	HIS	2.2
1	C	167	GLU	2.2
1	C	414	ARG	2.2
1	E	261	PHE	2.2
1	D	51	THR	2.2
1	E	190	TYR	2.2
1	C	392	ARG	2.2
1	A	265	ASP	2.1
1	F	161	LEU	2.1
1	C	28	GLU	2.1
1	F	117	ALA	2.1
1	B	434	ASN	2.1
1	C	152	ASP	2.1
1	C	196	ASN	2.1
1	C	227	ASN	2.1
1	F	141	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	GLU	2.1
1	B	224	ASP	2.1
1	C	385	ASP	2.1
1	A	136	GLN	2.1
1	C	295	TRP	2.1
1	C	415	ASP	2.1
1	D	327	ASP	2.1
1	E	92	ALA	2.1
1	D	232	GLU	2.1
1	B	118	GLN	2.1
1	C	342	LYS	2.1
1	E	324	LYS	2.1
1	F	270	SER	2.1
1	D	331	ASN	2.1
1	D	145	ILE	2.1
1	D	160	ALA	2.1
1	F	357	LEU	2.1
1	C	247	GLY	2.1
1	E	265	ASP	2.1
1	D	266	TRP	2.1
1	C	62	VAL	2.1
1	C	345	ARG	2.1
1	E	274	GLY	2.1
1	D	230	SER	2.1
1	B	260	ASP	2.1
1	D	357	LEU	2.1
1	C	219	MET	2.1
1	C	268	LYS	2.1
1	E	331	ASN	2.1
1	A	399	GLU	2.1
1	C	78	LEU	2.1
1	D	18	ALA	2.1
1	A	12	ASN	2.1
1	D	300	GLN	2.1
1	E	262	ALA	2.0
1	E	66	SER	2.0
1	A	264	GLU	2.0
1	B	255	LYS	2.0
1	D	367	LYS	2.0
1	D	425	PHE	2.0
1	F	144	GLU	2.0
1	C	424	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	22	SER	2.0
1	D	225	VAL	2.0
1	D	217	LYS	2.0
1	F	326	ASN	2.0
1	F	396	TYR	2.0
1	B	72	GLY	2.0
1	C	51	THR	2.0
1	F	403	LYS	2.0
1	C	327	ASP	2.0
1	A	153	ASP	2.0
1	F	110	LYS	2.0
1	F	367	LYS	2.0
1	D	309	ARG	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.