Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:02 AM EDT

PDB ID	:	2R6D
Title	:	Crystal Form B1
Authors	:	Bailey, S.; Eliason, W.K.; Steitz, T.A.
Deposited on	:	2007-09-05
Resolution	:	3.70 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:

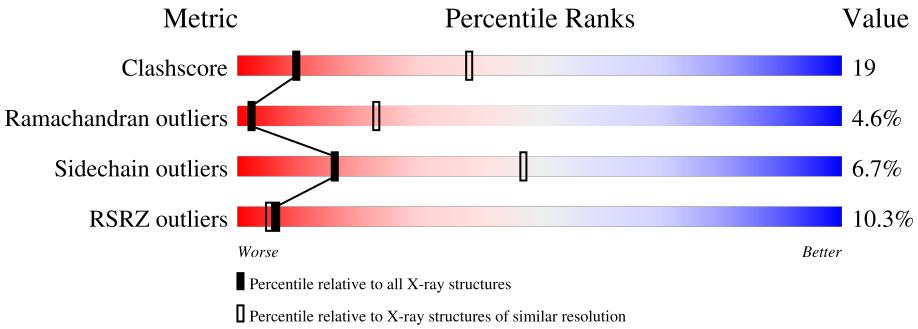
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	454	6% 57% 27% 5% • 11%
1	B	454	5% 55% 24% • 17%
1	C	454	8% 58% 25% 5% • 12%
1	D	454	8% 55% 23% • • 17%
1	E	454	17% 60% 22% 5% 14%
1	F	454	9% 60% 22% • • 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18085 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 Replicative helicase.

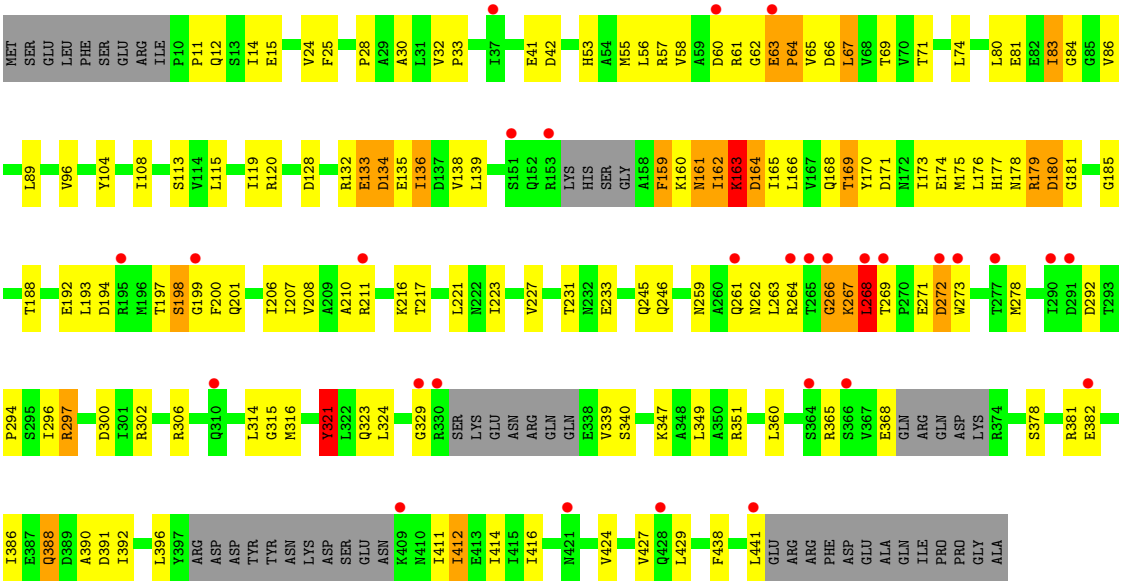
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3138	1969	544	611	14			
1	B	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	C	399	Total	C	N	O	S	0	0	0
			3089	1938	534	603	14			
1	D	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	E	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			
1	F	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			

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.

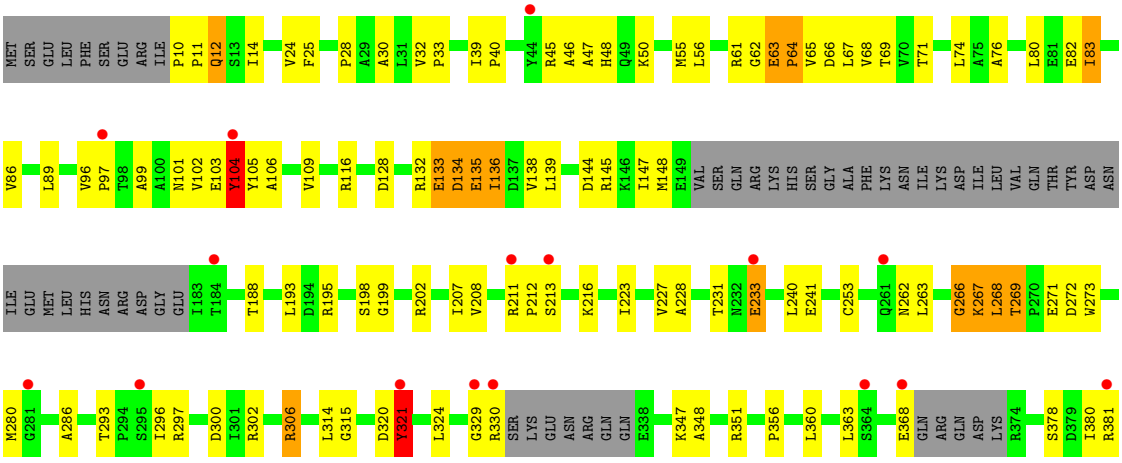
• Molecule 1: Replicative helicase

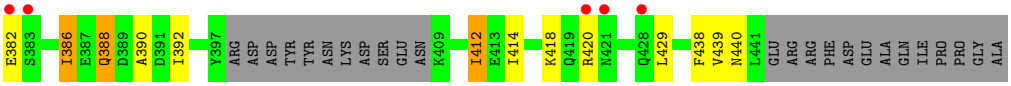
Chain A:



• Molecule 1: Replicative helicase

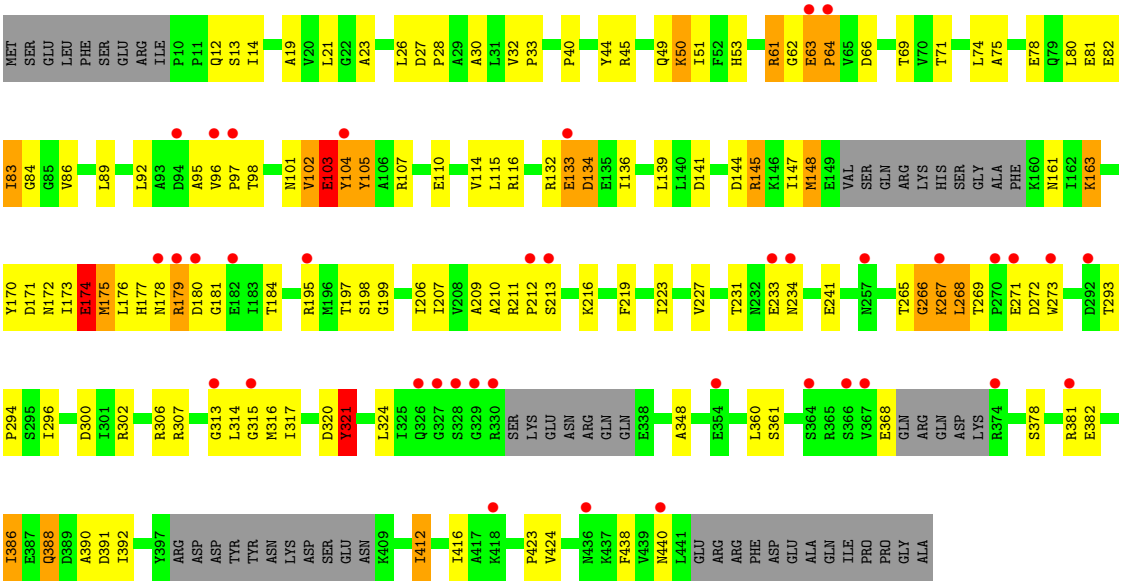
Chain B:





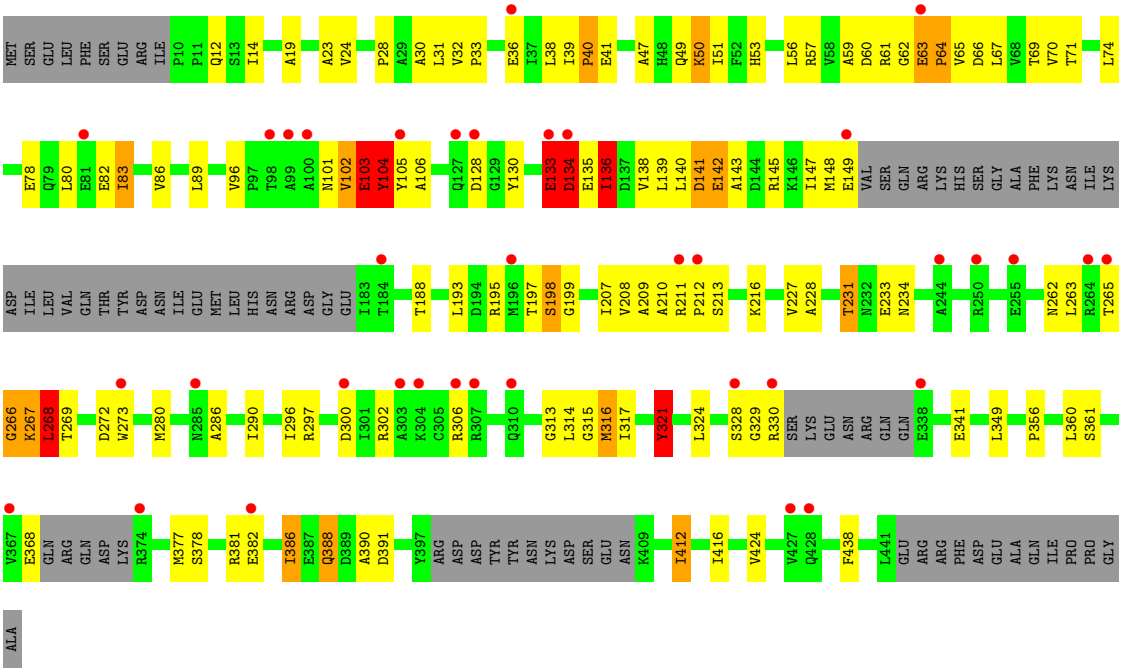
• Molecule 1: Replicative helicase

Chain C:



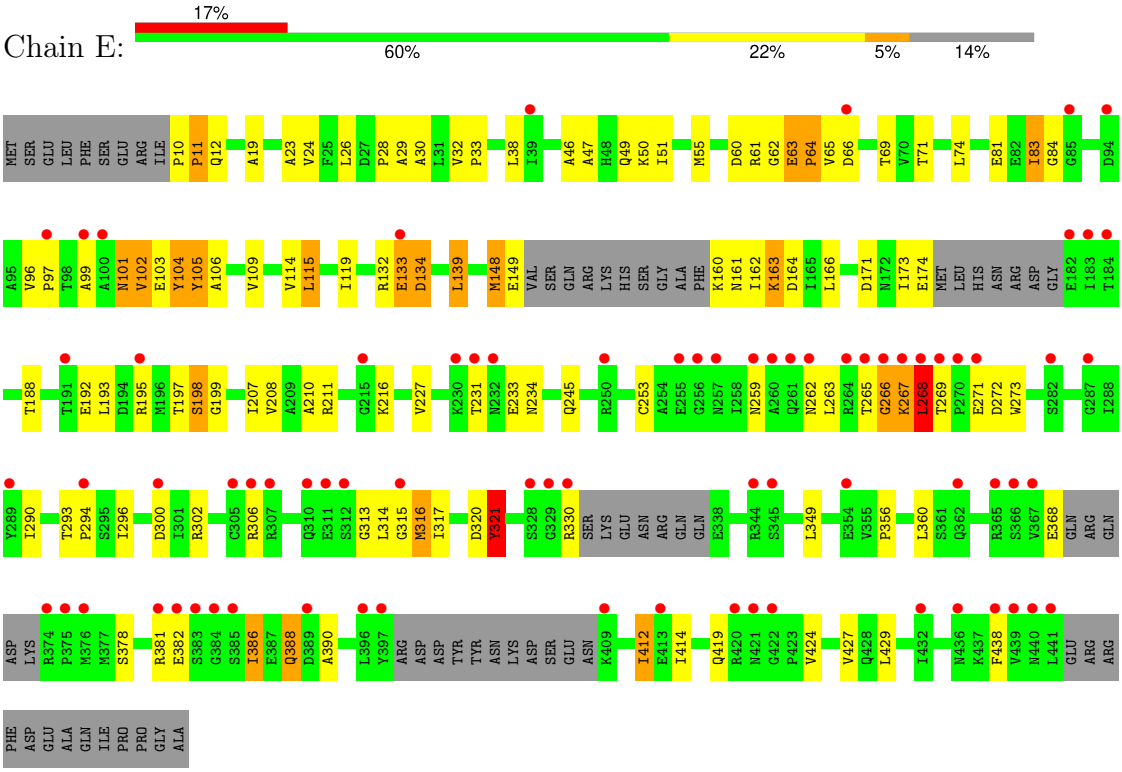
• Molecule 1: Replicative helicase

Chain D:



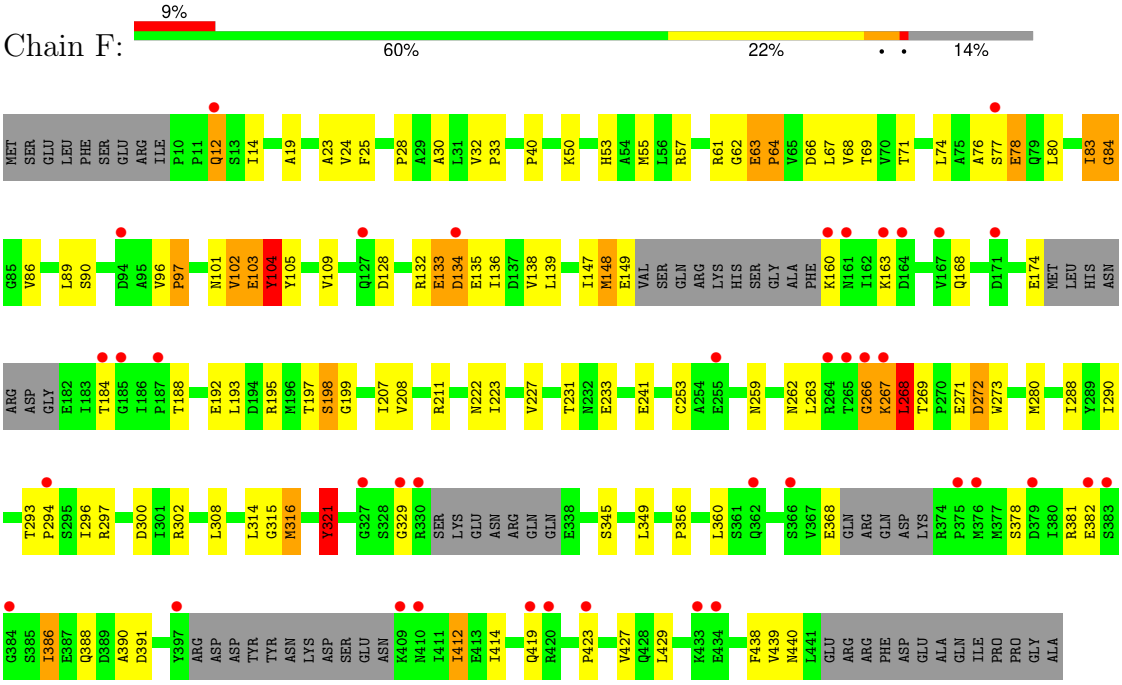
• Molecule 1: Replicative helicase

Chain E:



• Molecule 1: Replicative helicase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	371.26Å 110.30Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 19.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.70) 98.1 (19.99-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.309 , 0.322 0.288 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	145.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 189.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.077 for -h,l,k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18085	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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	0.45	0/3173	0.68	1/4285 (0.0%)
1	B	0.46	0/2929	0.72	1/3957 (0.0%)
1	C	0.47	1/3123 (0.0%)	0.70	4/4218 (0.1%)
1	D	0.41	0/2929	0.69	3/3957 (0.1%)
1	E	0.38	0/3064	0.64	0/4138
1	F	0.41	0/3064	0.69	2/4138 (0.0%)
All	All	0.43	1/18282 (0.0%)	0.69	11/24693 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	2
1	D	1	1
1	E	1	0
1	F	1	1
All	All	5	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	GLU	CD-OE2	6.40	1.32	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	GLY	N-CA-C	-6.08	97.91	113.10
1	C	174	GLU	O-C-N	5.89	132.12	122.70
1	A	321	TYR	N-CA-C	5.85	126.79	111.00
1	B	321	TYR	N-CA-C	5.79	126.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	321	TYR	N-CA-C	5.68	126.34	111.00
1	F	321	TYR	N-CA-C	5.50	125.85	111.00
1	C	103	GLU	N-CA-C	5.34	125.42	111.00
1	D	321	TYR	N-CA-C	5.19	125.00	111.00
1	F	84	GLY	N-CA-C	-5.13	100.26	113.10
1	D	103	GLU	C-N-CA	5.04	134.30	121.70
1	D	133	GLU	C-N-CA	5.02	134.25	121.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	104	TYR	CA
1	C	104	TYR	CA
1	D	104	TYR	CA
1	E	104	TYR	CA
1	F	104	TYR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	103	GLU	Peptide
1	C	174	GLU	Mainchain
1	D	104	TYR	Peptide
1	F	104	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3190	134	0
1	B	2897	0	2953	131	0
1	C	3089	0	3141	148	2
1	D	2897	0	2953	154	0
1	E	3032	0	3087	115	0
1	F	3032	0	3087	108	2
All	All	18085	0	18411	705	2

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 19.

All (705) 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:A:133:GLU:N	1:A:134:ASP:HB2	1.33	1.43
1:E:133:GLU:N	1:E:134:ASP:HB2	1.36	1.40
1:F:133:GLU:N	1:F:134:ASP:HB2	1.39	1.38
1:C:133:GLU:N	1:C:134:ASP:HB2	1.32	1.35
1:E:330:ARG:NH1	1:F:148:MET:O	1.63	1.32
1:C:133:GLU:H	1:C:134:ASP:CB	1.43	1.30
1:B:133:GLU:N	1:B:134:ASP:HB2	1.42	1.30
1:A:133:GLU:H	1:A:134:ASP:CB	1.45	1.27
1:D:133:GLU:N	1:D:134:ASP:HB2	1.47	1.26
1:E:133:GLU:H	1:E:134:ASP:CB	1.48	1.23
1:C:174:GLU:O	1:C:177:HIS:N	1.73	1.22
1:D:133:GLU:H	1:D:134:ASP:CB	1.51	1.22
1:C:294:PRO:HB2	1:D:381:ARG:NE	1.58	1.18
1:F:133:GLU:H	1:F:134:ASP:CB	1.57	1.17
1:B:133:GLU:H	1:B:134:ASP:CB	1.62	1.13
1:D:62:GLY:HA2	1:D:63:GLU:HB3	1.31	1.11
1:F:63:GLU:H	1:F:64:PRO:HA	1.14	1.10
1:D:63:GLU:H	1:D:64:PRO:HA	1.12	1.07
1:C:104:TYR:HB3	1:C:105:TYR:HB2	1.34	1.06
1:D:135:GLU:HG2	1:D:330:ARG:HH21	1.16	1.05
1:B:133:GLU:H	1:B:134:ASP:HB2	0.91	1.03
1:B:268:LEU:HB2	1:C:177:HIS:HE1	1.19	1.03
1:D:133:GLU:H	1:D:134:ASP:HB2	0.87	1.02
1:E:104:TYR:HA	1:E:105:TYR:HB2	1.38	1.01
1:E:61:ARG:HB2	1:E:62:GLY:HA3	1.39	1.01
1:A:294:PRO:HG3	1:B:348:ALA:HA	1.40	0.99
1:D:135:GLU:HG2	1:D:330:ARG:NH2	1.78	0.99
1:E:330:ARG:CZ	1:F:148:MET:O	2.10	0.99
1:F:61:ARG:HB2	1:F:62:GLY:HA3	1.44	0.98
1:E:19:ALA:HA	1:E:96:VAL:HG21	1.44	0.97
1:C:61:ARG:HB2	1:C:62:GLY:HA3	1.44	0.96
1:A:306:ARG:NH2	1:B:103:GLU:OE2	1.99	0.96
1:B:104:TYR:HB3	1:B:105:TYR:HB2	1.44	0.96
1:E:63:GLU:H	1:E:64:PRO:HA	1.27	0.96
1:F:207:ILE:HD12	1:F:390:ALA:HB2	1.48	0.94
1:D:61:ARG:HB2	1:D:62:GLY:HA3	1.50	0.94
1:A:61:ARG:CB	1:A:62:GLY:HA3	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ILE:HD12	1:E:390:ALA:HB2	1.50	0.92
1:C:294:PRO:HB2	1:D:381:ARG:CD	1.98	0.92
1:D:145:ARG:NH1	1:D:328:SER:H	1.66	0.92
1:D:145:ARG:HD3	1:D:328:SER:OG	1.70	0.91
1:C:171:ASP:O	1:C:175:MET:HG3	1.70	0.91
1:D:145:ARG:HG3	1:D:341:GLU:OE1	1.70	0.91
1:D:145:ARG:HH11	1:D:328:SER:H	0.93	0.91
1:C:61:ARG:CB	1:C:62:GLY:HA3	2.00	0.90
1:E:104:TYR:CA	1:E:105:TYR:HB2	2.03	0.89
1:A:207:ILE:HD12	1:A:390:ALA:HB2	1.51	0.88
1:B:268:LEU:HB2	1:C:177:HIS:CE1	2.09	0.87
1:C:174:GLU:CG	1:C:175:MET:N	2.35	0.87
1:E:330:ARG:HG3	1:F:149:GLU:HG2	1.53	0.87
1:D:104:TYR:HB3	1:D:105:TYR:HB2	1.57	0.86
1:E:265:THR:HG23	1:F:423:PRO:HB3	1.57	0.85
1:F:101:ASN:O	1:F:103:GLU:N	2.07	0.85
1:D:145:ARG:HH11	1:D:328:SER:N	1.73	0.85
1:F:61:ARG:CB	1:F:62:GLY:HA3	2.04	0.84
1:B:63:GLU:H	1:B:64:PRO:HA	1.42	0.84
1:F:32:VAL:HB	1:F:33:PRO:HD3	1.58	0.83
1:F:104:TYR:HB3	1:F:105:TYR:HB2	1.60	0.83
1:D:32:VAL:HB	1:D:33:PRO:HD3	1.60	0.83
1:E:61:ARG:CB	1:E:62:GLY:HA3	2.08	0.83
1:A:227:VAL:O	1:A:231:THR:HG22	1.79	0.83
1:C:294:PRO:HG2	1:D:381:ARG:CZ	2.09	0.83
1:C:174:GLU:OE2	1:C:178:ASN:HB3	1.79	0.83
1:E:104:TYR:HB3	1:E:105:TYR:HB2	1.61	0.82
1:F:67:LEU:O	1:F:71:THR:HG23	1.79	0.82
1:D:265:THR:HG23	1:E:424:VAL:H	1.44	0.81
1:C:207:ILE:HD13	1:C:386:ILE:HG22	1.62	0.81
1:D:135:GLU:CG	1:D:330:ARG:HH21	1.92	0.81
1:D:142:GLU:N	1:D:328:SER:HB2	1.95	0.81
1:F:302:ARG:HG2	1:F:349:LEU:HD13	1.63	0.81
1:A:198:SER:N	1:A:199:GLY:HA2	1.96	0.80
1:D:63:GLU:N	1:D:64:PRO:HA	1.96	0.80
1:A:246:GLN:NE2	1:B:420:ARG:HB3	1.97	0.80
1:D:19:ALA:HA	1:D:96:VAL:HG21	1.62	0.80
1:A:294:PRO:HG3	1:B:348:ALA:CA	2.11	0.79
1:D:62:GLY:HA2	1:D:63:GLU:CB	1.99	0.79
1:D:145:ARG:NH1	1:D:328:SER:N	2.30	0.79
1:F:198:SER:N	1:F:199:GLY:HA2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ASN:HA	1:C:175:MET:HB2	1.64	0.79
1:F:63:GLU:N	1:F:64:PRO:HA	1.96	0.79
1:C:175:MET:O	1:C:179:ARG:HD2	1.83	0.79
1:D:101:ASN:O	1:D:103:GLU:N	2.15	0.79
1:E:198:SER:N	1:E:199:GLY:HA2	1.98	0.78
1:C:198:SER:N	1:C:199:GLY:HA2	1.98	0.78
1:A:188:THR:HG21	1:A:193:LEU:HD23	1.65	0.78
1:E:32:VAL:HB	1:E:33:PRO:HD3	1.65	0.78
1:E:104:TYR:CB	1:E:105:TYR:HB2	2.13	0.78
1:B:347:LYS:HE3	1:B:351:ARG:CZ	2.14	0.78
1:E:207:ILE:HD13	1:E:386:ILE:HG22	1.67	0.77
1:C:104:TYR:CB	1:C:105:TYR:HB2	2.13	0.76
1:B:61:ARG:HB2	1:B:62:GLY:HA3	1.67	0.76
1:B:268:LEU:HD12	1:C:177:HIS:CE1	2.20	0.76
1:B:267:LYS:O	1:C:177:HIS:CE1	2.40	0.75
1:A:161:ASN:HD21	1:A:163:LYS:HG2	1.52	0.75
1:D:63:GLU:H	1:D:64:PRO:CA	1.98	0.75
1:C:306:ARG:HD3	1:D:32:VAL:HG13	1.69	0.75
1:D:62:GLY:CA	1:D:63:GLU:HB3	2.15	0.75
1:A:61:ARG:HB3	1:A:62:GLY:HA3	1.67	0.75
1:C:294:PRO:CB	1:D:381:ARG:NE	2.46	0.74
1:A:161:ASN:ND2	1:A:163:LYS:HG2	2.02	0.74
1:B:207:ILE:HD12	1:B:390:ALA:HB2	1.68	0.74
1:A:63:GLU:H	1:A:64:PRO:HA	1.52	0.74
1:C:241:GLU:HG3	1:D:378:SER:HB3	1.68	0.74
1:B:198:SER:N	1:B:199:GLY:HA2	2.01	0.74
1:E:66:ASP:H	1:E:69:THR:HG22	1.52	0.74
1:A:381:ARG:HH22	1:A:388:GLN:HE22	1.36	0.74
1:B:61:ARG:CB	1:B:62:GLY:HA3	2.18	0.73
1:F:207:ILE:HD13	1:F:386:ILE:HG22	1.70	0.73
1:B:67:LEU:O	1:B:71:THR:HG23	1.88	0.73
1:D:198:SER:N	1:D:199:GLY:HA2	2.03	0.72
1:D:273:TRP:CH2	1:E:173:ILE:HG22	2.24	0.72
1:C:63:GLU:H	1:C:64:PRO:HA	1.55	0.72
1:F:297:ARG:NH2	1:F:329:GLY:O	2.20	0.72
1:C:207:ILE:HD12	1:C:390:ALA:HB2	1.71	0.71
1:D:145:ARG:CG	1:D:341:GLU:OE1	2.39	0.71
1:A:245:GLN:HE22	1:B:202:ARG:HH12	1.39	0.70
1:F:269:THR:HB	1:F:272:ASP:HB2	1.72	0.70
1:C:28:PRO:C	1:C:30:ALA:H	1.95	0.70
1:C:175:MET:O	1:C:179:ARG:CD	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:MET:HE3	1:C:148:MET:HA	1.73	0.70
1:D:66:ASP:H	1:D:69:THR:HG22	1.55	0.69
1:D:40:PRO:O	1:D:49:GLN:HG2	1.92	0.69
1:C:40:PRO:O	1:C:49:GLN:HG3	1.92	0.69
1:D:32:VAL:HG12	1:D:36:GLU:OE1	1.93	0.69
1:F:64:PRO:O	1:F:69:THR:HG21	1.92	0.69
1:A:159:PHE:HD1	1:A:160:LYS:H	1.40	0.69
1:D:136:ILE:HD12	1:E:115:LEU:HG	1.74	0.69
1:E:63:GLU:N	1:E:64:PRO:HA	2.06	0.69
1:C:241:GLU:O	1:D:377:MET:HB2	1.93	0.68
1:B:207:ILE:HD13	1:B:386:ILE:HG22	1.74	0.68
1:D:66:ASP:H	1:D:69:THR:CG2	2.07	0.68
1:D:61:ARG:CB	1:D:62:GLY:HA3	2.15	0.68
1:C:294:PRO:HG2	1:D:381:ARG:NH2	2.09	0.68
1:A:61:ARG:HB2	1:A:62:GLY:HA3	1.72	0.68
1:C:148:MET:HA	1:C:148:MET:CE	2.22	0.68
1:A:269:THR:HB	1:A:272:ASP:HB2	1.76	0.67
1:D:67:LEU:O	1:D:71:THR:HG23	1.94	0.67
1:E:330:ARG:NH2	1:F:149:GLU:HA	2.09	0.67
1:A:197:THR:O	1:A:198:SER:HB2	1.94	0.67
1:C:306:ARG:HD3	1:D:32:VAL:CG1	2.25	0.67
1:D:290:ILE:O	1:E:160:LYS:HB3	1.94	0.67
1:C:19:ALA:HA	1:C:96:VAL:HG21	1.74	0.67
1:C:307:ARG:NH2	1:D:36:GLU:OE2	2.27	0.67
1:C:175:MET:HB3	1:C:423:PRO:HB3	1.77	0.67
1:D:227:VAL:O	1:D:231:THR:HG22	1.95	0.66
1:C:320:ASP:HA	1:C:360:LEU:HD12	1.76	0.66
1:C:227:VAL:O	1:C:231:THR:HG22	1.95	0.66
1:A:294:PRO:HA	1:B:351:ARG:NH1	2.10	0.66
1:A:65:VAL:HA	1:A:69:THR:HG21	1.78	0.66
1:D:302:ARG:HG2	1:D:349:LEU:HD13	1.78	0.66
1:F:412:ILE:HG21	1:F:438:PHE:HE2	1.62	0.65
1:B:211:ARG:HH11	1:B:368:GLU:HG3	1.60	0.65
1:C:174:GLU:HG3	1:C:175:MET:H	1.62	0.65
1:C:63:GLU:N	1:C:64:PRO:HA	2.11	0.65
1:A:133:GLU:CA	1:A:134:ASP:HB2	2.23	0.65
1:B:253:CYS:SG	1:B:263:LEU:HD12	2.37	0.65
1:C:174:GLU:HG3	1:C:175:MET:N	2.11	0.65
1:C:211:ARG:HH11	1:C:368:GLU:HG3	1.62	0.65
1:E:188:THR:HG21	1:E:193:LEU:HD23	1.77	0.65
1:F:23:ALA:HB1	1:F:102:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:O	1:C:133:GLU:HG3	1.96	0.64
1:E:330:ARG:HG3	1:F:149:GLU:CG	2.24	0.64
1:A:211:ARG:HH11	1:A:368:GLU:HG3	1.62	0.64
1:C:294:PRO:CG	1:D:381:ARG:CZ	2.75	0.64
1:D:269:THR:HB	1:D:272:ASP:HB2	1.79	0.64
1:B:227:VAL:O	1:B:231:THR:HG22	1.98	0.64
1:E:23:ALA:HB1	1:E:102:VAL:HG22	1.80	0.64
1:A:66:ASP:H	1:A:69:THR:HG22	1.63	0.64
1:F:211:ARG:HH11	1:F:368:GLU:HG3	1.63	0.64
1:B:104:TYR:CB	1:B:105:TYR:HB2	2.22	0.64
1:A:173:ILE:HD12	1:F:263:LEU:HD22	1.80	0.64
1:C:12:GLN:HE21	1:C:14:ILE:HG12	1.63	0.64
1:F:227:VAL:O	1:F:231:THR:HG22	1.98	0.64
1:F:63:GLU:H	1:F:64:PRO:CA	2.02	0.63
1:E:104:TYR:HA	1:E:105:TYR:CB	2.19	0.63
1:A:266:GLY:HA2	1:A:267:LYS:O	1.98	0.63
1:D:207:ILE:HD12	1:D:390:ALA:HB2	1.80	0.63
1:E:63:GLU:H	1:E:64:PRO:CA	2.05	0.63
1:C:381:ARG:HH22	1:C:388:GLN:HE22	1.47	0.63
1:D:41:GLU:HA	1:D:49:GLN:HE21	1.64	0.63
1:B:74:LEU:HD13	1:B:83:ILE:CD1	2.28	0.63
1:A:174:GLU:OE1	1:A:178:ASN:HB2	1.97	0.62
1:E:62:GLY:HA2	1:E:63:GLU:HB3	1.79	0.62
1:E:101:ASN:O	1:E:103:GLU:N	2.33	0.62
1:A:171:ASP:O	1:A:174:GLU:HG3	1.99	0.62
1:C:307:ARG:HE	1:D:36:GLU:CD	2.02	0.62
1:E:65:VAL:HA	1:E:69:THR:HG21	1.81	0.62
1:C:207:ILE:HD13	1:C:386:ILE:CG2	2.28	0.62
1:E:381:ARG:HH22	1:E:388:GLN:HE22	1.46	0.62
1:A:71:THR:HG22	1:A:89:LEU:HD13	1.82	0.62
1:E:227:VAL:O	1:E:231:THR:HG22	2.00	0.62
1:C:147:ILE:HG22	1:C:147:ILE:O	1.98	0.62
1:D:133:GLU:CA	1:D:134:ASP:HB2	2.30	0.62
1:D:188:THR:HG21	1:D:193:LEU:HD23	1.81	0.61
1:A:133:GLU:H	1:A:134:ASP:HB2	0.55	0.61
1:C:23:ALA:HB1	1:C:102:VAL:HG22	1.83	0.61
1:E:19:ALA:O	1:E:23:ALA:HB2	2.00	0.61
1:E:47:ALA:HB1	1:E:83:ILE:HG23	1.82	0.61
1:F:62:GLY:HA2	1:F:63:GLU:HB3	1.82	0.61
1:C:147:ILE:O	1:C:147:ILE:CG2	2.48	0.61
1:D:296:ILE:CG2	1:D:300:ASP:HB2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:CG2	1:A:300:ASP:HB2	2.30	0.61
1:F:267:LYS:O	1:F:268:LEU:HB2	2.01	0.60
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.82	0.60
1:B:39:ILE:HB	1:B:40:PRO:HD2	1.84	0.60
1:C:296:ILE:HG22	1:C:300:ASP:HB2	1.83	0.60
1:A:198:SER:H	1:A:199:GLY:HA2	1.66	0.60
1:A:296:ILE:HG22	1:A:300:ASP:HB2	1.83	0.60
1:A:162:ILE:O	1:A:164:ASP:N	2.35	0.60
1:C:174:GLU:C	1:C:176:LEU:N	2.54	0.60
1:D:141:ASP:C	1:D:143:ALA:H	2.04	0.60
1:D:266:GLY:HA2	1:D:267:LYS:O	2.02	0.60
1:A:67:LEU:O	1:A:71:THR:HG23	2.02	0.60
1:C:133:GLU:CA	1:C:134:ASP:HB2	2.27	0.60
1:C:171:ASP:O	1:C:175:MET:CG	2.48	0.60
1:B:63:GLU:N	1:B:64:PRO:HA	2.14	0.59
1:C:412:ILE:HG21	1:C:438:PHE:HE2	1.66	0.59
1:C:412:ILE:HG21	1:C:438:PHE:CE2	2.37	0.59
1:A:246:GLN:HE22	1:B:420:ARG:HB3	1.65	0.59
1:F:62:GLY:CA	1:F:63:GLU:HB3	2.32	0.59
1:C:294:PRO:CB	1:D:381:ARG:CD	2.78	0.59
1:D:135:GLU:HG2	1:D:330:ARG:CZ	2.32	0.59
1:D:296:ILE:HG22	1:D:300:ASP:HB2	1.82	0.59
1:F:188:THR:HG21	1:F:193:LEU:HD23	1.83	0.59
1:B:50:LYS:NZ	1:B:82:GLU:OE2	2.36	0.59
1:C:103:GLU:N	1:C:104:TYR:HB2	2.17	0.59
1:D:135:GLU:CG	1:D:330:ARG:NH2	2.55	0.59
1:D:62:GLY:CA	1:D:63:GLU:CB	2.76	0.59
1:E:101:ASN:C	1:E:103:GLU:H	2.06	0.58
1:F:296:ILE:CG2	1:F:300:ASP:HB2	2.33	0.58
1:A:61:ARG:CB	1:A:62:GLY:CA	2.79	0.58
1:B:25:PHE:HZ	1:B:89:LEU:HD22	1.68	0.58
1:B:381:ARG:HH22	1:B:388:GLN:HE22	1.51	0.58
1:D:207:ILE:HD13	1:D:386:ILE:HG22	1.83	0.58
1:F:412:ILE:HG21	1:F:438:PHE:CE2	2.38	0.58
1:B:66:ASP:H	1:B:69:THR:HG22	1.69	0.58
1:C:75:ALA:HB2	1:C:80:LEU:HD12	1.85	0.58
1:F:296:ILE:HG22	1:F:300:ASP:HB2	1.84	0.58
1:A:297:ARG:NH2	1:A:329:GLY:O	2.36	0.58
1:A:104:TYR:CG	1:B:63:GLU:O	2.57	0.58
1:A:412:ILE:HG21	1:A:438:PHE:HE2	1.69	0.58
1:F:233:GLU:CG	1:F:315:GLY:HA3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:TYR:H	1:E:360:LEU:HB2	1.69	0.58
1:B:133:GLU:CA	1:B:134:ASP:HB2	2.32	0.57
1:B:24:VAL:O	1:B:28:PRO:HB3	2.04	0.57
1:E:266:GLY:HA2	1:E:267:LYS:O	2.04	0.57
1:E:412:ILE:HG21	1:E:438:PHE:HE2	1.70	0.57
1:A:30:ALA:O	1:A:33:PRO:HD2	2.03	0.57
1:C:307:ARG:NE	1:D:36:GLU:CD	2.58	0.57
1:A:378:SER:O	1:A:382:GLU:HG2	2.04	0.57
1:B:314:LEU:HD23	1:B:315:GLY:N	2.20	0.57
1:C:296:ILE:CG2	1:C:300:ASP:HB2	2.34	0.57
1:C:174:GLU:CD	1:C:178:ASN:CB	2.73	0.56
1:D:104:TYR:CB	1:D:105:TYR:HB2	2.32	0.56
1:E:28:PRO:C	1:E:30:ALA:H	2.08	0.56
1:A:412:ILE:HG21	1:A:438:PHE:CE2	2.39	0.56
1:B:412:ILE:HG21	1:B:438:PHE:HE2	1.69	0.56
1:C:104:TYR:H	1:C:107:ARG:H	1.53	0.56
1:C:269:THR:HB	1:C:272:ASP:HB2	1.86	0.56
1:A:162:ILE:HD13	1:F:288:ILE:HB	1.86	0.56
1:F:133:GLU:CA	1:F:134:ASP:HB2	2.32	0.56
1:C:40:PRO:HG2	1:C:53:HIS:HD2	1.71	0.56
1:C:103:GLU:N	1:C:104:TYR:CB	2.69	0.56
1:A:246:GLN:HE22	1:B:420:ARG:CB	2.18	0.56
1:B:233:GLU:HG2	1:B:315:GLY:HA3	1.89	0.56
1:D:51:ILE:HD11	1:D:83:ILE:HG21	1.87	0.56
1:B:296:ILE:CG2	1:B:300:ASP:HB2	2.36	0.55
1:A:306:ARG:NH2	1:B:103:GLU:CD	2.59	0.55
1:C:302:ARG:HH12	1:D:60:ASP:HA	1.70	0.55
1:B:207:ILE:CD1	1:B:386:ILE:HG22	2.36	0.55
1:C:32:VAL:HB	1:C:33:PRO:HD3	1.88	0.55
1:A:231:THR:HG23	1:A:233:GLU:H	1.71	0.55
1:B:296:ILE:HG22	1:B:300:ASP:HB2	1.88	0.55
1:D:133:GLU:H	1:D:134:ASP:HB3	1.62	0.55
1:E:296:ILE:HG22	1:E:300:ASP:HB2	1.89	0.55
1:E:412:ILE:HG21	1:E:438:PHE:CE2	2.42	0.55
1:B:208:VAL:HB	1:B:360:LEU:HD23	1.87	0.55
1:B:268:LEU:CB	1:C:177:HIS:HE1	2.07	0.55
1:F:28:PRO:C	1:F:30:ALA:H	2.09	0.55
1:B:262:ASN:OD1	1:B:268:LEU:HG	2.07	0.55
1:C:21:LEU:HB3	1:C:92:LEU:HD13	1.88	0.55
1:F:316:MET:HG2	1:F:356:PRO:HG2	1.88	0.55
1:A:302:ARG:CG	1:A:349:LEU:HD13	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLU:CD	1:C:178:ASN:HB3	2.26	0.54
1:A:41:GLU:OE1	1:A:41:GLU:N	2.34	0.54
1:B:228:ALA:HB1	1:B:286:ALA:HB1	1.89	0.54
1:A:175:MET:O	1:A:179:ARG:HD2	2.06	0.54
1:B:267:LYS:O	1:B:268:LEU:HB2	2.08	0.54
1:E:302:ARG:HG2	1:E:349:LEU:HD13	1.89	0.54
1:A:292:ASP:O	1:B:351:ARG:CD	2.56	0.54
1:C:104:TYR:HD1	1:C:105:TYR:CG	2.26	0.54
1:B:132:ARG:NH1	1:B:135:GLU:OE1	2.39	0.54
1:F:381:ARG:HH22	1:F:388:GLN:HE22	1.55	0.54
1:E:105:TYR:HE2	1:F:68:VAL:HB	1.71	0.54
1:A:294:PRO:HD3	1:B:351:ARG:HD2	1.89	0.53
1:A:245:GLN:HE22	1:B:202:ARG:NH1	2.06	0.53
1:D:104:TYR:HB3	1:D:105:TYR:CB	2.35	0.53
1:C:294:PRO:HB2	1:D:381:ARG:CG	2.38	0.53
1:D:207:ILE:CD1	1:D:390:ALA:HB2	2.38	0.53
1:A:64:PRO:O	1:A:69:THR:HG21	2.08	0.53
1:E:133:GLU:CA	1:E:134:ASP:HB2	2.33	0.53
1:D:145:ARG:CD	1:D:328:SER:OG	2.52	0.53
1:C:231:THR:HG23	1:C:233:GLU:H	1.74	0.53
1:E:62:GLY:CA	1:E:63:GLU:HB3	2.39	0.53
1:A:262:ASN:HD21	1:A:268:LEU:HA	1.74	0.53
1:A:314:LEU:HD23	1:A:315:GLY:N	2.23	0.53
1:B:30:ALA:HB1	1:B:102:VAL:HG21	1.90	0.53
1:D:381:ARG:HH22	1:D:388:GLN:HE22	1.56	0.53
1:E:269:THR:HB	1:E:272:ASP:HB2	1.90	0.53
1:F:62:GLY:CA	1:F:63:GLU:CB	2.87	0.53
1:E:267:LYS:O	1:E:268:LEU:HB2	2.09	0.53
1:E:296:ILE:CG2	1:E:300:ASP:HB2	2.39	0.53
1:F:233:GLU:HG2	1:F:315:GLY:HA3	1.90	0.53
1:A:302:ARG:HG2	1:A:349:LEU:HD13	1.91	0.52
1:B:12:GLN:HE21	1:B:14:ILE:HG12	1.74	0.52
1:B:105:TYR:O	1:B:109:VAL:HG23	2.10	0.52
1:C:104:TYR:HE2	1:D:63:GLU:HB2	1.75	0.52
1:D:71:THR:HG22	1:D:89:LEU:HD13	1.90	0.52
1:D:228:ALA:HB1	1:D:286:ALA:HB1	1.91	0.52
1:B:320:ASP:HA	1:B:360:LEU:HD12	1.90	0.52
1:B:412:ILE:HG21	1:B:438:PHE:CE2	2.44	0.52
1:A:166:LEU:HD22	1:F:280:MET:HG2	1.91	0.52
1:C:294:PRO:HB2	1:D:381:ARG:HE	1.63	0.52
1:D:61:ARG:CB	1:D:62:GLY:CA	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ARG:NH2	1:B:348:ALA:HB1	2.24	0.52
1:E:330:ARG:CZ	1:F:149:GLU:HA	2.39	0.52
1:A:160:LYS:HB3	1:F:290:ILE:O	2.09	0.52
1:C:348:ALA:HB2	1:D:61:ARG:O	2.10	0.52
1:F:104:TYR:HB3	1:F:105:TYR:CB	2.35	0.52
1:F:104:TYR:CB	1:F:105:TYR:HB2	2.38	0.52
1:E:207:ILE:HD13	1:E:386:ILE:CG2	2.38	0.52
1:F:148:MET:O	1:F:149:GLU:HG3	2.10	0.52
1:A:162:ILE:HG22	1:A:163:LYS:N	2.25	0.52
1:D:141:ASP:C	1:D:328:SER:HB2	2.30	0.52
1:E:265:THR:HB	1:E:267:LYS:HD2	1.92	0.52
1:E:265:THR:CG2	1:F:423:PRO:HB3	2.33	0.52
1:B:392:ILE:HA	1:B:418:LYS:O	2.10	0.52
1:D:211:ARG:HH11	1:D:368:GLU:HG3	1.75	0.52
1:C:161:ASN:ND2	1:C:163:LYS:HG2	2.25	0.52
1:F:197:THR:O	1:F:198:SER:HB2	2.10	0.52
1:A:104:TYR:CD2	1:B:63:GLU:O	2.62	0.51
1:B:104:TYR:HA	1:B:106:ALA:H	1.75	0.51
1:C:348:ALA:CB	1:D:61:ARG:O	2.58	0.51
1:E:83:ILE:HG22	1:E:84:GLY:H	1.76	0.51
1:C:28:PRO:C	1:C:30:ALA:N	2.63	0.51
1:D:31:LEU:HD22	1:D:65:VAL:HG21	1.93	0.51
1:F:105:TYR:O	1:F:109:VAL:HG23	2.10	0.51
1:D:197:THR:O	1:D:198:SER:HB2	2.11	0.51
1:B:269:THR:HB	1:B:272:ASP:HB2	1.93	0.51
1:C:63:GLU:H	1:C:64:PRO:CA	2.21	0.51
1:F:12:GLN:HE21	1:F:14:ILE:HD11	1.75	0.51
1:C:174:GLU:OE1	1:C:178:ASN:ND2	2.33	0.51
1:A:162:ILE:O	1:A:165:ILE:N	2.44	0.51
1:E:51:ILE:HD11	1:E:83:ILE:HG21	1.92	0.51
1:E:61:ARG:CB	1:E:62:GLY:CA	2.87	0.51
1:B:45:ARG:O	1:B:46:ALA:C	2.50	0.50
1:B:266:GLY:HA2	1:B:267:LYS:O	2.11	0.50
1:F:71:THR:HG22	1:F:89:LEU:HD12	1.93	0.50
1:A:173:ILE:O	1:A:173:ILE:HG22	2.11	0.50
1:B:25:PHE:CZ	1:B:89:LEU:HD22	2.46	0.50
1:B:74:LEU:HD13	1:B:83:ILE:HD11	1.93	0.50
1:C:74:LEU:HD22	1:C:83:ILE:HD11	1.93	0.50
1:E:103:GLU:N	1:E:104:TYR:HB2	2.26	0.50
1:E:321:TYR:HA	1:E:360:LEU:O	2.12	0.50
1:A:378:SER:CB	1:F:241:GLU:HG3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLU:HB3	1:B:138:VAL:HB	1.94	0.50
1:C:50:LYS:NZ	1:C:82:GLU:OE2	2.32	0.50
1:D:262:ASN:HD21	1:D:268:LEU:HA	1.75	0.50
1:D:265:THR:O	1:D:265:THR:HG22	2.11	0.50
1:B:216:LYS:HB2	1:B:360:LEU:HD22	1.93	0.50
1:D:32:VAL:HB	1:D:33:PRO:CD	2.36	0.50
1:D:412:ILE:HG21	1:D:438:PHE:HE2	1.76	0.50
1:F:66:ASP:OD1	1:F:66:ASP:C	2.48	0.50
1:B:133:GLU:N	1:B:134:ASP:CB	2.33	0.50
1:B:280:MET:SD	1:C:170:TYR:CD1	3.04	0.50
1:A:128:ASP:HB3	1:A:139:LEU:HD21	1.92	0.50
1:A:321:TYR:CE1	1:A:324:LEU:HG	2.47	0.50
1:B:378:SER:O	1:B:382:GLU:HG2	2.12	0.50
1:C:175:MET:O	1:C:179:ARG:HD3	2.12	0.50
1:A:294:PRO:HA	1:B:351:ARG:HH12	1.77	0.49
1:A:294:PRO:CA	1:B:351:ARG:NH1	2.74	0.49
1:E:290:ILE:O	1:F:160:LYS:HB3	2.12	0.49
1:A:162:ILE:HG23	1:A:166:LEU:HD12	1.94	0.49
1:D:412:ILE:HG21	1:D:438:PHE:CE2	2.47	0.49
1:C:66:ASP:H	1:C:69:THR:HG22	1.77	0.49
1:C:241:GLU:HG3	1:D:378:SER:CB	2.40	0.49
1:A:58:VAL:HG13	1:A:63:GLU:HG2	1.95	0.49
1:D:28:PRO:C	1:D:30:ALA:H	2.16	0.49
1:E:74:LEU:HD22	1:E:83:ILE:HD11	1.94	0.49
1:D:38:LEU:HD11	1:D:106:ALA:HA	1.93	0.49
1:D:61:ARG:HB2	1:D:62:GLY:CA	2.33	0.49
1:E:104:TYR:OH	1:F:63:GLU:HB2	2.11	0.49
1:F:74:LEU:HD13	1:F:83:ILE:CD1	2.42	0.49
1:F:259:ASN:O	1:F:262:ASN:HB3	2.12	0.49
1:C:266:GLY:HA2	1:C:267:LYS:O	2.13	0.49
1:E:198:SER:H	1:E:199:GLY:HA2	1.76	0.49
1:C:197:THR:O	1:C:198:SER:HB2	2.12	0.49
1:D:234:ASN:HB2	1:D:313:GLY:O	2.13	0.49
1:E:104:TYR:CD1	1:E:104:TYR:C	2.84	0.49
1:F:378:SER:O	1:F:382:GLU:HG2	2.13	0.49
1:A:414:ILE:HD11	1:A:429:LEU:HD12	1.95	0.49
1:D:231:THR:HG23	1:D:233:GLU:H	1.78	0.49
1:D:314:LEU:HD23	1:D:315:GLY:N	2.27	0.49
1:B:212:PRO:O	1:B:213:SER:HB2	2.13	0.48
1:C:267:LYS:O	1:C:268:LEU:HB2	2.12	0.48
1:A:161:ASN:O	1:A:162:ILE:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:O	1:A:306:ARG:HB2	2.13	0.48
1:C:51:ILE:HD11	1:C:83:ILE:HG21	1.94	0.48
1:A:134:ASP:O	1:A:135:GLU:HG3	2.13	0.48
1:C:71:THR:HG22	1:C:89:LEU:HD13	1.96	0.48
1:C:144:ASP:O	1:C:145:ARG:C	2.51	0.48
1:F:147:ILE:O	1:F:147:ILE:CG2	2.61	0.48
1:F:233:GLU:HG3	1:F:315:GLY:HA3	1.96	0.48
1:B:68:VAL:HG12	1:B:69:THR:N	2.28	0.48
1:B:273:TRP:HZ3	1:C:177:HIS:ND1	2.11	0.48
1:A:263:LEU:HD23	1:A:268:LEU:HD11	1.96	0.48
1:C:378:SER:O	1:C:382:GLU:HG2	2.13	0.48
1:A:294:PRO:HG3	1:B:348:ALA:CB	2.44	0.48
1:B:28:PRO:C	1:B:30:ALA:H	2.16	0.48
1:D:23:ALA:HB1	1:D:102:VAL:HG22	1.94	0.48
1:D:135:GLU:HB3	1:D:138:VAL:HB	1.95	0.48
1:E:30:ALA:O	1:E:33:PRO:HD2	2.13	0.48
1:E:316:MET:HG2	1:E:356:PRO:HG2	1.96	0.48
1:F:101:ASN:HB3	1:F:105:TYR:CD1	2.48	0.48
1:B:132:ARG:HD2	1:B:139:LEU:HG	1.95	0.48
1:E:66:ASP:H	1:E:69:THR:CG2	2.21	0.48
1:B:297:ARG:NH2	1:B:329:GLY:O	2.47	0.48
1:D:53:HIS:HE1	1:D:57:ARG:NH1	2.11	0.48
1:A:104:TYR:O	1:A:108:ILE:HG12	2.14	0.48
1:D:262:ASN:OD1	1:D:268:LEU:HG	2.14	0.48
1:A:160:LYS:CB	1:F:290:ILE:O	2.62	0.48
1:C:302:ARG:NH1	1:D:59:ALA:O	2.47	0.48
1:D:263:LEU:HD23	1:D:268:LEU:HD11	1.95	0.48
1:D:316:MET:HG2	1:D:356:PRO:HG2	1.96	0.48
1:D:314:LEU:HD21	1:D:317:ILE:HG13	1.96	0.47
1:E:414:ILE:HD11	1:E:429:LEU:HD12	1.96	0.47
1:F:184:THR:N	1:F:198:SER:O	2.47	0.47
1:D:33:PRO:HA	1:D:36:GLU:OE2	2.14	0.47
1:D:50:LYS:NZ	1:D:82:GLU:OE2	2.46	0.47
1:E:211:ARG:HH11	1:E:368:GLU:HG3	1.79	0.47
1:E:268:LEU:HD13	1:E:273:TRP:CE3	2.50	0.47
1:A:296:ILE:HG22	1:A:297:ARG:O	2.14	0.47
1:C:102:VAL:H	1:C:105:TYR:HD1	1.63	0.47
1:E:259:ASN:O	1:E:262:ASN:HB3	2.15	0.47
1:B:62:GLY:HA2	1:B:63:GLU:HA	1.59	0.47
1:D:268:LEU:HD13	1:D:273:TRP:CE3	2.49	0.47
1:A:12:GLN:HE21	1:A:14:ILE:HG12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASN:HD22	1:C:163:LYS:HG2	1.80	0.47
1:D:267:LYS:O	1:D:268:LEU:HB2	2.14	0.47
1:A:86:VAL:HA	1:A:89:LEU:HD12	1.97	0.47
1:A:206:ILE:HA	1:A:392:ILE:HG23	1.97	0.47
1:B:263:LEU:HD23	1:B:268:LEU:HD11	1.95	0.47
1:B:439:VAL:HG12	1:B:440:ASN:N	2.29	0.47
1:E:233:GLU:HG2	1:E:315:GLY:HA3	1.97	0.47
1:A:233:GLU:CG	1:A:315:GLY:HA3	2.44	0.47
1:C:174:GLU:OE2	1:C:178:ASN:CB	2.59	0.47
1:C:234:ASN:HB2	1:C:313:GLY:O	2.15	0.47
1:D:216:LYS:HB2	1:D:360:LEU:HD22	1.96	0.47
1:A:174:GLU:OE2	1:A:175:MET:HG2	2.15	0.47
1:B:145:ARG:HD2	1:B:330:ARG:CZ	2.45	0.47
1:D:198:SER:H	1:D:199:GLY:HA2	1.75	0.47
1:F:19:ALA:O	1:F:23:ALA:HB2	2.15	0.47
1:C:293:THR:HA	1:C:294:PRO:HD2	1.54	0.46
1:B:102:VAL:O	1:B:105:TYR:HB2	2.15	0.46
1:E:10:PRO:HA	1:E:11:PRO:HD2	1.77	0.46
1:E:24:VAL:HG11	1:E:55:MET:SD	2.55	0.46
1:C:219:PHE:CE2	1:C:223:ILE:HD11	2.50	0.46
1:C:302:ARG:NH1	1:D:60:ASP:HA	2.30	0.46
1:E:207:ILE:CD1	1:E:386:ILE:HG22	2.43	0.46
1:C:14:ILE:CD1	1:C:45:ARG:HG3	2.45	0.46
1:A:198:SER:N	1:A:199:GLY:CA	2.75	0.46
1:A:416:ILE:O	1:A:424:VAL:HG13	2.15	0.46
1:D:61:ARG:HD3	1:D:63:GLU:OE2	2.16	0.46
1:D:208:VAL:HB	1:D:360:LEU:HD23	1.98	0.46
1:E:245:GLN:NE2	1:F:168:GLN:OE1	2.48	0.46
1:F:207:ILE:HD12	1:F:390:ALA:CB	2.34	0.46
1:E:197:THR:O	1:E:198:SER:HB2	2.15	0.46
1:F:32:VAL:HB	1:F:33:PRO:CD	2.39	0.46
1:A:63:GLU:N	1:A:64:PRO:HA	2.28	0.46
1:D:64:PRO:HB2	1:D:65:VAL:H	1.59	0.46
1:D:74:LEU:HD22	1:D:83:ILE:HD11	1.98	0.46
1:E:216:LYS:HB2	1:E:360:LEU:HD22	1.97	0.45
1:F:74:LEU:HD13	1:F:83:ILE:HD11	1.98	0.45
1:E:233:GLU:CG	1:E:315:GLY:HA3	2.46	0.45
1:F:207:ILE:CD1	1:F:390:ALA:HB2	2.33	0.45
1:A:168:GLN:O	1:A:170:TYR:N	2.49	0.45
1:C:174:GLU:CD	1:C:178:ASN:HB2	2.37	0.45
1:D:47:ALA:HB1	1:D:83:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ASN:HB2	1:E:105:TYR:CE1	2.51	0.45
1:F:76:ALA:C	1:F:78:GLU:H	2.20	0.45
1:B:11:PRO:HG2	1:B:116:ARG:HG2	1.97	0.45
1:C:184:THR:N	1:C:198:SER:O	2.50	0.45
1:D:273:TRP:CH2	1:E:173:ILE:CG2	2.98	0.45
1:E:302:ARG:O	1:E:306:ARG:HB2	2.16	0.45
1:F:135:GLU:HB3	1:F:138:VAL:HB	1.97	0.45
1:A:25:PHE:HZ	1:A:89:LEU:HD22	1.82	0.45
1:A:176:LEU:HB2	1:A:177:HIS:HD2	1.81	0.45
1:B:263:LEU:HD22	1:C:173:ILE:HG23	1.99	0.45
1:B:102:VAL:O	1:B:105:TYR:CB	2.64	0.45
1:B:202:ARG:HA	1:B:356:PRO:HD3	1.99	0.45
1:C:268:LEU:HD13	1:C:273:TRP:CE3	2.51	0.45
1:D:32:VAL:CB	1:D:33:PRO:HD3	2.41	0.45
1:F:24:VAL:HG11	1:F:55:MET:SD	2.57	0.45
1:A:53:HIS:HE1	1:A:57:ARG:HH11	1.62	0.45
1:A:169:THR:O	1:A:169:THR:HG22	2.17	0.45
1:D:321:TYR:CZ	1:D:324:LEU:HG	2.52	0.45
1:E:208:VAL:HB	1:E:360:LEU:HD23	1.98	0.45
1:B:363:LEU:HD23	1:B:380:ILE:HG23	1.99	0.45
1:C:86:VAL:HA	1:C:89:LEU:HD12	1.99	0.45
1:D:53:HIS:CE1	1:D:57:ARG:HH11	2.35	0.45
1:E:163:LYS:HG3	1:E:164:ASP:N	2.32	0.45
1:E:268:LEU:HD13	1:E:273:TRP:CZ3	2.52	0.45
1:B:105:TYR:HD2	1:B:105:TYR:HA	1.71	0.45
1:B:386:ILE:H	1:B:386:ILE:HG13	1.44	0.45
1:E:234:ASN:HB2	1:E:313:GLY:O	2.16	0.45
1:E:262:ASN:HD21	1:E:268:LEU:HA	1.82	0.45
1:F:132:ARG:NH1	1:F:135:GLU:OE1	2.50	0.45
1:B:347:LYS:HE3	1:B:351:ARG:NH2	2.32	0.44
1:C:71:THR:HG22	1:C:89:LEU:CD1	2.47	0.44
1:C:97:PRO:HD2	1:C:98:THR:HG22	1.99	0.44
1:B:269:THR:CB	1:B:272:ASP:HB2	2.47	0.44
1:C:110:GLU:O	1:C:114:VAL:HG23	2.16	0.44
1:C:206:ILE:HA	1:C:392:ILE:HG23	1.98	0.44
1:C:302:ARG:O	1:C:306:ARG:HB2	2.17	0.44
1:D:416:ILE:O	1:D:424:VAL:HG13	2.16	0.44
1:F:24:VAL:HA	1:F:30:ALA:HB3	2.00	0.44
1:A:381:ARG:HH22	1:A:388:GLN:NE2	2.09	0.44
1:C:30:ALA:HB1	1:C:102:VAL:HG21	1.99	0.44
1:E:99:ALA:O	1:E:102:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HB3	1:A:427:VAL:CG1	2.48	0.44
1:A:15:GLU:OE2	1:B:86:VAL:HG11	2.17	0.44
1:B:414:ILE:HD11	1:B:429:LEU:HD12	2.00	0.44
1:D:302:ARG:O	1:D:306:ARG:HB2	2.17	0.44
1:E:314:LEU:HD23	1:E:315:GLY:N	2.32	0.44
1:A:11:PRO:HG3	1:A:119:ILE:CD1	2.47	0.44
1:C:294:PRO:HB2	1:D:381:ARG:HG2	2.00	0.44
1:A:28:PRO:C	1:A:30:ALA:H	2.20	0.44
1:A:159:PHE:HD1	1:A:160:LYS:N	2.13	0.44
1:A:200:PHE:HE2	1:A:223:ILE:HD13	1.82	0.44
1:A:411:ILE:HD11	1:A:441:LEU:HD21	1.99	0.44
1:B:262:ASN:HD21	1:B:268:LEU:HA	1.82	0.44
1:C:212:PRO:O	1:C:213:SER:HB2	2.17	0.44
1:C:307:ARG:NE	1:D:36:GLU:OE2	2.50	0.44
1:C:321:TYR:H	1:C:360:LEU:HB2	1.83	0.44
1:A:246:GLN:NE2	1:B:420:ARG:CB	2.70	0.44
1:D:141:ASP:C	1:D:143:ALA:N	2.69	0.44
1:F:268:LEU:HD13	1:F:273:TRP:CE3	2.52	0.44
1:B:145:ARG:HD2	1:B:330:ARG:NH2	2.33	0.43
1:C:63:GLU:N	1:C:64:PRO:CA	2.81	0.43
1:D:138:VAL:HG22	1:D:297:ARG:NH1	2.33	0.43
1:F:262:ASN:O	1:F:266:GLY:HA2	2.18	0.43
1:F:267:LYS:O	1:F:268:LEU:CB	2.65	0.43
1:B:32:VAL:HB	1:B:33:PRO:HD3	2.00	0.43
1:C:40:PRO:HG2	1:C:53:HIS:CD2	2.52	0.43
1:D:210:ALA:HB3	1:D:216:LYS:HB3	1.99	0.43
1:E:132:ARG:HD2	1:E:139:LEU:HG	2.00	0.43
1:E:314:LEU:HD21	1:E:317:ILE:HG13	2.00	0.43
1:B:11:PRO:HG2	1:B:116:ARG:CG	2.47	0.43
1:F:223:ILE:HG22	1:F:316:MET:HE1	2.01	0.43
1:B:231:THR:HG23	1:B:233:GLU:H	1.83	0.43
1:D:212:PRO:O	1:D:213:SER:HB2	2.18	0.43
1:D:321:TYR:CE1	1:D:324:LEU:HG	2.53	0.43
1:F:53:HIS:HE1	1:F:57:ARG:NH1	2.17	0.43
1:B:188:THR:HG23	1:B:223:ILE:HG23	2.00	0.43
1:B:268:LEU:HD13	1:B:273:TRP:CE3	2.53	0.43
1:B:268:LEU:CD1	1:C:177:HIS:CE1	2.98	0.43
1:B:347:LYS:HG3	1:B:351:ARG:NH1	2.33	0.43
1:C:74:LEU:HD13	1:C:83:ILE:HD11	2.01	0.43
1:D:280:MET:HG2	1:E:166:LEU:HD22	2.01	0.43
1:E:19:ALA:O	1:E:23:ALA:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:HG3	1:A:65:VAL:HG11	2.01	0.43
1:A:268:LEU:HD13	1:A:273:TRP:CZ3	2.54	0.43
1:B:99:ALA:O	1:B:102:VAL:HG23	2.19	0.43
1:F:208:VAL:HB	1:F:360:LEU:HD23	2.01	0.43
1:F:293:THR:HA	1:F:294:PRO:HD2	1.81	0.43
1:A:302:ARG:HG3	1:A:349:LEU:HD13	2.01	0.43
1:B:61:ARG:CB	1:B:62:GLY:CA	2.93	0.43
1:C:210:ALA:HB3	1:C:216:LYS:HB3	2.00	0.43
1:D:14:ILE:HD13	1:D:14:ILE:HA	1.90	0.43
1:A:259:ASN:O	1:A:262:ASN:HB3	2.19	0.43
1:B:188:THR:HG21	1:B:193:LEU:HD23	2.00	0.43
1:C:233:GLU:HG2	1:C:315:GLY:HA3	2.00	0.43
1:C:321:TYR:CE1	1:C:324:LEU:HG	2.54	0.43
1:E:104:TYR:OH	1:F:63:GLU:CG	2.67	0.43
1:E:253:CYS:SG	1:E:263:LEU:HD12	2.59	0.43
1:F:74:LEU:HD22	1:F:83:ILE:HD11	2.01	0.43
1:F:439:VAL:HG12	1:F:440:ASN:N	2.34	0.43
1:A:179:ARG:O	1:A:180:ASP:C	2.57	0.43
1:C:61:ARG:CB	1:C:62:GLY:CA	2.84	0.43
1:D:39:ILE:O	1:D:41:GLU:N	2.52	0.43
1:F:308:LEU:HD23	1:F:314:LEU:HD12	1.99	0.43
1:D:148:MET:O	1:D:149:GLU:HG3	2.19	0.42
1:D:209:ALA:HA	1:D:361:SER:O	2.19	0.42
1:E:148:MET:O	1:E:149:GLU:HG3	2.18	0.42
1:E:293:THR:HB	1:E:296:ILE:HG12	2.00	0.42
1:B:321:TYR:CZ	1:B:324:LEU:HG	2.55	0.42
1:C:62:GLY:HA2	1:C:63:GLU:HA	1.83	0.42
1:B:96:VAL:HA	1:B:97:PRO:HD3	1.91	0.42
1:B:240:LEU:HD22	1:B:293:THR:O	2.18	0.42
1:B:273:TRP:HZ3	1:C:177:HIS:CE1	2.37	0.42
1:D:66:ASP:N	1:D:69:THR:HG22	2.28	0.42
1:D:69:THR:HG23	1:D:70:VAL:N	2.34	0.42
1:E:71:THR:HA	1:E:74:LEU:HD12	2.02	0.42
1:F:53:HIS:CE1	1:F:57:ARG:HH11	2.37	0.42
1:F:266:GLY:HA2	1:F:267:LYS:O	2.20	0.42
1:C:265:THR:HB	1:C:267:LYS:HD2	2.02	0.42
1:D:135:GLU:HG2	1:D:330:ARG:NE	2.35	0.42
1:D:378:SER:O	1:D:382:GLU:HG2	2.19	0.42
1:A:161:ASN:O	1:A:163:LYS:N	2.52	0.42
1:A:185:GLY:HA3	1:A:201:GLN:HG2	2.02	0.42
1:A:210:ALA:HB2	1:A:396:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLU:H	1:C:104:TYR:HB2	1.84	0.42
1:F:32:VAL:CB	1:F:33:PRO:HD3	2.39	0.42
1:C:96:VAL:HA	1:C:97:PRO:HD3	1.83	0.42
1:C:314:LEU:HD21	1:C:317:ILE:HG13	2.02	0.42
1:E:161:ASN:OD1	1:E:162:ILE:N	2.53	0.42
1:B:76:ALA:HA	1:F:133:GLU:HB3	2.00	0.42
1:C:14:ILE:HD11	1:C:45:ARG:HG3	2.02	0.42
1:D:24:VAL:HG13	1:D:31:LEU:HB2	2.01	0.42
1:D:53:HIS:HE1	1:D:57:ARG:HH11	1.68	0.42
1:F:198:SER:H	1:F:199:GLY:HA2	1.80	0.42
1:A:132:ARG:HD3	1:A:135:GLU:OE1	2.20	0.42
1:B:65:VAL:HA	1:B:69:THR:HG21	2.02	0.42
1:B:302:ARG:O	1:B:306:ARG:HB2	2.20	0.42
1:C:61:ARG:HD3	1:C:63:GLU:CD	2.40	0.42
1:C:74:LEU:HD13	1:C:83:ILE:CD1	2.50	0.42
1:C:179:ARG:NE	1:C:179:ARG:HA	2.35	0.42
1:F:28:PRO:C	1:F:30:ALA:N	2.72	0.42
1:C:13:SER:O	1:C:14:ILE:C	2.59	0.42
1:D:388:GLN:HE21	1:D:388:GLN:HB2	1.57	0.42
1:E:267:LYS:O	1:E:268:LEU:CB	2.68	0.42
1:E:378:SER:O	1:E:382:GLU:HG2	2.20	0.42
1:A:259:ASN:HB3	1:A:262:ASN:HB3	2.01	0.41
1:A:347:LYS:HE3	1:A:351:ARG:CZ	2.50	0.41
1:B:64:PRO:O	1:B:69:THR:HG21	2.20	0.41
1:A:188:THR:OG1	1:A:194:ASP:OD1	2.32	0.41
1:B:10:PRO:HA	1:B:11:PRO:HD2	1.86	0.41
1:B:263:LEU:CD2	1:B:268:LEU:HD11	2.50	0.41
1:C:267:LYS:O	1:C:268:LEU:CB	2.67	0.41
1:E:192:GLU:HB3	1:E:427:VAL:HG13	2.02	0.41
1:F:207:ILE:CD1	1:F:386:ILE:HG22	2.46	0.41
1:A:216:LYS:HB2	1:A:360:LEU:HD22	2.02	0.41
1:B:132:ARG:O	1:B:133:GLU:CB	2.68	0.41
1:B:241:GLU:HG3	1:C:378:SER:HB3	2.02	0.41
1:C:294:PRO:CB	1:D:381:ARG:CZ	2.99	0.41
1:D:297:ARG:NH2	1:D:329:GLY:O	2.53	0.41
1:E:28:PRO:C	1:E:30:ALA:N	2.72	0.41
1:E:210:ALA:HB3	1:E:216:LYS:HB3	2.03	0.41
1:D:141:ASP:OD2	1:D:297:ARG:HB2	2.21	0.41
1:E:262:ASN:OD1	1:E:268:LEU:HG	2.20	0.41
1:C:233:GLU:CG	1:C:315:GLY:HA3	2.51	0.41
1:D:142:GLU:CA	1:D:328:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:PHE:CE1	1:F:67:LEU:HD23	2.56	0.41
1:D:267:LYS:O	1:D:268:LEU:CB	2.68	0.41
1:F:197:THR:HA	1:F:419:GLN:OE1	2.21	0.41
1:D:136:ILE:C	1:D:138:VAL:H	2.24	0.41
1:E:198:SER:N	1:E:199:GLY:CA	2.77	0.41
1:F:96:VAL:HG22	1:F:97:PRO:HD2	2.03	0.41
1:F:253:CYS:SG	1:F:263:LEU:HD12	2.60	0.41
1:A:104:TYR:CD1	1:B:63:GLU:O	2.73	0.41
1:D:130:TYR:CE1	1:E:119:ILE:HD13	2.56	0.41
1:E:133:GLU:N	1:E:134:ASP:CB	2.32	0.41
1:E:293:THR:HA	1:E:294:PRO:HD2	1.79	0.41
1:A:74:LEU:HD22	1:A:83:ILE:HD11	2.03	0.41
1:A:233:GLU:HG3	1:A:315:GLY:HA3	2.02	0.41
1:A:233:GLU:HG2	1:A:315:GLY:HA3	2.03	0.41
1:A:321:TYR:H	1:A:360:LEU:HB2	1.86	0.41
1:B:267:LYS:O	1:B:268:LEU:CB	2.68	0.41
1:C:209:ALA:HA	1:C:361:SER:O	2.21	0.41
1:C:416:ILE:O	1:C:424:VAL:HG13	2.21	0.41
1:E:197:THR:HA	1:E:419:GLN:OE1	2.21	0.41
1:F:53:HIS:HE1	1:F:57:ARG:HH11	1.68	0.41
1:F:414:ILE:HD11	1:F:429:LEU:HD12	2.02	0.41
1:A:207:ILE:HD12	1:A:390:ALA:CB	2.37	0.41
1:A:208:VAL:HB	1:A:360:LEU:HD23	2.03	0.41
1:A:262:ASN:O	1:A:266:GLY:HA2	2.21	0.41
1:E:46:ALA:O	1:E:50:LYS:HD3	2.21	0.41
1:E:104:TYR:HA	1:E:106:ALA:H	1.86	0.41
1:F:83:ILE:HB	1:F:84:GLY:H	1.62	0.41
1:F:148:MET:CE	1:F:148:MET:HA	2.50	0.41
1:F:222:ASN:N	1:F:222:ASN:HD22	2.18	0.41
1:A:42:ASP:HA	1:A:113:SER:OG	2.21	0.40
1:A:74:LEU:HD13	1:A:83:ILE:CD1	2.51	0.40
1:B:47:ALA:HB1	1:B:83:ILE:HG23	2.03	0.40
1:B:48:HIS:CD2	1:B:48:HIS:H	2.39	0.40
1:B:102:VAL:O	1:B:106:ALA:N	2.51	0.40
1:D:65:VAL:HA	1:D:69:THR:HG21	2.03	0.40
1:F:192:GLU:HB3	1:F:427:VAL:HG13	2.04	0.40
1:A:53:HIS:HE1	1:A:57:ARG:NH1	2.19	0.40
1:A:83:ILE:HB	1:A:84:GLY:H	1.73	0.40
1:A:217:THR:O	1:A:221:LEU:HG	2.20	0.40
1:B:67:LEU:O	1:B:71:THR:CG2	2.66	0.40
1:F:231:THR:HG23	1:F:233:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:HB3	1:A:138:VAL:HB	2.04	0.40
1:B:207:ILE:HD13	1:B:386:ILE:CG2	2.46	0.40
1:D:145:ARG:HH12	1:D:329:GLY:H	1.69	0.40
1:D:211:ARG:NH1	1:D:368:GLU:HG3	2.36	0.40
1:E:38:LEU:HD21	1:E:109:VAL:HB	2.03	0.40
1:A:24:VAL:HG11	1:A:55:MET:SD	2.62	0.40
1:A:261:GLN:HA	1:A:264:ARG:HD2	2.04	0.40
1:B:240:LEU:HD21	1:B:296:ILE:HG13	2.04	0.40
1:D:71:THR:HG22	1:D:89:LEU:CD1	2.52	0.40
1:A:168:GLN:C	1:A:170:TYR:N	2.75	0.40
1:C:294:PRO:CB	1:D:381:ARG:HG2	2.52	0.40
1:E:320:ASP:HA	1:E:360:LEU:HD12	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ASN:ND2	1:F:97:PRO:CB[1_565]	2.12	0.08
1:C:178:ASN:CG	1:F:97:PRO:CB[1_565]	2.13	0.07

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	395/454 (87%)	334 (85%)	43 (11%)	18 (5%)	2 23
1	B	366/454 (81%)	308 (84%)	46 (13%)	12 (3%)	4 31
1	C	389/454 (86%)	327 (84%)	37 (10%)	25 (6%)	1 17
1	D	366/454 (81%)	308 (84%)	42 (12%)	16 (4%)	2 24
1	E	380/454 (84%)	325 (86%)	38 (10%)	17 (4%)	2 23
1	F	380/454 (84%)	331 (87%)	33 (9%)	16 (4%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2276/2724 (84%)	1933 (85%)	239 (10%)	104 (5%)	2 23

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	134	ASP
1	A	162	ILE
1	A	179	ARG
1	A	180	ASP
1	A	266	GLY
1	A	268	LEU
1	A	321	TYR
1	B	83	ILE
1	B	104	TYR
1	B	133	GLU
1	B	268	LEU
1	B	321	TYR
1	C	63	GLU
1	C	104	TYR
1	C	133	GLU
1	C	134	ASP
1	C	179	ARG
1	C	180	ASP
1	C	266	GLY
1	C	268	LEU
1	C	321	TYR
1	D	63	GLU
1	D	64	PRO
1	D	83	ILE
1	D	102	VAL
1	D	104	TYR
1	D	134	ASP
1	D	268	LEU
1	D	321	TYR
1	E	63	GLU
1	E	83	ILE
1	E	102	VAL
1	E	134	ASP
1	E	266	GLY
1	E	268	LEU
1	E	321	TYR

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Mol	Chain	Res	Type
1	F	63	GLU
1	F	64	PRO
1	F	102	VAL
1	F	104	TYR
1	F	134	ASP
1	F	266	GLY
1	F	268	LEU
1	F	321	TYR
1	A	163	LYS
1	A	169	THR
1	A	198	SER
1	B	63	GLU
1	B	134	ASP
1	B	136	ILE
1	B	266	GLY
1	C	44	TYR
1	C	101	ASN
1	C	145	ARG
1	C	175	MET
1	D	133	GLU
1	D	136	ILE
1	D	198	SER
1	D	266	GLY
1	A	133	GLU
1	A	267	LYS
1	C	116	ARG
1	C	440	ASN
1	D	78	GLU
1	E	11	PRO
1	E	133	GLU
1	E	198	SER
1	F	78	GLU
1	F	97	PRO
1	F	198	SER
1	A	64	PRO
1	B	64	PRO
1	B	101	ASN
1	B	267	LYS
1	C	64	PRO
1	C	78	GLU
1	C	95	ALA
1	C	181	GLY

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Mol	Chain	Res	Type
1	D	40	PRO
1	D	267	LYS
1	E	49	GLN
1	E	97	PRO
1	E	104	TYR
1	E	267	LYS
1	A	365	ARG
1	C	27	ASP
1	C	83	ILE
1	C	105	TYR
1	C	267	LYS
1	E	29	ALA
1	E	101	ASN
1	F	133	GLU
1	F	267	LYS
1	A	83	ILE
1	A	136	ILE
1	D	142	GLU
1	E	64	PRO
1	A	181	GLY
1	C	102	VAL
1	C	136	ILE
1	F	40	PRO
1	F	83	ILE
1	F	136	ILE

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	341/386 (88%)	314 (92%)	27 (8%)	12 42
1	B	314/386 (81%)	294 (94%)	20 (6%)	17 48
1	C	336/386 (87%)	318 (95%)	18 (5%)	22 54
1	D	314/386 (81%)	291 (93%)	23 (7%)	14 44
1	E	330/386 (86%)	310 (94%)	20 (6%)	18 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	330/386 (86%)	307 (93%)	23 (7%)	15 45
All	All	1965/2316 (85%)	1834 (93%)	131 (7%)	16 47

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	60	ASP
1	A	67	LEU
1	A	80	LEU
1	A	81	GLU
1	A	96	VAL
1	A	115	LEU
1	A	120	ARG
1	A	136	ILE
1	A	159	PHE
1	A	161	ASN
1	A	163	LYS
1	A	164	ASP
1	A	268	LEU
1	A	271	GLU
1	A	272	ASP
1	A	278	MET
1	A	297	ARG
1	A	316	MET
1	A	321	TYR
1	A	323	GLN
1	A	339	VAL
1	A	340	SER
1	A	386	ILE
1	A	388	GLN
1	A	391	ASP
1	A	412	ILE
1	B	12	GLN
1	B	55	MET
1	B	56	LEU
1	B	80	LEU
1	B	104	TYR
1	B	128	ASP
1	B	135	GLU
1	B	136	ILE
1	B	144	ASP

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Mol	Chain	Res	Type
1	B	147	ILE
1	B	148	MET
1	B	195	ARG
1	B	233	GLU
1	B	269	THR
1	B	271	GLU
1	B	306	ARG
1	B	321	TYR
1	B	386	ILE
1	B	388	GLN
1	B	412	ILE
1	C	26	LEU
1	C	50	LYS
1	C	61	ARG
1	C	81	GLU
1	C	115	LEU
1	C	139	LEU
1	C	141	ASP
1	C	148	MET
1	C	163	LYS
1	C	174	GLU
1	C	195	ARG
1	C	271	GLU
1	C	316	MET
1	C	321	TYR
1	C	386	ILE
1	C	388	GLN
1	C	391	ASP
1	C	412	ILE
1	D	12	GLN
1	D	50	LYS
1	D	56	LEU
1	D	80	LEU
1	D	86	VAL
1	D	103	GLU
1	D	104	TYR
1	D	128	ASP
1	D	134	ASP
1	D	136	ILE
1	D	139	LEU
1	D	140	LEU
1	D	141	ASP

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Mol	Chain	Res	Type
1	D	147	ILE
1	D	195	ARG
1	D	231	THR
1	D	268	LEU
1	D	316	MET
1	D	321	TYR
1	D	386	ILE
1	D	388	GLN
1	D	391	ASP
1	D	412	ILE
1	E	12	GLN
1	E	26	LEU
1	E	60	ASP
1	E	81	GLU
1	E	105	TYR
1	E	114	VAL
1	E	115	LEU
1	E	139	LEU
1	E	148	MET
1	E	163	LYS
1	E	171	ASP
1	E	174	GLU
1	E	195	ARG
1	E	268	LEU
1	E	271	GLU
1	E	316	MET
1	E	321	TYR
1	E	386	ILE
1	E	388	GLN
1	E	412	ILE
1	F	12	GLN
1	F	50	LYS
1	F	77	SER
1	F	80	LEU
1	F	86	VAL
1	F	90	SER
1	F	103	GLU
1	F	104	TYR
1	F	128	ASP
1	F	139	LEU
1	F	148	MET
1	F	163	LYS

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Mol	Chain	Res	Type
1	F	174	GLU
1	F	195	ARG
1	F	268	LEU
1	F	271	GLU
1	F	272	ASP
1	F	316	MET
1	F	321	TYR
1	F	345	SER
1	F	386	ILE
1	F	391	ASP
1	F	412	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	53	HIS
1	A	79	GLN
1	A	152	GLN
1	A	177	HIS
1	A	225	GLN
1	A	226	ASN
1	A	245	GLN
1	A	246	GLN
1	A	323	GLN
1	A	388	GLN
1	A	436	ASN
1	B	12	GLN
1	B	53	HIS
1	B	79	GLN
1	B	225	GLN
1	B	226	ASN
1	B	323	GLN
1	B	388	GLN
1	C	12	GLN
1	C	53	HIS
1	C	172	ASN
1	C	177	HIS
1	C	225	GLN
1	C	323	GLN
1	C	388	GLN
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	53	HIS
1	D	79	GLN
1	D	225	GLN
1	D	226	ASN
1	D	323	GLN
1	D	388	GLN
1	E	53	HIS
1	E	79	GLN
1	E	225	GLN
1	E	226	ASN
1	E	245	GLN
1	E	323	GLN
1	E	388	GLN
1	F	12	GLN
1	F	53	HIS
1	F	225	GLN
1	F	323	GLN
1	F	388	GLN

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

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	405/454 (89%)	0.15	29 (7%) 15 11	153, 178, 179, 207	0
1	B	376/454 (82%)	0.16	21 (5%) 24 17	175, 178, 179, 186	0
1	C	399/454 (87%)	0.32	38 (9%) 8 6	145, 178, 179, 209	0
1	D	376/454 (82%)	0.33	37 (9%) 7 6	165, 178, 179, 184	0
1	E	392/454 (86%)	0.97	77 (19%) 1 1	169, 178, 179, 198	0
1	F	392/454 (86%)	0.41	39 (9%) 7 6	176, 178, 180, 189	0
All	All	2340/2724 (85%)	0.39	241 (10%) 6 5	145, 178, 179, 209	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	265	THR	12.4
1	E	384	GLY	12.3
1	F	409	LYS	9.0
1	E	409	LYS	8.9
1	E	421	ASN	8.6
1	D	264	ARG	8.0
1	E	374	ARG	7.7
1	E	266	GLY	7.6
1	F	330	ARG	7.5
1	A	265	THR	7.5
1	E	420	ARG	7.5
1	F	160	LYS	7.3
1	E	383	SER	7.2
1	E	261	GLN	7.1
1	D	330	ARG	7.1
1	A	409	LYS	7.1
1	E	310	GLN	6.9
1	F	265	THR	6.7
1	E	397	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	267	LYS	6.0
1	F	382	GLU	5.9
1	E	294	PRO	5.8
1	D	328	SER	5.8
1	D	184	THR	5.7
1	F	397	TYR	5.6
1	C	327	GLY	5.6
1	E	382	GLU	5.5
1	E	307	ARG	5.4
1	A	268	LEU	5.2
1	C	213	SER	5.1
1	B	381	ARG	5.0
1	C	178	ASN	5.0
1	E	385	SER	5.0
1	E	183	ILE	5.0
1	E	259	ASN	4.9
1	E	182	GLU	4.9
1	C	270	PRO	4.9
1	C	330	ARG	4.9
1	C	97	PRO	4.8
1	E	231	THR	4.7
1	F	184	THR	4.6
1	E	262	ASN	4.6
1	F	423	PRO	4.5
1	A	261	GLN	4.4
1	B	420	ARG	4.3
1	F	384	GLY	4.3
1	F	255	GLU	4.3
1	E	365	ARG	4.2
1	A	264	ARG	4.2
1	E	256	GLY	4.2
1	B	382	GLU	4.1
1	C	364	SER	4.1
1	A	273	TRP	4.0
1	A	329	GLY	4.0
1	F	164	ASP	4.0
1	E	311	GLU	3.9
1	E	232	ASN	3.9
1	E	260	ALA	3.9
1	F	12	GLN	3.9
1	E	396	LEU	3.9
1	D	100	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	432	ILE	3.8
1	F	362	GLN	3.8
1	D	265	THR	3.8
1	A	330	ARG	3.7
1	C	273	TRP	3.7
1	E	422	GLY	3.6
1	F	379	ASP	3.6
1	E	264	ARG	3.6
1	C	234	ASN	3.6
1	E	271	GLU	3.6
1	E	268	LEU	3.6
1	D	285	ASN	3.6
1	E	376	MET	3.6
1	F	383	SER	3.6
1	E	345	SER	3.6
1	C	418	LYS	3.5
1	D	99	ALA	3.5
1	E	329	GLY	3.5
1	F	434	GLU	3.5
1	D	273	TRP	3.5
1	E	195	ARG	3.5
1	F	327	GLY	3.5
1	F	420	ARG	3.5
1	C	179	ARG	3.4
1	C	381	ARG	3.4
1	E	413	GLU	3.4
1	A	266	GLY	3.4
1	E	230	LYS	3.4
1	F	127	GLN	3.4
1	B	329	GLY	3.4
1	A	364	SER	3.3
1	A	441	LEU	3.3
1	D	133	GLU	3.3
1	E	270	PRO	3.3
1	E	287	GLY	3.3
1	F	161	ASN	3.2
1	C	180	ASP	3.2
1	D	300	ASP	3.2
1	B	281	GLY	3.2
1	C	233	GLU	3.2
1	B	368	GLU	3.2
1	E	255	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	375	PRO	3.1
1	E	94	ASP	3.1
1	A	366	SER	3.1
1	F	187	PRO	3.1
1	D	149	GLU	3.1
1	E	257	ASN	3.0
1	F	329	GLY	3.0
1	C	328	SER	3.0
1	B	421	ASN	3.0
1	E	99	ALA	3.0
1	F	134	ASP	3.0
1	B	261	GLN	3.0
1	D	127	GLN	3.0
1	E	215	GLY	3.0
1	C	267	LYS	3.0
1	B	213	SER	2.9
1	B	383	SER	2.9
1	D	307	ARG	2.9
1	D	338	GLU	2.9
1	D	105	TYR	2.9
1	E	367	VAL	2.9
1	E	366	SER	2.9
1	E	289	TYR	2.9
1	C	257	ASN	2.9
1	E	250	ARG	2.8
1	E	305	CYS	2.8
1	A	211	ARG	2.8
1	E	381	ARG	2.8
1	E	39	ILE	2.8
1	C	133	GLU	2.8
1	D	212	PRO	2.8
1	F	376	MET	2.8
1	F	163	LYS	2.7
1	C	366	SER	2.7
1	B	330	ARG	2.7
1	D	36	GLU	2.7
1	D	306	ARG	2.7
1	B	211	ARG	2.7
1	C	326	GLN	2.7
1	A	291	ASP	2.7
1	C	271	GLU	2.7
1	B	364	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	167	VAL	2.6
1	A	151	SER	2.6
1	E	438	PHE	2.6
1	C	212	PRO	2.6
1	E	440	ASN	2.6
1	E	354	GLU	2.6
1	E	315	GLY	2.6
1	F	77	SER	2.5
1	E	362	GLN	2.5
1	F	94	ASP	2.5
1	E	389	ASP	2.5
1	D	310	GLN	2.5
1	D	428	GLN	2.5
1	A	277	THR	2.5
1	C	63	GLU	2.5
1	A	63	GLU	2.5
1	F	264	ARG	2.5
1	C	96	VAL	2.5
1	D	63	GLU	2.5
1	A	199	GLY	2.5
1	D	196	MET	2.5
1	D	250	ARG	2.5
1	F	294	PRO	2.5
1	F	410	ASN	2.5
1	D	382	GLU	2.5
1	E	439	VAL	2.5
1	E	184	THR	2.4
1	C	64	PRO	2.4
1	E	191	THR	2.4
1	B	97	PRO	2.4
1	B	44	TYR	2.4
1	E	436	ASN	2.4
1	C	182	GLU	2.4
1	E	441	LEU	2.4
1	D	128	ASP	2.4
1	A	382	GLU	2.4
1	E	100	ALA	2.4
1	A	310	GLN	2.4
1	D	255	GLU	2.4
1	C	195	ARG	2.4
1	C	374	ARG	2.3
1	E	306	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	367	VAL	2.3
1	C	367	VAL	2.3
1	F	419	GLN	2.3
1	E	344	ARG	2.3
1	F	267	LYS	2.3
1	C	315	GLY	2.3
1	D	134	ASP	2.3
1	C	329	GLY	2.3
1	B	184	THR	2.3
1	C	104	TYR	2.3
1	B	428	GLN	2.3
1	C	94	ASP	2.3
1	F	366	SER	2.2
1	C	292	ASP	2.2
1	F	185	GLY	2.2
1	B	104	TYR	2.2
1	E	312	SER	2.2
1	A	153	ARG	2.2
1	E	66	ASP	2.2
1	F	375	PRO	2.2
1	E	269	THR	2.2
1	B	233	GLU	2.2
1	C	354	GLU	2.2
1	D	81	GLU	2.2
1	F	433	LYS	2.2
1	C	313	GLY	2.1
1	D	374	ARG	2.1
1	A	60	ASP	2.1
1	A	290	ILE	2.1
1	A	37	ILE	2.1
1	F	171	ASP	2.1
1	A	269	THR	2.1
1	D	244	ALA	2.1
1	B	295	SER	2.1
1	E	282	SER	2.1
1	B	321	TYR	2.1
1	A	428	GLN	2.1
1	A	272	ASP	2.1
1	D	98	THR	2.1
1	C	440	ASN	2.1
1	E	133	GLU	2.1
1	E	330	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	304	LYS	2.1
1	A	421	ASN	2.1
1	D	427	VAL	2.1
1	E	328	SER	2.0
1	D	303	ALA	2.0
1	E	85	GLY	2.0
1	A	195	ARG	2.0
1	C	436	ASN	2.0
1	E	97	PRO	2.0
1	E	300	ASP	2.0
1	F	266	GLY	2.0
1	D	211	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.