Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 09:34 AM EDT

PDB ID	:	3I6W
Title	:	Structure and Activation Mechanism of the CHK2 DNA-Damage Checkpoint Kinase
Authors	:	Pavletich, N.P.
Deposited on	:	2009-07-07
Resolution	:	3.25 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:

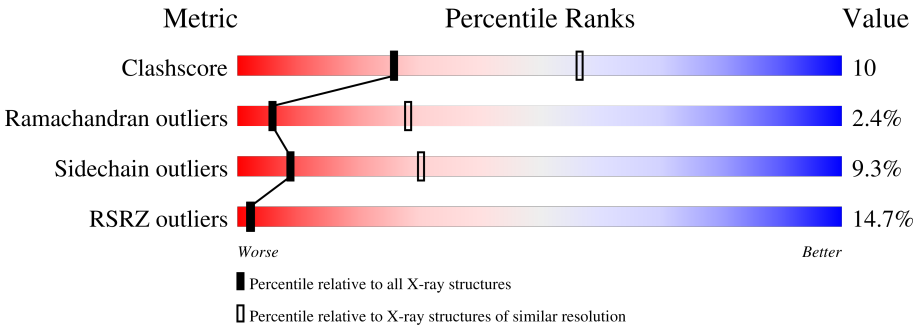
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.25 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	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	443	8% 60% 19% · 17%
1	B	443	9% 63% 21% · 14%
1	C	443	6% 58% 21% · 17%
1	D	443	13% 63% 21% · 14%
1	E	443	17% 60% 20% · 17%
1	F	443	21% 65% 18% · 14%
1	G	443	12% 59% 20% · 17%

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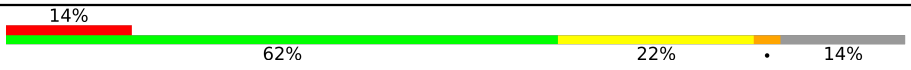
Mol	Chain	Length	Quality of chain
1	H	443	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24560 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 Serine/threonine-protein kinase Chk2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	B	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	C	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	D	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	E	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	F	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	G	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	H	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			

There are 8 discrepancies between the modelled and reference sequences:

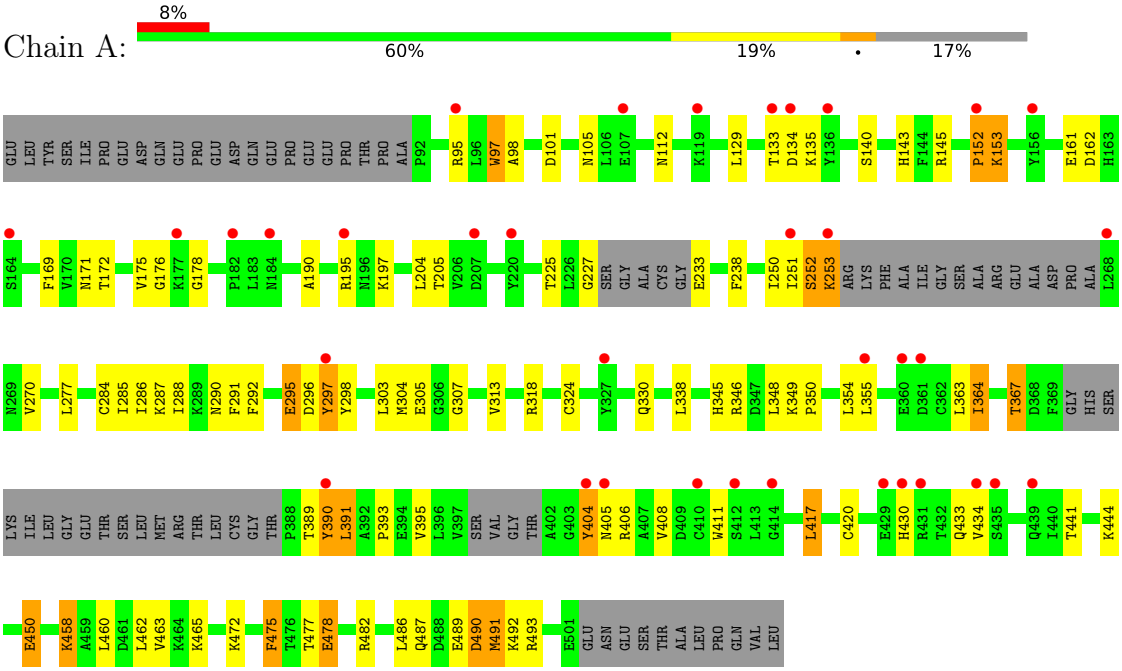
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ARG	LYS	engineered mutation	UNP O96017
B	249	ARG	LYS	engineered mutation	UNP O96017
C	249	ARG	LYS	engineered mutation	UNP O96017
D	249	ARG	LYS	engineered mutation	UNP O96017
E	249	ARG	LYS	engineered mutation	UNP O96017
F	249	ARG	LYS	engineered mutation	UNP O96017
G	249	ARG	LYS	engineered mutation	UNP O96017
H	249	ARG	LYS	engineered mutation	UNP O96017

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.

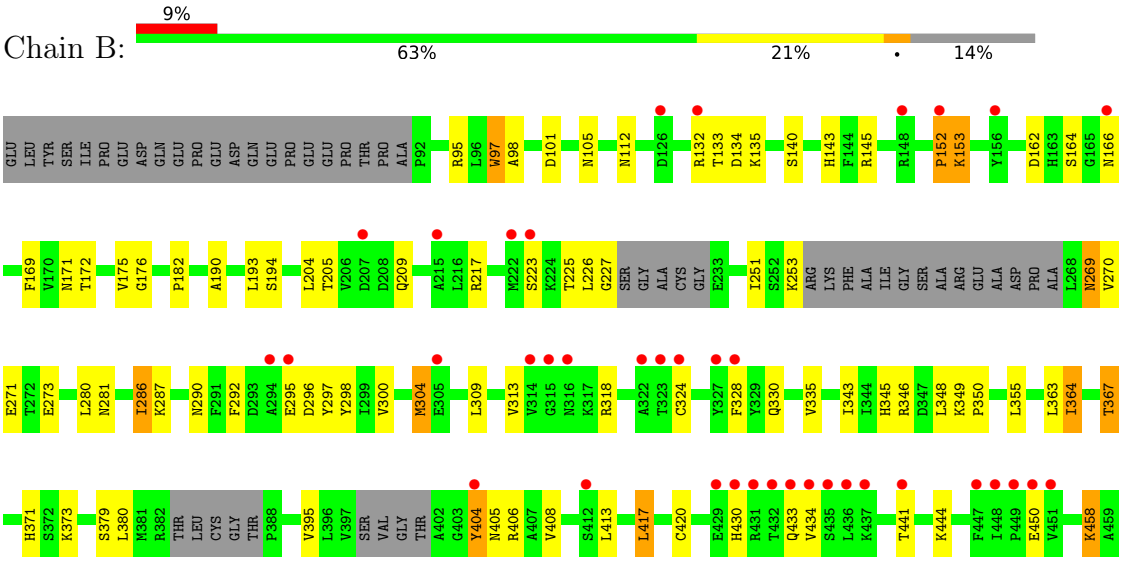
• Molecule 1: Serine/threonine-protein kinase Chk2

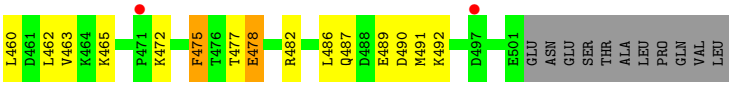
Chain A:



• Molecule 1: Serine/threonine-protein kinase Chk2

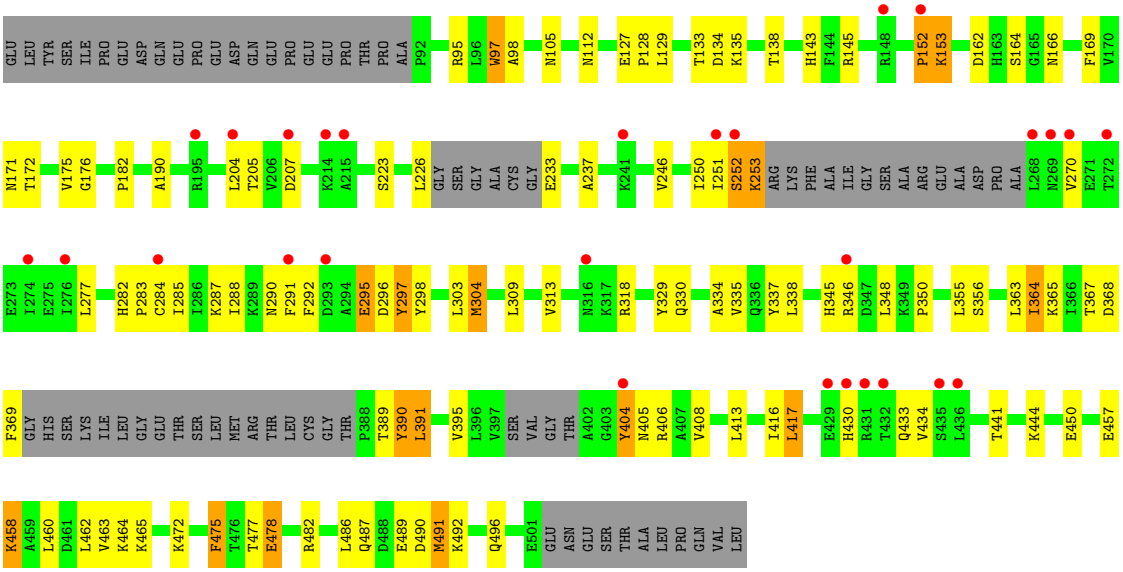
Chain B:





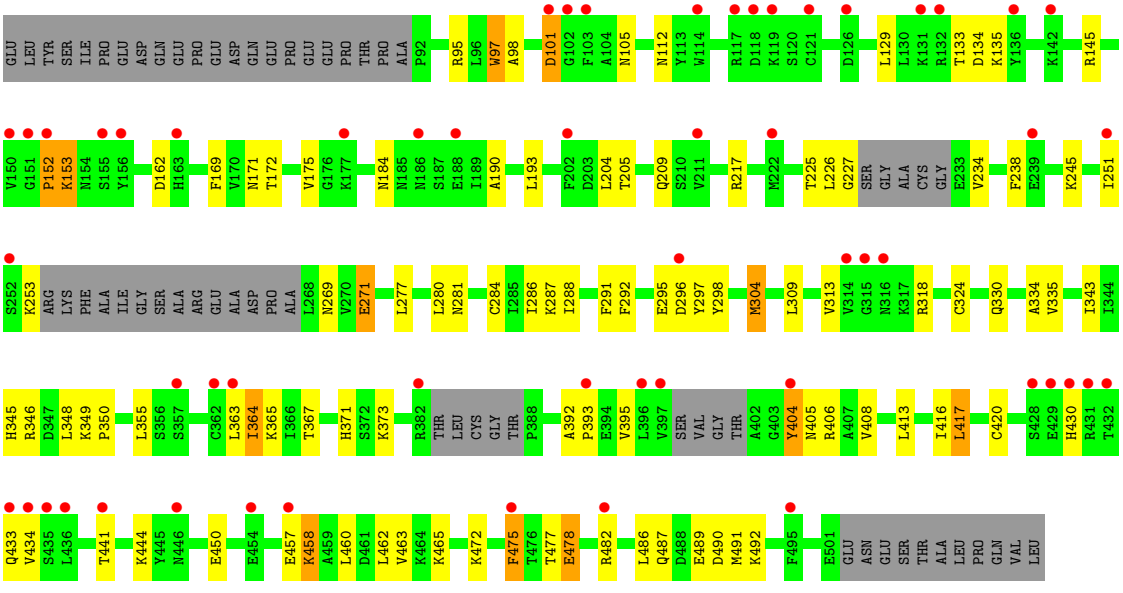
• Molecule 1: Serine/threonine-protein kinase Chk2

Chain C:



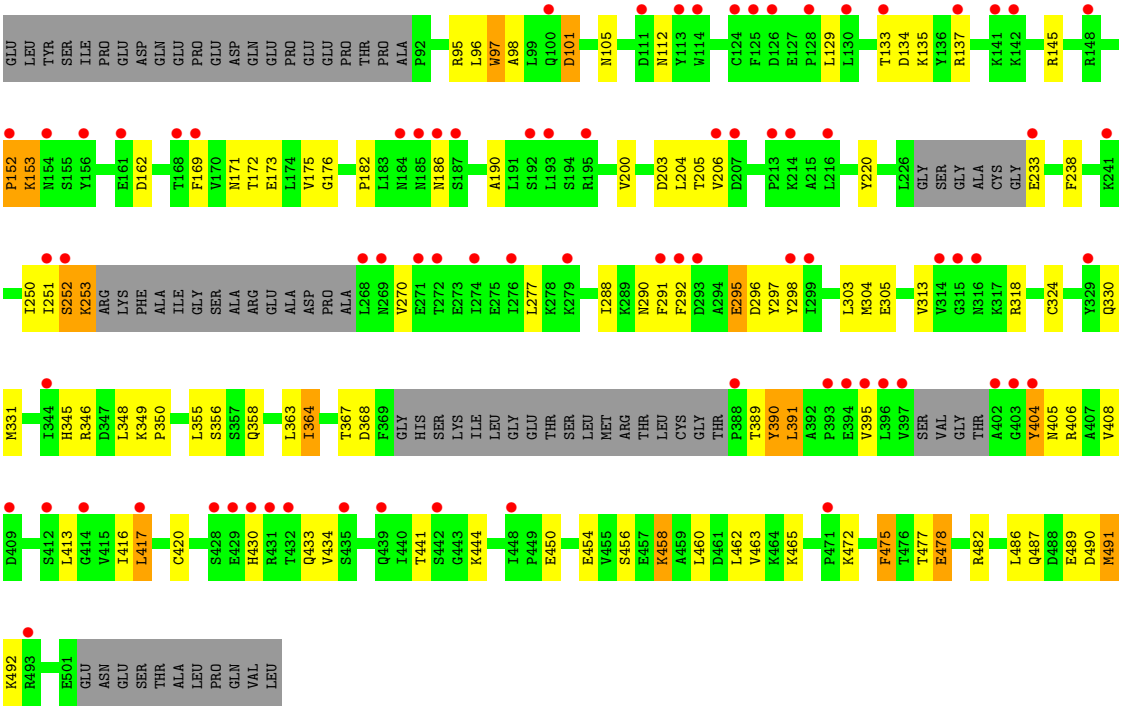
• Molecule 1: Serine/threonine-protein kinase Chk2

Chain D:



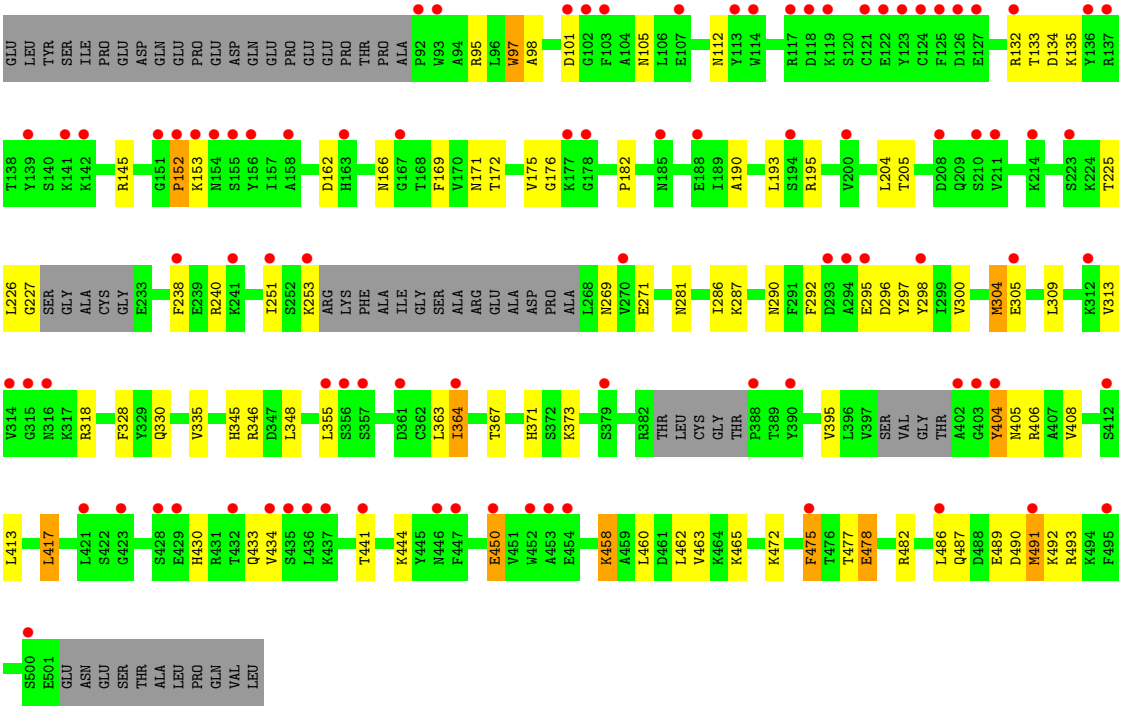
• Molecule 1: Serine/threonine-protein kinase Chk2

Chain E:



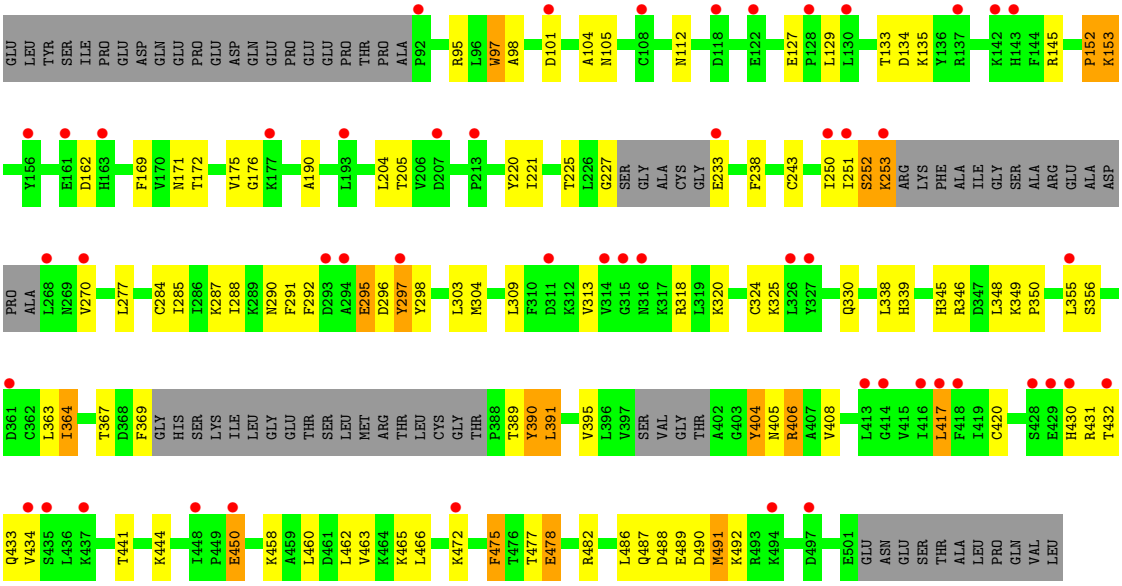
• Molecule 1: Serine/threonine-protein kinase Chk2

Chain F:



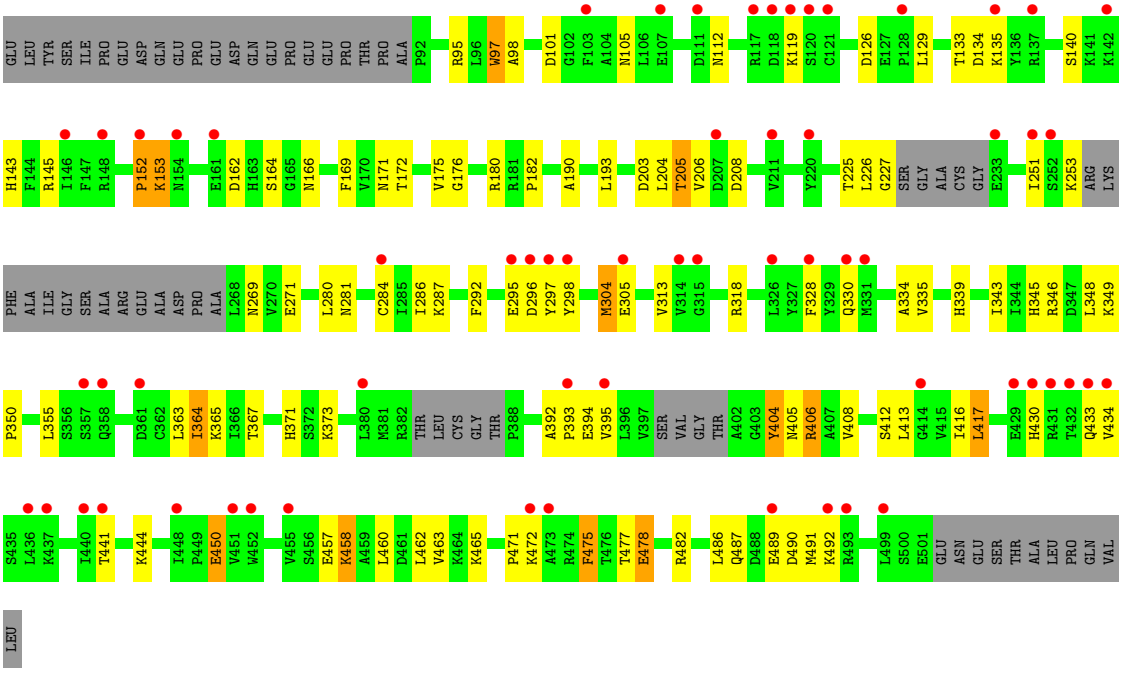
• Molecule 1: Serine/threonine-protein kinase Chk2

Chain G:



• Molecule 1: Serine/threonine-protein kinase Chk2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.20Å 114.70Å 123.00Å 84.10° 81.20° 80.70°	Depositor
Resolution (Å)	30.00 – 3.25 29.86 – 3.25	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.00-3.25) 90.9 (29.86-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.251 , 0.287 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	119.5	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 172.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24560	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.48	0/3087	0.59	0/4163
1	B	0.49	0/3186	0.60	1/4294 (0.0%)
1	C	0.55	0/3083	0.63	1/4158 (0.0%)
1	D	0.46	0/3186	0.60	1/4294 (0.0%)
1	E	0.44	0/3083	0.58	0/4158
1	F	0.41	0/3186	0.57	1/4294 (0.0%)
1	G	0.43	0/3087	0.58	1/4163 (0.0%)
1	H	0.40	0/3186	0.57	0/4294
All	All	0.46	0/25084	0.59	5/33818 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	309	LEU	CA-CB-CG	5.17	127.20	115.30
1	G	309	LEU	CA-CB-CG	5.12	127.07	115.30
1	C	309	LEU	CA-CB-CG	5.09	127.01	115.30
1	F	309	LEU	CA-CB-CG	5.05	126.92	115.30
1	D	309	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3022	0	3026	80	6
1	B	3120	0	3130	79	0
1	C	3018	0	3023	74	5
1	D	3120	0	3130	71	0
1	E	3018	0	3023	81	6
1	F	3120	0	3130	69	8
1	G	3022	0	3026	69	5
1	H	3120	0	3130	84	4
All	All	24560	0	24618	516	20

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 10.

All (516) 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:129:LEU:HD23	1:D:193:LEU:CD2	1.47	1.44
1:A:129:LEU:CD2	1:D:193:LEU:HD21	1.52	1.40
1:F:132:ARG:CD	1:H:129:LEU:HD13	1.74	1.16
1:B:166:ASN:HD22	1:C:129:LEU:HB2	1.15	1.09
1:F:132:ARG:HD2	1:H:129:LEU:CD1	1.84	1.07
1:F:132:ARG:HD2	1:H:129:LEU:HD13	1.12	1.04
1:A:129:LEU:CD2	1:D:193:LEU:CD2	2.21	1.02
1:E:129:LEU:HD23	1:H:193:LEU:CD2	1.90	1.01
1:A:97:TRP:NE1	1:B:97:TRP:NE1	2.08	1.01
1:A:97:TRP:CD1	1:B:97:TRP:NE1	2.30	1.00
1:E:346:ARG:HG3	1:E:404:TYR:HE2	1.24	0.99
1:A:97:TRP:CE2	1:B:97:TRP:CD1	2.51	0.99
1:B:478:GLU:HB2	1:B:482:ARG:HH12	1.31	0.96
1:D:457:GLU:OE2	1:H:119:LYS:HD2	1.66	0.95
1:B:132:ARG:HH11	1:D:129:LEU:HD22	1.29	0.94
1:D:478:GLU:HB2	1:D:482:ARG:HH12	1.33	0.94
1:H:478:GLU:HB2	1:H:482:ARG:HH12	1.33	0.93
1:F:478:GLU:HB2	1:F:482:ARG:HH12	1.32	0.93
1:E:478:GLU:HB2	1:E:482:ARG:HH12	1.32	0.93
1:G:346:ARG:HG3	1:G:404:TYR:HE2	1.33	0.93
1:H:346:ARG:HG3	1:H:404:TYR:HE2	1.34	0.92
1:C:478:GLU:HB2	1:C:482:ARG:HH12	1.34	0.92
1:B:166:ASN:ND2	1:C:129:LEU:HB2	1.85	0.92
1:A:478:GLU:HB2	1:A:482:ARG:HH12	1.32	0.92
1:A:478:GLU:OE2	1:E:456:SER:HB2	1.70	0.91
1:D:346:ARG:HG3	1:D:404:TYR:HE2	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:LEU:HD23	1:H:193:LEU:HD21	1.53	0.90
1:A:346:ARG:HG3	1:A:404:TYR:HE2	1.37	0.89
1:G:478:GLU:HB2	1:G:482:ARG:HH12	1.40	0.87
1:B:166:ASN:HD21	1:C:129:LEU:HD13	1.39	0.87
1:A:238:PHE:CD1	1:B:182:PRO:HG3	2.11	0.85
1:B:346:ARG:HG3	1:B:404:TYR:HE2	1.42	0.84
1:C:98:ALA:H	1:C:105:ASN:ND2	1.76	0.83
1:H:394:GLU:OE2	1:H:471:PRO:HB3	1.78	0.82
1:G:225:THR:HG22	1:G:227:GLY:H	1.44	0.82
1:G:98:ALA:H	1:G:105:ASN:ND2	1.79	0.81
1:A:97:TRP:NE1	1:B:97:TRP:CD1	2.47	0.81
1:A:98:ALA:H	1:A:105:ASN:ND2	1.78	0.81
1:D:98:ALA:H	1:D:105:ASN:ND2	1.79	0.81
1:G:98:ALA:H	1:G:105:ASN:HD22	1.30	0.80
1:H:98:ALA:H	1:H:105:ASN:ND2	1.79	0.80
1:H:98:ALA:H	1:H:105:ASN:HD22	1.30	0.79
1:B:193:LEU:HA	1:C:127:GLU:OE1	1.82	0.79
1:C:98:ALA:H	1:C:105:ASN:HD22	1.30	0.79
1:G:238:PHE:CD1	1:H:182:PRO:HG3	2.18	0.79
1:E:129:LEU:HD23	1:H:193:LEU:HD23	1.65	0.79
1:B:132:ARG:NH1	1:D:129:LEU:HD22	1.98	0.78
1:E:98:ALA:H	1:E:105:ASN:ND2	1.81	0.78
1:F:98:ALA:H	1:F:105:ASN:HD22	1.32	0.78
1:F:98:ALA:H	1:F:105:ASN:ND2	1.83	0.77
1:B:269:ASN:ND2	1:B:380:LEU:HD13	2.00	0.77
1:D:98:ALA:H	1:D:105:ASN:HD22	1.30	0.77
1:B:98:ALA:H	1:B:105:ASN:HD22	1.33	0.77
1:E:98:ALA:H	1:E:105:ASN:HD22	1.31	0.76
1:E:182:PRO:HG3	1:F:238:PHE:CD1	2.21	0.76
1:B:98:ALA:H	1:B:105:ASN:ND2	1.84	0.75
1:A:98:ALA:H	1:A:105:ASN:HD22	1.30	0.75
1:B:273:GLU:OE1	1:B:379:SER:HB2	1.87	0.74
1:C:346:ARG:HG3	1:C:404:TYR:HE2	1.53	0.73
1:B:112:ASN:ND2	1:B:145:ARG:HH11	1.88	0.71
1:B:280:LEU:HD21	1:B:343:ILE:HD12	1.70	0.71
1:E:129:LEU:CD2	1:H:193:LEU:CD2	2.68	0.71
1:E:101:ASP:O	1:H:193:LEU:HD21	1.89	0.71
1:A:277:LEU:HB3	1:A:288:ILE:HD12	1.73	0.70
1:C:285:ILE:HD11	1:C:338:LEU:HG	1.73	0.70
1:G:277:LEU:HB3	1:G:288:ILE:HD12	1.73	0.70
1:B:193:LEU:HD23	1:C:127:GLU:OE1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PHE:HB2	1:A:190:ALA:HB3	1.74	0.69
1:H:112:ASN:ND2	1:H:145:ARG:HH11	1.90	0.69
1:H:281:ASN:HA	1:H:287:LYS:HE2	1.75	0.69
1:G:112:ASN:ND2	1:G:145:ARG:HH11	1.90	0.69
1:B:166:ASN:ND2	1:C:129:LEU:HD13	2.07	0.69
1:B:281:ASN:HA	1:B:287:LYS:HE2	1.74	0.69
1:D:112:ASN:ND2	1:D:145:ARG:HH11	1.90	0.69
1:D:225:THR:HG22	1:D:227:GLY:H	1.58	0.68
1:F:132:ARG:HD3	1:H:129:LEU:HD13	1.73	0.68
1:A:112:ASN:ND2	1:A:145:ARG:HH11	1.92	0.68
1:D:281:ASN:HA	1:D:287:LYS:HE2	1.74	0.68
1:G:169:PHE:HB2	1:G:190:ALA:HB3	1.75	0.68
1:A:129:LEU:HD22	1:D:193:LEU:CD2	2.22	0.67
1:D:169:PHE:HB2	1:D:190:ALA:HB3	1.77	0.67
1:F:166:ASN:HD22	1:G:129:LEU:HB2	1.58	0.67
1:C:292:PHE:HB2	1:C:298:TYR:HB2	1.76	0.67
1:A:330:GLN:NE2	1:A:364:ILE:H	1.92	0.67
1:C:277:LEU:HB3	1:C:288:ILE:HD12	1.76	0.67
1:A:277:LEU:HB3	1:A:288:ILE:CD1	2.25	0.67
1:E:346:ARG:HG3	1:E:404:TYR:CE2	2.17	0.67
1:F:281:ASN:HA	1:F:287:LYS:HE2	1.77	0.67
1:A:97:TRP:CZ2	1:B:97:TRP:CD1	2.83	0.66
1:B:478:GLU:HB2	1:B:482:ARG:NH1	2.09	0.66
1:F:112:ASN:ND2	1:F:145:ARG:HH11	1.91	0.66
1:B:225:THR:HG22	1:B:227:GLY:H	1.60	0.66
1:E:292:PHE:HB2	1:E:298:TYR:HB2	1.77	0.66
1:E:112:ASN:ND2	1:E:145:ARG:HH11	1.92	0.66
1:E:277:LEU:HB3	1:E:288:ILE:HD12	1.76	0.66
1:E:478:GLU:HB2	1:E:482:ARG:NH1	2.09	0.66
1:A:292:PHE:HB2	1:A:298:TYR:HB2	1.78	0.66
1:B:132:ARG:HH11	1:D:129:LEU:CD2	2.05	0.66
1:E:101:ASP:O	1:H:193:LEU:CD2	2.43	0.66
1:G:346:ARG:HG3	1:G:404:TYR:CE2	2.24	0.66
1:C:112:ASN:ND2	1:C:145:ARG:HH11	1.94	0.66
1:C:169:PHE:HB2	1:C:190:ALA:HB3	1.77	0.66
1:A:405:ASN:O	1:A:408:VAL:HG12	1.96	0.66
1:E:169:PHE:HB2	1:E:190:ALA:HB3	1.78	0.65
1:C:405:ASN:O	1:C:408:VAL:HG12	1.97	0.65
1:A:129:LEU:HD22	1:D:193:LEU:HG	1.76	0.65
1:G:277:LEU:HB3	1:G:288:ILE:CD1	2.27	0.65
1:H:169:PHE:HB2	1:H:190:ALA:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PHE:HB2	1:B:190:ALA:HB3	1.78	0.64
1:F:169:PHE:HB2	1:F:190:ALA:HB3	1.78	0.64
1:E:200:VAL:HG21	1:F:97:TRP:CH2	2.32	0.64
1:F:478:GLU:HB2	1:F:482:ARG:NH1	2.11	0.64
1:A:478:GLU:HB2	1:A:482:ARG:NH1	2.10	0.64
1:E:277:LEU:HB3	1:E:288:ILE:CD1	2.28	0.64
1:G:292:PHE:HB2	1:G:298:TYR:HB2	1.79	0.64
1:B:330:GLN:NE2	1:B:364:ILE:H	1.96	0.64
1:C:277:LEU:HB3	1:C:288:ILE:CD1	2.28	0.64
1:E:305:GLU:O	1:F:152:PRO:CG	2.46	0.64
1:H:330:GLN:NE2	1:H:364:ILE:H	1.96	0.64
1:H:346:ARG:HG3	1:H:404:TYR:CE2	2.25	0.64
1:A:478:GLU:OE2	1:E:456:SER:CB	2.46	0.63
1:G:330:GLN:NE2	1:G:364:ILE:H	1.96	0.63
1:C:182:PRO:HG3	1:D:238:PHE:CD1	2.34	0.63
1:H:405:ASN:O	1:H:408:VAL:HG12	1.99	0.63
1:E:405:ASN:O	1:E:408:VAL:HG12	1.99	0.63
1:F:346:ARG:HG3	1:F:404:TYR:HE2	1.64	0.63
1:B:166:ASN:HD21	1:C:129:LEU:CD1	2.10	0.63
1:B:166:ASN:O	1:C:128:PRO:HG2	1.98	0.63
1:E:304:MET:HE3	1:E:356:SER:HA	1.78	0.63
1:G:405:ASN:O	1:G:408:VAL:HG12	1.99	0.63
1:B:465:LYS:HD3	1:B:475:PHE:CE1	2.34	0.63
1:F:405:ASN:O	1:F:408:VAL:HG12	1.99	0.62
1:G:277:LEU:CB	1:G:288:ILE:HD12	2.29	0.62
1:E:129:LEU:CD2	1:H:193:LEU:HD21	2.27	0.62
1:A:129:LEU:HD23	1:D:193:LEU:HD21	0.69	0.62
1:C:478:GLU:HB2	1:C:482:ARG:NH1	2.11	0.62
1:H:478:GLU:HB2	1:H:482:ARG:NH1	2.11	0.62
1:D:405:ASN:O	1:D:408:VAL:HG12	1.99	0.62
1:C:330:GLN:NE2	1:C:364:ILE:H	1.99	0.61
1:F:330:GLN:NE2	1:F:364:ILE:H	1.97	0.61
1:A:277:LEU:CB	1:A:288:ILE:HD12	2.30	0.61
1:B:405:ASN:O	1:B:408:VAL:HG12	2.00	0.61
1:G:152:PRO:HG3	1:H:305:GLU:HG3	1.81	0.61
1:E:465:LYS:HD3	1:E:475:PHE:CE1	2.35	0.61
1:C:277:LEU:CB	1:C:288:ILE:HD12	2.30	0.61
1:G:465:LYS:HD3	1:G:475:PHE:CE1	2.35	0.61
1:D:330:GLN:NE2	1:D:364:ILE:H	1.99	0.61
1:H:280:LEU:HD21	1:H:343:ILE:HD12	1.83	0.61
1:H:335:VAL:HG21	1:H:413:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:NH1	1:D:129:LEU:HD13	2.16	0.61
1:E:330:GLN:NE2	1:E:364:ILE:H	1.98	0.61
1:A:465:LYS:HD3	1:A:475:PHE:CE1	2.36	0.60
1:B:269:ASN:ND2	1:B:380:LEU:CD1	2.63	0.60
1:D:465:LYS:HD3	1:D:475:PHE:CE1	2.36	0.60
1:F:465:LYS:HD3	1:F:475:PHE:CE1	2.36	0.60
1:A:129:LEU:CD2	1:D:193:LEU:CG	2.79	0.60
1:C:465:LYS:HD3	1:C:475:PHE:CE1	2.36	0.60
1:H:465:LYS:HD3	1:H:475:PHE:CE1	2.36	0.60
1:A:129:LEU:HD23	1:D:193:LEU:HD23	1.72	0.60
1:A:330:GLN:HE22	1:A:364:ILE:H	1.48	0.60
1:C:251:ILE:O	1:C:252:SER:HB3	2.02	0.60
1:E:277:LEU:CB	1:E:288:ILE:HD12	2.31	0.60
1:A:129:LEU:HD22	1:D:193:LEU:CG	2.32	0.60
1:A:251:ILE:O	1:A:252:SER:HB3	2.02	0.59
1:A:405:ASN:ND2	1:E:454:GLU:HB3	2.17	0.59
1:B:346:ARG:HD2	1:B:371:HIS:O	2.02	0.59
1:B:304:MET:HA	1:B:304:MET:CE	2.33	0.59
1:D:478:GLU:HB2	1:D:482:ARG:NH1	2.11	0.59
1:D:133:THR:O	1:D:135:LYS:N	2.35	0.59
1:E:350:PRO:HD3	1:E:416:ILE:HG12	1.84	0.58
1:E:251:ILE:O	1:E:252:SER:HB3	2.04	0.58
1:F:335:VAL:HG21	1:F:413:LEU:HD11	1.85	0.58
1:A:330:GLN:HE22	1:A:363:LEU:HA	1.69	0.58
1:F:330:GLN:HE22	1:F:363:LEU:HA	1.69	0.58
1:C:133:THR:O	1:C:135:LYS:N	2.35	0.57
1:A:346:ARG:HG3	1:A:404:TYR:CE2	2.28	0.57
1:D:304:MET:CE	1:D:304:MET:HA	2.34	0.57
1:B:330:GLN:HE22	1:B:364:ILE:H	1.52	0.57
1:G:330:GLN:HE22	1:G:363:LEU:HA	1.70	0.57
1:D:330:GLN:HE22	1:D:363:LEU:HA	1.69	0.56
1:G:251:ILE:O	1:G:252:SER:HB3	2.05	0.56
1:H:304:MET:HE3	1:H:304:MET:HA	1.87	0.56
1:A:225:THR:HG22	1:A:227:GLY:H	1.69	0.56
1:B:166:ASN:ND2	1:C:129:LEU:CB	2.63	0.56
1:G:133:THR:O	1:G:135:LYS:N	2.35	0.56
1:A:405:ASN:HD21	1:E:454:GLU:HB3	1.70	0.56
1:C:282:HIS:HD2	1:C:337:TYR:CD1	2.23	0.56
1:G:330:GLN:HE22	1:G:364:ILE:H	1.53	0.56
1:H:330:GLN:HE22	1:H:363:LEU:HA	1.70	0.56
1:C:95:ARG:HD3	1:C:97:TRP:HZ3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:LEU:HD22	1:E:364:ILE:HD11	1.87	0.56
1:H:330:GLN:HE22	1:H:364:ILE:H	1.53	0.56
1:C:355:LEU:HD22	1:C:364:ILE:HD11	1.87	0.56
1:B:355:LEU:HD22	1:B:364:ILE:HD11	1.87	0.56
1:E:305:GLU:HG3	1:F:152:PRO:HG3	1.87	0.55
1:F:304:MET:CE	1:F:304:MET:HA	2.36	0.55
1:B:330:GLN:HE22	1:B:363:LEU:HA	1.71	0.55
1:D:355:LEU:HD22	1:D:364:ILE:HD11	1.88	0.55
1:E:330:GLN:HE22	1:E:364:ILE:H	1.54	0.55
1:E:358:GLN:HE22	1:F:152:PRO:HB3	1.72	0.55
1:H:304:MET:HA	1:H:304:MET:CE	2.37	0.55
1:C:389:THR:O	1:C:391:LEU:N	2.39	0.55
1:F:355:LEU:HD22	1:F:364:ILE:HD11	1.88	0.55
1:D:280:LEU:HD21	1:D:343:ILE:HD12	1.89	0.55
1:H:304:MET:SD	1:H:365:LYS:HD2	2.47	0.55
1:A:97:TRP:CD1	1:B:97:TRP:CE2	2.96	0.54
1:B:171:ASN:O	1:B:172:THR:HB	2.06	0.54
1:A:296:ASP:O	1:A:297:TYR:HB2	2.06	0.54
1:B:346:ARG:NH1	1:B:371:HIS:ND1	2.55	0.54
1:F:304:MET:HA	1:F:304:MET:HE3	1.87	0.54
1:D:346:ARG:HG3	1:D:404:TYR:CE2	2.26	0.54
1:E:389:THR:O	1:E:391:LEU:N	2.40	0.54
1:H:355:LEU:HD22	1:H:364:ILE:HD11	1.89	0.54
1:C:330:GLN:HE22	1:C:363:LEU:HA	1.73	0.54
1:G:95:ARG:HD3	1:G:97:TRP:HZ3	1.72	0.54
1:C:296:ASP:O	1:C:297:TYR:HB2	2.08	0.54
1:F:133:THR:O	1:F:135:LYS:N	2.36	0.54
1:A:389:THR:O	1:A:391:LEU:N	2.40	0.54
1:G:225:THR:HG22	1:G:227:GLY:N	2.19	0.54
1:F:95:ARG:HD3	1:F:97:TRP:HZ3	1.72	0.54
1:D:284:CYS:CB	1:D:334:ALA:HB2	2.38	0.54
1:G:355:LEU:HD22	1:G:364:ILE:HD11	1.90	0.53
1:D:292:PHE:HB2	1:D:298:TYR:HB2	1.90	0.53
1:F:292:PHE:HB2	1:F:298:TYR:HB2	1.90	0.53
1:B:273:GLU:OE2	1:B:380:LEU:N	2.41	0.53
1:A:133:THR:O	1:A:135:LYS:N	2.35	0.53
1:C:171:ASN:O	1:C:172:THR:HB	2.09	0.53
1:E:330:GLN:HE22	1:E:363:LEU:HA	1.72	0.53
1:G:296:ASP:O	1:G:297:TYR:HB2	2.08	0.53
1:A:97:TRP:CE2	1:B:97:TRP:NE1	2.68	0.53
1:G:389:THR:O	1:G:391:LEU:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HD3	1:A:97:TRP:HZ3	1.73	0.53
1:D:304:MET:HA	1:D:304:MET:HE3	1.91	0.53
1:H:292:PHE:HB2	1:H:298:TYR:HB2	1.91	0.53
1:E:95:ARG:HD3	1:E:97:TRP:HZ3	1.73	0.53
1:B:346:ARG:HG3	1:B:404:TYR:CE2	2.33	0.53
1:D:95:ARG:HD3	1:D:97:TRP:HZ3	1.74	0.53
1:E:238:PHE:CD1	1:F:182:PRO:HG3	2.44	0.53
1:E:346:ARG:CG	1:E:404:TYR:HE2	2.11	0.53
1:F:330:GLN:HE22	1:F:364:ILE:H	1.55	0.52
1:A:171:ASN:O	1:A:172:THR:HB	2.09	0.52
1:E:296:ASP:O	1:E:297:TYR:HB2	2.08	0.52
1:G:152:PRO:HD2	1:G:153:LYS:HZ2	1.74	0.52
1:F:132:ARG:CD	1:H:129:LEU:CD1	2.61	0.52
1:G:284:CYS:SG	1:G:330:GLN:HB3	2.50	0.52
1:H:284:CYS:CB	1:H:334:ALA:HB2	2.39	0.52
1:B:209:GLN:O	1:B:217:ARG:HD2	2.08	0.52
1:F:171:ASN:O	1:F:172:THR:HB	2.09	0.52
1:H:95:ARG:HD3	1:H:97:TRP:HZ3	1.74	0.52
1:H:152:PRO:HD2	1:H:153:LYS:HZ2	1.75	0.52
1:C:282:HIS:CD2	1:C:337:TYR:CG	2.98	0.52
1:G:304:MET:HE3	1:G:356:SER:HA	1.92	0.52
1:A:355:LEU:HD22	1:A:364:ILE:HD11	1.89	0.52
1:A:482:ARG:NH2	1:E:458:LYS:NZ	2.58	0.52
1:D:330:GLN:HE22	1:D:364:ILE:H	1.57	0.52
1:E:171:ASN:O	1:E:172:THR:HB	2.10	0.52
1:F:304:MET:HB3	1:F:355:LEU:O	2.10	0.52
1:F:417:LEU:HD13	1:F:463:VAL:HG22	1.91	0.52
1:C:417:LEU:HD13	1:C:463:VAL:HG22	1.92	0.51
1:B:133:THR:O	1:B:135:LYS:N	2.37	0.51
1:B:95:ARG:HD3	1:B:97:TRP:HZ3	1.74	0.51
1:G:152:PRO:HB2	1:H:305:GLU:O	2.10	0.51
1:C:253:LYS:HE2	1:C:253:LYS:C	2.31	0.51
1:C:330:GLN:HE22	1:C:364:ILE:H	1.57	0.51
1:E:203:ASP:HB3	1:E:206:VAL:CG2	2.41	0.51
1:G:478:GLU:HB2	1:G:482:ARG:NH1	2.18	0.51
1:B:112:ASN:HD21	1:B:145:ARG:HH11	1.59	0.51
1:C:350:PRO:HD3	1:C:416:ILE:HG12	1.92	0.51
1:H:171:ASN:O	1:H:172:THR:HB	2.10	0.51
1:A:284:CYS:SG	1:A:330:GLN:HB3	2.51	0.51
1:E:277:LEU:CB	1:E:288:ILE:CD1	2.89	0.51
1:A:286:ILE:HG13	1:A:367:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:ARG:HG3	1:G:104:ALA:HB1	1.92	0.50
1:G:489:GLU:HA	1:G:492:LYS:HB2	1.93	0.50
1:H:296:ASP:O	1:H:297:TYR:HB2	2.10	0.50
1:B:296:ASP:O	1:B:297:TYR:HB2	2.11	0.50
1:F:491:MET:C	1:F:491:MET:HE3	2.31	0.50
1:H:346:ARG:HD2	1:H:371:HIS:O	2.12	0.50
1:H:350:PRO:HD3	1:H:416:ILE:HG12	1.93	0.50
1:D:296:ASP:O	1:D:297:TYR:HB2	2.11	0.50
1:G:277:LEU:CB	1:G:288:ILE:CD1	2.89	0.50
1:E:133:THR:O	1:E:135:LYS:N	2.38	0.50
1:G:95:ARG:HG3	1:G:204:LEU:HD11	1.94	0.50
1:D:171:ASN:O	1:D:172:THR:HB	2.10	0.50
1:F:95:ARG:HG3	1:F:204:LEU:HD11	1.94	0.50
1:F:489:GLU:HA	1:F:492:LYS:HB2	1.94	0.50
1:C:284:CYS:CB	1:C:334:ALA:HB2	2.42	0.49
1:D:284:CYS:HB3	1:D:334:ALA:HB2	1.94	0.49
1:E:417:LEU:HD13	1:E:463:VAL:HG22	1.94	0.49
1:A:417:LEU:HD13	1:A:463:VAL:HG22	1.94	0.49
1:A:489:GLU:HA	1:A:492:LYS:HB2	1.94	0.49
1:B:292:PHE:HB2	1:B:298:TYR:HB2	1.93	0.49
1:D:417:LEU:HD13	1:D:463:VAL:HG22	1.94	0.49
1:H:328:PHE:CD1	1:H:417:LEU:HG	2.47	0.49
1:G:285:ILE:HD11	1:G:338:LEU:HG	1.93	0.49
1:D:95:ARG:HG3	1:D:204:LEU:HD11	1.94	0.49
1:D:350:PRO:HD3	1:D:416:ILE:HG12	1.94	0.49
1:D:489:GLU:HA	1:D:492:LYS:HB2	1.95	0.49
1:A:395:VAL:HG12	1:A:395:VAL:O	2.12	0.49
1:F:166:ASN:HD21	1:G:129:LEU:HD13	1.77	0.49
1:A:277:LEU:CB	1:A:288:ILE:CD1	2.88	0.49
1:E:349:LYS:HB2	1:E:350:PRO:HD2	1.95	0.49
1:H:162:ASP:HB3	1:H:176:GLY:O	2.13	0.49
1:C:489:GLU:HA	1:C:492:LYS:HB2	1.94	0.49
1:A:417:LEU:HD13	1:A:463:VAL:CG2	2.43	0.49
1:B:95:ARG:HG3	1:B:204:LEU:HD11	1.94	0.49
1:F:346:ARG:HD2	1:F:371:HIS:O	2.13	0.48
1:A:458:LYS:H	1:A:458:LYS:HG2	1.47	0.48
1:C:417:LEU:HD13	1:C:463:VAL:CG2	2.43	0.48
1:D:152:PRO:HD2	1:D:153:LYS:HZ2	1.78	0.48
1:E:152:PRO:HD2	1:E:153:LYS:HZ2	1.78	0.48
1:F:491:MET:HE3	1:F:491:MET:O	2.14	0.48
1:G:171:ASN:O	1:G:172:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LEU:HD13	1:B:463:VAL:HG22	1.96	0.48
1:E:417:LEU:HD13	1:E:463:VAL:CG2	2.43	0.48
1:E:489:GLU:HA	1:E:492:LYS:HB2	1.94	0.48
1:G:284:CYS:HA	1:G:364:ILE:O	2.13	0.48
1:H:489:GLU:HA	1:H:492:LYS:HB2	1.95	0.48
1:E:95:ARG:HG3	1:E:204:LEU:HD11	1.94	0.48
1:C:277:LEU:CB	1:C:288:ILE:CD1	2.89	0.48
1:F:417:LEU:HD13	1:F:463:VAL:CG2	2.42	0.48
1:G:395:VAL:HG12	1:G:395:VAL:O	2.13	0.48
1:A:129:LEU:CD2	1:D:193:LEU:HD23	2.34	0.48
1:B:489:GLU:HA	1:B:492:LYS:HB2	1.94	0.48
1:D:335:VAL:HG21	1:D:413:LEU:HD11	1.96	0.48
1:E:305:GLU:O	1:F:152:PRO:HG2	2.13	0.48
1:H:95:ARG:HG3	1:H:204:LEU:HD11	1.95	0.48
1:B:270:VAL:HG13	1:B:380:LEU:HB2	1.96	0.48
1:B:273:GLU:CD	1:B:379:SER:HB2	2.34	0.48
1:H:133:THR:O	1:H:135:LYS:N	2.36	0.48
1:D:417:LEU:HD13	1:D:463:VAL:CG2	2.44	0.48
1:F:296:ASP:O	1:F:297:TYR:HB2	2.14	0.48
1:C:95:ARG:HG3	1:C:204:LEU:HD11	1.96	0.47
1:C:162:ASP:HB3	1:C:176:GLY:O	2.14	0.47
1:G:112:ASN:HD21	1:G:145:ARG:HH11	1.61	0.47
1:H:417:LEU:HD13	1:H:463:VAL:HG22	1.95	0.47
1:B:286:ILE:HG21	1:B:367:THR:HG23	1.97	0.47
1:C:207:ASP:OD1	1:C:223:SER:HA	2.14	0.47
1:E:173:GLU:CD	1:F:240:ARG:HH21	2.17	0.47
1:E:304:MET:HB3	1:E:355:LEU:O	2.15	0.47
1:H:284:CYS:HB3	1:H:334:ALA:HB2	1.95	0.47
1:D:457:GLU:OE2	1:H:119:LYS:CD	2.51	0.47
1:F:132:ARG:HH11	1:H:129:LEU:HB2	1.79	0.47
1:H:417:LEU:HD13	1:H:463:VAL:CG2	2.45	0.47
1:B:280:LEU:HD21	1:B:343:ILE:CD1	2.41	0.47
1:D:112:ASN:HD21	1:D:145:ARG:HH11	1.61	0.47
1:G:152:PRO:CB	1:H:305:GLU:O	2.62	0.47
1:H:349:LYS:HB2	1:H:350:PRO:HD2	1.97	0.47
1:C:355:LEU:CD2	1:C:364:ILE:HD11	2.45	0.47
1:B:458:LYS:H	1:B:458:LYS:HG2	1.47	0.47
1:E:152:PRO:HG3	1:F:305:GLU:HG3	1.96	0.47
1:E:458:LYS:H	1:E:458:LYS:HG2	1.47	0.47
1:F:166:ASN:ND2	1:G:129:LEU:HD13	2.30	0.47
1:F:225:THR:HG22	1:F:227:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:CYS:HA	1:A:364:ILE:O	2.15	0.46
1:G:349:LYS:HB2	1:G:350:PRO:HD2	1.97	0.46
1:H:203:ASP:HB3	1:H:206:VAL:HG23	1.96	0.46
1:F:458:LYS:H	1:F:458:LYS:HG2	1.47	0.46
1:H:203:ASP:HB3	1:H:206:VAL:CG2	2.45	0.46
1:E:358:GLN:NE2	1:F:152:PRO:HB3	2.30	0.46
1:E:253:LYS:C	1:E:253:LYS:HE2	2.36	0.46
1:C:284:CYS:HB3	1:C:334:ALA:HB2	1.98	0.46
1:D:349:LYS:HB2	1:D:350:PRO:HD2	1.97	0.46
1:G:253:LYS:C	1:G:253:LYS:HE2	2.36	0.46
1:G:417:LEU:HD13	1:G:463:VAL:HG22	1.96	0.46
1:H:112:ASN:HD21	1:H:145:ARG:HH11	1.62	0.46
1:D:346:ARG:HD2	1:D:371:HIS:O	2.16	0.46
1:E:200:VAL:HG21	1:F:97:TRP:HH2	1.76	0.46
1:B:417:LEU:HD13	1:B:463:VAL:CG2	2.46	0.46
1:H:348:LEU:HB3	1:H:412:SER:HB3	1.97	0.46
1:B:162:ASP:HB3	1:B:176:GLY:O	2.15	0.45
1:C:395:VAL:HG12	1:C:395:VAL:O	2.15	0.45
1:A:152:PRO:HD2	1:A:153:LYS:HZ2	1.81	0.45
1:C:304:MET:HE2	1:C:356:SER:HB3	1.96	0.45
1:F:112:ASN:HD21	1:F:145:ARG:HH11	1.62	0.45
1:A:162:ASP:HB2	1:A:175:VAL:HB	1.98	0.45
1:E:112:ASN:HD21	1:E:145:ARG:HH11	1.64	0.45
1:E:345:HIS:CG	1:E:348:LEU:HD13	2.51	0.45
1:B:345:HIS:CG	1:B:348:LEU:HD13	2.51	0.45
1:F:328:PHE:CD1	1:F:417:LEU:HG	2.50	0.45
1:G:304:MET:CE	1:G:356:SER:HA	2.46	0.45
1:A:253:LYS:HE2	1:A:253:LYS:C	2.37	0.45
1:A:345:HIS:CG	1:A:348:LEU:HD13	2.52	0.45
1:D:227:GLY:C	1:D:234:VAL:HG12	2.37	0.45
1:E:358:GLN:HE22	1:F:152:PRO:CB	2.30	0.45
1:C:345:HIS:CG	1:C:348:LEU:HD13	2.52	0.45
1:D:395:VAL:HG12	1:D:395:VAL:O	2.17	0.45
1:E:395:VAL:HG12	1:E:395:VAL:O	2.17	0.45
1:F:395:VAL:HG12	1:F:395:VAL:O	2.17	0.45
1:B:395:VAL:O	1:B:395:VAL:HG12	2.16	0.45
1:C:290:ASN:OD1	1:C:291:PHE:N	2.50	0.45
1:G:152:PRO:HG3	1:H:305:GLU:CG	2.45	0.45
1:G:221:ILE:HG21	1:H:182:PRO:HG2	1.99	0.45
1:G:417:LEU:HD13	1:G:463:VAL:CG2	2.46	0.45
1:A:491:MET:HE2	1:A:492:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASP:HB2	1:B:175:VAL:HB	2.00	0.44
1:C:304:MET:SD	1:C:365:LYS:HD2	2.57	0.44
1:H:395:VAL:HG12	1:H:395:VAL:O	2.17	0.44
1:E:162:ASP:HB2	1:E:175:VAL:HB	2.00	0.44
1:A:478:GLU:OE2	1:E:456:SER:CA	2.65	0.44
1:D:284:CYS:HB2	1:D:334:ALA:HB2	2.00	0.44
1:D:457:GLU:HG3	1:H:126:ASP:OD2	2.18	0.44
1:E:129:LEU:HD13	1:H:166:ASN:HD22	1.83	0.44
1:E:491:MET:HE2	1:E:492:LYS:HA	2.00	0.44
1:G:491:MET:HE2	1:G:492:LYS:HA	1.99	0.44
1:C:282:HIS:CG	1:C:283:PRO:HD2	2.53	0.44
1:F:95:ARG:HD3	1:F:97:TRP:CZ3	2.53	0.44
1:F:162:ASP:HB2	1:F:175:VAL:HB	2.00	0.44
1:G:233:GLU:HG3	1:G:250:ILE:HB	2.00	0.44
1:G:450:GLU:H	1:G:450:GLU:HG3	1.52	0.44
1:H:339:HIS:CG	1:H:406:ARG:HD2	2.53	0.44
1:C:335:VAL:HG21	1:C:413:LEU:HD11	1.99	0.44
1:F:345:HIS:CG	1:F:348:LEU:HD13	2.53	0.44
1:A:95:ARG:HG3	1:A:204:LEU:HD11	2.00	0.43
1:D:345:HIS:CG	1:D:348:LEU:HD13	2.53	0.43
1:F:162:ASP:HB3	1:F:176:GLY:O	2.18	0.43
1:A:225:THR:HG22	1:A:227:GLY:N	2.32	0.43
1:B:132:ARG:HG3	1:D:101:ASP:OD1	2.18	0.43
1:C:95:ARG:HD3	1:C:97:TRP:CZ3	2.51	0.43
1:A:393:PRO:HD3	1:A:411:TRP:CD2	2.54	0.43
1:D:304:MET:SD	1:D:365:LYS:HD2	2.59	0.43
1:A:162:ASP:HB3	1:A:176:GLY:O	2.18	0.43
1:C:282:HIS:CD2	1:C:337:TYR:HB2	2.53	0.43
1:C:162:ASP:HB2	1:C:175:VAL:HB	2.01	0.43
1:C:282:HIS:HD2	1:C:337:TYR:CG	2.36	0.43
1:D:324:CYS:SG	1:D:420:CYS:HB3	2.59	0.43
1:G:325:LYS:NZ	1:G:488:ASP:OD2	2.47	0.43
1:G:95:ARG:HD3	1:G:97:TRP:CZ3	2.53	0.43
1:H:284:CYS:HB2	1:H:334:ALA:HB2	2.01	0.43
1:B:152:PRO:HD2	1:B:153:LYS:HZ2	1.83	0.43
1:F:193:LEU:HD23	1:G:127:GLU:OE1	2.19	0.43
1:H:458:LYS:H	1:H:458:LYS:HG2	1.47	0.43
1:A:285:ILE:HD11	1:A:338:LEU:HG	2.01	0.43
1:A:304:MET:HB2	1:A:354:LEU:HD13	2.00	0.43
1:A:349:LYS:HB2	1:A:350:PRO:HD2	2.01	0.42
1:E:186:ASN:OD1	1:F:204:LEU:HD22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:PRO:CG	1:H:305:GLU:O	2.67	0.42
1:G:339:HIS:CG	1:G:406:ARG:HD2	2.54	0.42
1:A:233:GLU:HG3	1:A:250:ILE:HB	2.01	0.42
1:C:152:PRO:HD2	1:C:153:LYS:HZ2	1.82	0.42
1:B:140:SER:HB2	1:B:143:HIS:HA	2.01	0.42
1:E:290:ASN:OD1	1:E:291:PHE:N	2.53	0.42
1:G:162:ASP:HB2	1:G:175:VAL:HB	2.00	0.42
1:G:243:CYS:SG	1:H:180:ARG:O	2.78	0.42
1:H:345:HIS:CG	1:H:348:LEU:HD13	2.54	0.42
1:D:162:ASP:HB2	1:D:175:VAL:HB	2.00	0.42
1:D:209:GLN:O	1:D:217:ARG:HD2	2.20	0.42
1:F:290:ASN:HB3	1:F:300:VAL:HB	2.02	0.42
1:H:205:THR:HA	1:H:208:ASP:HB2	2.00	0.42
1:A:290:ASN:OD1	1:A:291:PHE:N	2.52	0.42
1:C:233:GLU:HG3	1:C:250:ILE:HB	2.01	0.42
1:A:393:PRO:HD3	1:A:411:TRP:CE2	2.54	0.42
1:A:450:GLU:H	1:A:450:GLU:HG3	1.49	0.42
1:E:305:GLU:O	1:F:152:PRO:HB2	2.19	0.42
1:E:324:CYS:SG	1:E:420:CYS:HB3	2.60	0.42
1:B:328:PHE:CD1	1:B:417:LEU:HG	2.55	0.42
1:H:162:ASP:HB2	1:H:175:VAL:HB	2.00	0.42
1:C:458:LYS:H	1:C:458:LYS:HG2	1.43	0.42
1:C:491:MET:HE2	1:C:492:LYS:HA	2.02	0.42
1:C:207:ASP:HB3	1:D:184:ASN:ND2	2.35	0.41
1:D:458:LYS:H	1:D:458:LYS:HG2	1.48	0.41
1:B:355:LEU:CD2	1:B:364:ILE:HD11	2.50	0.41
1:D:271:GLU:HG2	1:D:291:PHE:CE2	2.55	0.41
1:G:290:ASN:OD1	1:G:291:PHE:N	2.53	0.41
1:B:143:HIS:CD2	1:B:164:SER:HB3	2.55	0.41
1:B:324:CYS:SG	1:B:420:CYS:HB3	2.60	0.41
1:C:143:HIS:CD2	1:C:164:SER:HB3	2.55	0.41
1:C:282:HIS:CD2	1:C:337:TYR:CB	3.02	0.41
1:B:349:LYS:HB2	1:B:350:PRO:HD2	2.01	0.41
1:E:233:GLU:HG3	1:E:250:ILE:HB	2.02	0.41
1:F:450:GLU:H	1:F:450:GLU:HG3	1.51	0.41
1:G:345:HIS:CG	1:G:348:LEU:HD13	2.56	0.41
1:H:95:ARG:HD3	1:H:97:TRP:CZ3	2.55	0.41
1:H:450:GLU:H	1:H:450:GLU:HG3	1.51	0.41
1:B:194:SER:H	1:C:127:GLU:CD	2.24	0.41
1:B:290:ASN:HB3	1:B:300:VAL:HB	2.03	0.41
1:E:162:ASP:HB3	1:E:176:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:THR:HG22	1:H:227:GLY:H	1.85	0.41
1:H:346:ARG:NH1	1:H:371:HIS:ND1	2.68	0.41
1:A:287:LYS:HA	1:A:287:LYS:HD3	1.94	0.41
1:A:324:CYS:SG	1:A:420:CYS:HB3	2.61	0.41
1:E:331:MET:CE	1:E:413:LEU:HD22	2.50	0.41
1:A:140:SER:HB2	1:A:143:HIS:HA	2.02	0.41
1:C:491:MET:HE3	1:C:491:MET:O	2.19	0.41
1:E:220:TYR:HA	1:E:238:PHE:O	2.21	0.41
1:G:220:TYR:HA	1:G:238:PHE:O	2.21	0.41
1:A:97:TRP:CZ2	1:B:97:TRP:HD1	2.37	0.41
1:C:253:LYS:H	1:C:253:LYS:HG3	1.73	0.41
1:E:305:GLU:O	1:F:152:PRO:CB	2.69	0.41
1:G:466:LEU:HD12	1:G:466:LEU:HA	1.96	0.41
1:H:140:SER:HB2	1:H:143:HIS:HA	2.03	0.41
1:B:269:ASN:HD21	1:B:380:LEU:HD13	1.83	0.41
1:G:162:ASP:HB3	1:G:176:GLY:O	2.21	0.41
1:B:335:VAL:HG21	1:B:413:LEU:HD11	2.01	0.40
1:C:237:ALA:HB3	1:C:246:VAL:HG23	2.03	0.40
1:C:284:CYS:HB2	1:C:334:ALA:HB2	2.02	0.40
1:D:238:PHE:CE2	1:D:245:LYS:HG2	2.56	0.40
1:G:431:ARG:HB3	1:G:432:THR:H	1.77	0.40
1:C:226:LEU:HD22	1:D:153:LYS:HG2	2.02	0.40
1:D:277:LEU:HB3	1:D:288:ILE:HD12	2.03	0.40
1:A:112:ASN:HD21	1:A:145:ARG:HH11	1.65	0.40
1:A:305:GLU:C	1:A:307:GLY:H	2.25	0.40
1:C:287:LYS:HA	1:C:287:LYS:HD3	1.97	0.40
1:D:392:ALA:HA	1:D:393:PRO:HD3	1.95	0.40
1:E:129:LEU:HD13	1:H:166:ASN:ND2	2.37	0.40
1:F:364:ILE:HD12	1:F:364:ILE:HA	1.91	0.40
1:G:287:LYS:HA	1:G:287:LYS:HD3	1.95	0.40
1:G:324:CYS:SG	1:G:420:CYS:HB3	2.60	0.40
1:E:96:LEU:HD23	1:E:96:LEU:HA	1.94	0.40
1:B:364:ILE:HD12	1:B:364:ILE:HA	1.90	0.40
1:C:329:TYR:CE1	1:C:492:LYS:HE2	2.57	0.40
1:D:392:ALA:HB2	1:D:408:VAL:HG23	2.03	0.40
1:E:101:ASP:C	1:H:193:LEU:HD21	2.42	0.40
1:F:132:ARG:HH11	1:H:129:LEU:HD13	1.86	0.40
1:H:143:HIS:CD2	1:H:164:SER:HB3	2.57	0.40
1:H:392:ALA:HA	1:H:393:PRO:HD3	1.96	0.40

All (20) 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:G:320:LYS:CD	1:H:457:GLU:OE2[1_455]	0.80	1.40
1:C:138:THR:CG2	1:C:496:GLN:NE2[1_655]	1.64	0.56
1:E:137:ARG:CD	1:F:450:GLU:CG[1_455]	1.64	0.56
1:G:320:LYS:CE	1:H:457:GLU:OE2[1_455]	1.71	0.49
1:A:195:ARG:O	1:F:493:ARG:NH1[1_456]	1.73	0.47
1:C:166:ASN:ND2	1:C:496:GLN:OE1[1_655]	1.76	0.44
1:G:320:LYS:CG	1:H:457:GLU:OE2[1_455]	1.76	0.44
1:E:137:ARG:CG	1:F:450:GLU:OE2[1_455]	1.78	0.42
1:A:178:GLY:O	1:A:490:ASP:OD1[1_455]	1.81	0.39
1:E:137:ARG:NE	1:F:450:GLU:CD[1_455]	1.89	0.31
1:A:161:GLU:OE2	1:A:493:ARG:NH1[1_455]	1.90	0.30
1:A:178:GLY:C	1:A:490:ASP:OD1[1_455]	1.94	0.26
1:A:197:LYS:NZ	1:F:489:GLU:OE2[1_456]	1.99	0.21
1:E:137:ARG:NE	1:F:450:GLU:OE2[1_455]	2.00	0.20
1:G:320:LYS:CD	1:H:457:GLU:CD[1_455]	2.02	0.18
1:A:450:GLU:OE2	1:C:464:LYS:NZ[1_665]	2.03	0.17
1:E:137:ARG:CD	1:F:450:GLU:CD[1_455]	2.05	0.15
1:C:138:THR:CB	1:C:496:GLN:NE2[1_655]	2.09	0.11
1:C:457:GLU:OE1	1:G:482:ARG:NH2[1_456]	2.12	0.08
1:E:137:ARG:CD	1:F:450:GLU:OE2[1_455]	2.15	0.05

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	359/443 (81%)	326 (91%)	23 (6%)	10 (3%)	5 25
1	B	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	8 34
1	C	358/443 (81%)	326 (91%)	21 (6%)	11 (3%)	4 24
1	D	372/443 (84%)	334 (90%)	31 (8%)	7 (2%)	8 34
1	E	358/443 (81%)	327 (91%)	21 (6%)	10 (3%)	5 25
1	F	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	8 34
1	G	359/443 (81%)	328 (91%)	21 (6%)	10 (3%)	5 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	372/443 (84%)	335 (90%)	30 (8%)	7 (2%)	8 34
All	All	2922/3544 (82%)	2650 (91%)	203 (7%)	69 (2%)	6 28

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	390	TYR
1	A	433	GLN
1	B	134	ASP
1	B	433	GLN
1	C	134	ASP
1	C	390	TYR
1	C	433	GLN
1	D	134	ASP
1	D	433	GLN
1	E	134	ASP
1	E	390	TYR
1	E	433	GLN
1	F	134	ASP
1	F	433	GLN
1	G	134	ASP
1	G	390	TYR
1	G	433	GLN
1	H	134	ASP
1	H	433	GLN
1	A	252	SER
1	A	295	GLU
1	A	434	VAL
1	B	434	VAL
1	C	295	GLU
1	C	434	VAL
1	D	434	VAL
1	E	434	VAL
1	F	434	VAL
1	G	252	SER
1	G	434	VAL
1	H	434	VAL
1	B	251	ILE
1	B	271	GLU
1	C	252	SER
1	D	271	GLU

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Mol	Chain	Res	Type
1	E	252	SER
1	E	295	GLU
1	F	271	GLU
1	G	295	GLU
1	H	251	ILE
1	H	271	GLU
1	A	430	HIS
1	C	430	HIS
1	D	251	ILE
1	E	430	HIS
1	F	251	ILE
1	G	430	HIS
1	B	430	HIS
1	C	368	ASP
1	D	430	HIS
1	E	368	ASP
1	F	430	HIS
1	H	430	HIS
1	A	297	TYR
1	C	297	TYR
1	G	297	TYR
1	A	270	VAL
1	G	270	VAL
1	C	270	VAL
1	E	270	VAL
1	C	152	PRO
1	A	152	PRO
1	B	152	PRO
1	D	152	PRO
1	E	152	PRO
1	F	152	PRO
1	G	152	PRO
1	H	152	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	333/395 (84%)	303 (91%)	30 (9%)	9	32
1	B	344/395 (87%)	311 (90%)	33 (10%)	8	29
1	C	333/395 (84%)	302 (91%)	31 (9%)	9	30
1	D	344/395 (87%)	312 (91%)	32 (9%)	9	30
1	E	333/395 (84%)	303 (91%)	30 (9%)	9	32
1	F	344/395 (87%)	312 (91%)	32 (9%)	9	30
1	G	333/395 (84%)	302 (91%)	31 (9%)	9	30
1	H	344/395 (87%)	312 (91%)	32 (9%)	9	30
All	All	2708/3160 (86%)	2457 (91%)	251 (9%)	9	30

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	TRP
1	A	101	ASP
1	A	153	LYS
1	A	205	THR
1	A	253	LYS
1	A	295	GLU
1	A	303	LEU
1	A	313	VAL
1	A	318	ARG
1	A	364	ILE
1	A	367	THR
1	A	390	TYR
1	A	391	LEU
1	A	404	TYR
1	A	406	ARG
1	A	417	LEU
1	A	441	THR
1	A	444	LYS
1	A	450	GLU
1	A	458	LYS
1	A	460	LEU
1	A	462	LEU
1	A	472	LYS
1	A	475	PHE
1	A	477	THR
1	A	478	GLU
1	A	486	LEU

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Mol	Chain	Res	Type
1	A	487	GLN
1	A	490	ASP
1	A	491	MET
1	B	97	TRP
1	B	101	ASP
1	B	153	LYS
1	B	205	THR
1	B	223	SER
1	B	226	LEU
1	B	253	LYS
1	B	269	ASN
1	B	286	ILE
1	B	295	GLU
1	B	304	MET
1	B	313	VAL
1	B	318	ARG
1	B	364	ILE
1	B	367	THR
1	B	373	LYS
1	B	404	TYR
1	B	406	ARG
1	B	417	LEU
1	B	441	THR
1	B	444	LYS
1	B	450	GLU
1	B	458	LYS
1	B	460	LEU
1	B	462	LEU
1	B	472	LYS
1	B	475	PHE
1	B	477	THR
1	B	478	GLU
1	B	486	LEU
1	B	487	GLN
1	B	490	ASP
1	B	491	MET
1	C	97	TRP
1	C	153	LYS
1	C	205	THR
1	C	253	LYS
1	C	295	GLU
1	C	303	LEU

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Mol	Chain	Res	Type
1	C	304	MET
1	C	313	VAL
1	C	318	ARG
1	C	364	ILE
1	C	367	THR
1	C	369	PHE
1	C	390	TYR
1	C	391	LEU
1	C	404	TYR
1	C	406	ARG
1	C	417	LEU
1	C	441	THR
1	C	444	LYS
1	C	450	GLU
1	C	458	LYS
1	C	460	LEU
1	C	462	LEU
1	C	472	LYS
1	C	475	PHE
1	C	477	THR
1	C	478	GLU
1	C	486	LEU
1	C	487	GLN
1	C	490	ASP
1	C	491	MET
1	D	97	TRP
1	D	101	ASP
1	D	153	LYS
1	D	205	THR
1	D	226	LEU
1	D	253	LYS
1	D	269	ASN
1	D	286	ILE
1	D	295	GLU
1	D	304	MET
1	D	313	VAL
1	D	318	ARG
1	D	364	ILE
1	D	367	THR
1	D	373	LYS
1	D	404	TYR
1	D	406	ARG

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Mol	Chain	Res	Type
1	D	417	LEU
1	D	441	THR
1	D	444	LYS
1	D	450	GLU
1	D	458	LYS
1	D	460	LEU
1	D	462	LEU
1	D	472	LYS
1	D	475	PHE
1	D	477	THR
1	D	478	GLU
1	D	486	LEU
1	D	487	GLN
1	D	490	ASP
1	D	491	MET
1	E	97	TRP
1	E	101	ASP
1	E	153	LYS
1	E	205	THR
1	E	253	LYS
1	E	295	GLU
1	E	303	LEU
1	E	313	VAL
1	E	318	ARG
1	E	364	ILE
1	E	367	THR
1	E	390	TYR
1	E	391	LEU
1	E	404	TYR
1	E	406	ARG
1	E	417	LEU
1	E	441	THR
1	E	444	LYS
1	E	450	GLU
1	E	458	LYS
1	E	460	LEU
1	E	462	LEU
1	E	472	LYS
1	E	475	PHE
1	E	477	THR
1	E	478	GLU
1	E	486	LEU

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Mol	Chain	Res	Type
1	E	487	GLN
1	E	490	ASP
1	E	491	MET
1	F	97	TRP
1	F	101	ASP
1	F	153	LYS
1	F	205	THR
1	F	226	LEU
1	F	253	LYS
1	F	269	ASN
1	F	286	ILE
1	F	295	GLU
1	F	304	MET
1	F	313	VAL
1	F	318	ARG
1	F	364	ILE
1	F	367	THR
1	F	373	LYS
1	F	404	TYR
1	F	406	ARG
1	F	417	LEU
1	F	441	THR
1	F	444	LYS
1	F	450	GLU
1	F	458	LYS
1	F	460	LEU
1	F	462	LEU
1	F	472	LYS
1	F	475	PHE
1	F	477	THR
1	F	478	GLU
1	F	486	LEU
1	F	487	GLN
1	F	490	ASP
1	F	491	MET
1	G	97	TRP
1	G	101	ASP
1	G	153	LYS
1	G	205	THR
1	G	253	LYS
1	G	295	GLU
1	G	303	LEU

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Mol	Chain	Res	Type
1	G	313	VAL
1	G	318	ARG
1	G	364	ILE
1	G	367	THR
1	G	369	PHE
1	G	390	TYR
1	G	391	LEU
1	G	404	TYR
1	G	406	ARG
1	G	417	LEU
1	G	441	THR
1	G	444	LYS
1	G	450	GLU
1	G	458	LYS
1	G	460	LEU
1	G	462	LEU
1	G	472	LYS
1	G	475	PHE
1	G	477	THR
1	G	478	GLU
1	G	486	LEU
1	G	487	GLN
1	G	490	ASP
1	G	491	MET
1	H	97	TRP
1	H	101	ASP
1	H	153	LYS
1	H	205	THR
1	H	226	LEU
1	H	253	LYS
1	H	269	ASN
1	H	286	ILE
1	H	295	GLU
1	H	304	MET
1	H	313	VAL
1	H	318	ARG
1	H	364	ILE
1	H	367	THR
1	H	373	LYS
1	H	404	TYR
1	H	406	ARG
1	H	417	LEU

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Mol	Chain	Res	Type
1	H	441	THR
1	H	444	LYS
1	H	450	GLU
1	H	458	LYS
1	H	460	LEU
1	H	462	LEU
1	H	472	LYS
1	H	475	PHE
1	H	477	THR
1	H	478	GLU
1	H	486	LEU
1	H	487	GLN
1	H	490	ASP
1	H	491	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	105	ASN
1	A	112	ASN
1	A	186	ASN
1	A	196	ASN
1	A	330	GLN
1	A	405	ASN
1	B	100	GLN
1	B	105	ASN
1	B	112	ASN
1	B	166	ASN
1	B	186	ASN
1	B	196	ASN
1	B	269	ASN
1	B	330	GLN
1	C	100	GLN
1	C	105	ASN
1	C	112	ASN
1	C	186	ASN
1	C	196	ASN
1	C	330	GLN
1	D	100	GLN
1	D	105	ASN
1	D	112	ASN

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Mol	Chain	Res	Type
1	D	196	ASN
1	D	269	ASN
1	D	330	GLN
1	E	100	GLN
1	E	105	ASN
1	E	112	ASN
1	E	196	ASN
1	E	330	GLN
1	E	358	GLN
1	F	100	GLN
1	F	105	ASN
1	F	112	ASN
1	F	166	ASN
1	F	186	ASN
1	F	196	ASN
1	F	269	ASN
1	F	330	GLN
1	G	100	GLN
1	G	105	ASN
1	G	112	ASN
1	G	186	ASN
1	G	196	ASN
1	G	330	GLN
1	H	100	GLN
1	H	105	ASN
1	H	112	ASN
1	H	166	ASN
1	H	196	ASN
1	H	269	ASN
1	H	330	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	369/443 (83%)	0.65	35 (9%) 8 9	118, 136, 157, 175	0
1	B	382/443 (86%)	0.58	40 (10%) 6 6	115, 136, 154, 182	0
1	C	368/443 (83%)	0.56	28 (7%) 13 12	119, 134, 158, 178	0
1	D	382/443 (86%)	0.72	56 (14%) 2 2	118, 136, 154, 182	0
1	E	368/443 (83%)	1.15	77 (20%) 1 1	118, 136, 157, 180	0
1	F	382/443 (86%)	1.07	91 (23%) 0 0	118, 137, 153, 182	0
1	G	369/443 (83%)	0.96	51 (13%) 2 2	115, 137, 156, 178	0
1	H	382/443 (86%)	0.93	62 (16%) 1 2	119, 136, 153, 181	0
All	All	3002/3544 (84%)	0.82	440 (14%) 2 2	115, 136, 156, 182	0

All (440) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	10.2
1	A	434	VAL	9.6
1	G	434	VAL	8.7
1	E	432	THR	8.5
1	E	241	LYS	7.0
1	D	314	VAL	6.9
1	E	126	ASP	6.8
1	H	452	TRP	6.8
1	F	102	GLY	6.6
1	G	430	HIS	6.5
1	E	402	ALA	6.4
1	F	452	TRP	6.4
1	F	475	PHE	6.4
1	E	269	ASN	6.3
1	C	431	ARG	5.9
1	G	450	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	154	ASN	5.7
1	D	429	GLU	5.7
1	F	177	LYS	5.7
1	G	207	ASP	5.6
1	F	210	SER	5.5
1	H	455	VAL	5.5
1	H	451	VAL	5.5
1	B	156	TYR	5.4
1	C	316	ASN	5.4
1	H	161	GLU	5.4
1	B	152	PRO	5.3
1	F	152	PRO	5.3
1	G	268	LEU	5.2
1	E	111	ASP	5.2
1	E	293	ASP	5.2
1	C	268	LEU	5.2
1	H	432	THR	5.1
1	F	158	ALA	5.1
1	G	108	CYS	5.1
1	H	251	ILE	5.1
1	E	268	LEU	5.0
1	F	432	THR	5.0
1	G	497	ASP	5.0
1	E	431	ARG	4.9
1	D	428	SER	4.9
1	D	114	TRP	4.8
1	H	493	ARG	4.8
1	H	120	SER	4.8
1	B	471	PRO	4.7
1	A	207	ASP	4.7
1	H	152	PRO	4.7
1	E	315	GLY	4.7
1	D	357	SER	4.7
1	E	252	SER	4.6
1	F	253	LYS	4.6
1	F	124	CYS	4.6
1	C	269	ASN	4.5
1	E	251	ILE	4.5
1	D	397	VAL	4.5
1	E	272	THR	4.5
1	H	297	TYR	4.5
1	H	295	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	142	LYS	4.4
1	G	429	GLU	4.4
1	F	126	ASP	4.4
1	E	428	SER	4.4
1	F	312	LYS	4.3
1	C	429	GLU	4.3
1	G	316	ASN	4.3
1	H	433	GLN	4.3
1	D	316	ASN	4.3
1	B	430	HIS	4.3
1	E	213	PRO	4.3
1	F	315	GLY	4.2
1	G	101	ASP	4.2
1	D	142	LYS	4.2
1	E	298	TYR	4.2
1	H	441	THR	4.2
1	E	395	VAL	4.1
1	D	435	SER	4.1
1	F	314	VAL	4.1
1	E	393	PRO	4.1
1	E	404	TYR	4.1
1	D	454	GLU	4.0
1	H	111	ASP	4.0
1	E	192	SER	4.0
1	H	233	GLU	4.0
1	H	361	ASP	4.0
1	B	448	ILE	3.9
1	G	156	TYR	3.9
1	F	446	ASN	3.9
1	D	163	HIS	3.8
1	D	382	ARG	3.8
1	F	429	GLU	3.8
1	G	128	PRO	3.8
1	G	137	ARG	3.8
1	G	253	LYS	3.8
1	F	114	TRP	3.8
1	A	177	LYS	3.8
1	B	132	ARG	3.8
1	F	294	ALA	3.8
1	F	298	TYR	3.8
1	B	324	CYS	3.7
1	B	436	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	440	ILE	3.7
1	D	118	ASP	3.7
1	F	123	TYR	3.7
1	D	101	ASP	3.7
1	F	155	SER	3.7
1	F	178	GLY	3.7
1	A	431	ARG	3.7
1	B	215	ALA	3.7
1	H	431	ARG	3.7
1	F	214	LYS	3.6
1	D	404	TYR	3.6
1	C	272	THR	3.6
1	G	326	LEU	3.6
1	E	184	ASN	3.6
1	H	207	ASP	3.6
1	B	315	GLY	3.6
1	C	152	PRO	3.5
1	G	122	GLU	3.5
1	C	274	ILE	3.5
1	H	142	LYS	3.5
1	F	428	SER	3.5
1	D	177	LYS	3.5
1	F	436	LEU	3.5
1	G	142	LYS	3.5
1	F	125	PHE	3.5
1	E	292	PHE	3.5
1	D	156	TYR	3.4
1	E	187	SER	3.4
1	E	397	VAL	3.4
1	D	119	LYS	3.4
1	F	122	GLU	3.4
1	F	403	GLY	3.4
1	F	270	VAL	3.4
1	G	92	PRO	3.4
1	H	437	LYS	3.3
1	H	314	VAL	3.3
1	D	457	GLU	3.3
1	B	126	ASP	3.3
1	H	211	VAL	3.3
1	F	93	TRP	3.3
1	B	451	VAL	3.3
1	A	268	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	137	ARG	3.3
1	F	434	VAL	3.3
1	D	121	CYS	3.3
1	B	432	THR	3.3
1	D	252	SER	3.3
1	G	314	VAL	3.3
1	H	298	TYR	3.3
1	E	316	ASN	3.3
1	D	315	GLY	3.2
1	E	291	PHE	3.2
1	B	314	VAL	3.2
1	E	493	ARG	3.2
1	H	117	ARG	3.2
1	G	177	LYS	3.2
1	E	396	LEU	3.2
1	B	305	GLU	3.2
1	E	100	GLN	3.2
1	C	293	ASP	3.2
1	H	357	SER	3.2
1	F	402	ALA	3.2
1	F	447	PHE	3.2
1	E	394	GLU	3.2
1	H	414	GLY	3.1
1	C	270	VAL	3.1
1	E	130	LEU	3.1
1	D	251	ILE	3.1
1	F	167	GLY	3.1
1	B	429	GLU	3.1
1	E	161	GLU	3.1
1	E	414	GLY	3.1
1	F	356	SER	3.1
1	F	388	PRO	3.1
1	D	434	VAL	3.1
1	H	331	MET	3.1
1	A	107	GLU	3.1
1	C	432	THR	3.1
1	C	195	ARG	3.1
1	C	430	HIS	3.1
1	D	396	LEU	3.1
1	H	436	LEU	3.1
1	H	118	ASP	3.1
1	A	164	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	409	ASP	3.0
1	A	404	TYR	3.0
1	C	284	CYS	3.0
1	E	125	PHE	3.0
1	F	454	GLU	3.0
1	H	393	PRO	3.0
1	H	137	ARG	3.0
1	A	297	TYR	3.0
1	E	156	TYR	3.0
1	E	299	ILE	3.0
1	B	207	ASP	3.0
1	F	316	ASN	3.0
1	F	495	PHE	3.0
1	E	271	GLU	3.0
1	F	412	SER	3.0
1	A	119	LYS	3.0
1	H	448	ILE	3.0
1	A	95	ARG	3.0
1	E	206	VAL	3.0
1	B	447	PHE	3.0
1	H	148	ARG	2.9
1	G	297	TYR	2.9
1	A	430	HIS	2.9
1	E	276	ILE	2.9
1	C	215	ALA	2.9
1	D	102	GLY	2.9
1	E	403	GLY	2.9
1	G	432	THR	2.9
1	E	279	LYS	2.9
1	A	156	TYR	2.9
1	F	357	SER	2.9
1	G	233	GLU	2.9
1	B	322	ALA	2.9
1	A	361	ASP	2.9
1	B	497	ASP	2.9
1	D	136	TYR	2.9
1	F	450	GLU	2.9
1	F	119	LYS	2.9
1	E	430	HIS	2.8
1	C	207	ASP	2.8
1	C	404	TYR	2.8
1	B	431	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	132	ARG	2.8
1	E	128	PRO	2.8
1	G	163	HIS	2.8
1	H	128	PRO	2.8
1	F	127	GLU	2.8
1	G	161	GLU	2.8
1	E	169	PHE	2.8
1	F	435	SER	2.8
1	H	220	TYR	2.8
1	G	414	GLY	2.8
1	F	379	SER	2.8
1	D	103	PHE	2.8
1	D	211	VAL	2.8
1	H	305	GLU	2.8
1	H	429	GLU	2.8
1	G	361	ASP	2.8
1	E	114	TRP	2.8
1	F	163	HIS	2.8
1	F	437	LYS	2.7
1	F	188	GLU	2.7
1	H	472	LYS	2.7
1	E	185	ASN	2.7
1	G	327	TYR	2.7
1	H	358	GLN	2.7
1	H	499	LEU	2.7
1	H	473	ALA	2.7
1	D	117	ARG	2.7
1	C	435	SER	2.7
1	G	413	LEU	2.7
1	H	252	SER	2.7
1	E	137	ARG	2.7
1	H	135	LYS	2.7
1	D	441	THR	2.7
1	E	168	THR	2.7
1	E	207	ASP	2.7
1	F	361	ASP	2.7
1	G	251	ILE	2.7
1	G	293	ASP	2.7
1	F	113	TYR	2.7
1	A	355	LEU	2.7
1	B	316	ASN	2.7
1	H	430	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	446	ASN	2.6
1	D	131	LYS	2.6
1	B	433	GLN	2.6
1	F	151	GLY	2.6
1	E	113	TYR	2.6
1	A	251	ILE	2.6
1	H	146	ILE	2.6
1	G	428	SER	2.6
1	E	214	LYS	2.6
1	F	194	SER	2.6
1	G	494	LYS	2.6
1	H	330	GLN	2.6
1	D	430	HIS	2.6
1	E	195	ARG	2.6
1	E	329	TYR	2.6
1	H	492	LYS	2.6
1	F	154	ASN	2.6
1	A	220	TYR	2.6
1	E	141	LYS	2.6
1	D	151	GLY	2.6
1	B	323	THR	2.6
1	E	412	SER	2.5
1	G	270	VAL	2.5
1	A	253	LYS	2.5
1	G	193	LEU	2.5
1	F	141	LYS	2.5
1	F	364	ILE	2.5
1	C	252	SER	2.5
1	F	185	ASN	2.5
1	D	188	GLU	2.5
1	F	107	GLU	2.5
1	E	314	VAL	2.5
1	F	156	TYR	2.5
1	F	117	ARG	2.5
1	B	412	SER	2.5
1	E	435	SER	2.5
1	A	184	ASN	2.5
1	D	433	GLN	2.5
1	F	211	VAL	2.5
1	F	121	CYS	2.5
1	E	233	GLU	2.5
1	B	434	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	150	VAL	2.4
1	C	251	ILE	2.4
1	F	208	ASP	2.4
1	H	119	LYS	2.4
1	A	414	GLY	2.4
1	A	182	PRO	2.4
1	E	133	THR	2.4
1	G	437	LYS	2.4
1	E	388	PRO	2.4
1	D	296	ASP	2.4
1	E	417	LEU	2.4
1	G	355	LEU	2.4
1	F	101	ASP	2.4
1	F	103	PHE	2.4
1	G	311	ASP	2.4
1	E	124	CYS	2.4
1	H	328	PHE	2.4
1	D	152	PRO	2.4
1	E	186	ASN	2.4
1	F	441	THR	2.4
1	A	435	SER	2.4
1	D	495	PHE	2.4
1	G	416	ILE	2.4
1	B	328	PHE	2.3
1	B	404	TYR	2.3
1	D	436	LEU	2.3
1	H	434	VAL	2.3
1	A	134	ASP	2.3
1	C	241	LYS	2.3
1	H	121	CYS	2.3
1	H	154	ASN	2.3
1	B	295	GLU	2.3
1	H	315	GLY	2.3
1	G	118	ASP	2.3
1	H	380	LEU	2.3
1	F	136	TYR	2.3
1	G	435	SER	2.3
1	D	432	THR	2.3
1	F	153	LYS	2.3
1	H	107	GLU	2.3
1	F	421	LEU	2.3
1	B	222	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	344	ILE	2.3
1	F	139	TYR	2.3
1	F	142	LYS	2.3
1	E	152	PRO	2.3
1	G	213	PRO	2.3
1	C	346	ARG	2.3
1	C	436	LEU	2.3
1	A	439	GLN	2.3
1	H	395	VAL	2.3
1	A	360	GLU	2.3
1	F	295	GLU	2.3
1	A	327	TYR	2.3
1	A	429	GLU	2.2
1	D	362	CYS	2.2
1	D	186	ASN	2.2
1	E	274	ILE	2.2
1	G	315	GLY	2.2
1	E	216	LEU	2.2
1	D	363	LEU	2.2
1	G	448	ILE	2.2
1	D	431	ARG	2.2
1	E	442	SER	2.2
1	H	103	PHE	2.2
1	A	195	ARG	2.2
1	B	148	ARG	2.2
1	E	439	GLN	2.2
1	E	471	PRO	2.2
1	H	296	ASP	2.2
1	C	204	LEU	2.2
1	A	410	CYS	2.2
1	B	223	SER	2.2
1	F	486	LEU	2.2
1	D	202	PHE	2.2
1	G	418	PHE	2.2
1	F	423	GLY	2.2
1	D	482	ARG	2.2
1	D	126	ASP	2.2
1	D	222	MET	2.2
1	F	241	LYS	2.2
1	D	239	GLU	2.2
1	F	200	VAL	2.2
1	F	238	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	500	SER	2.1
1	A	136	TYR	2.1
1	F	355	LEU	2.1
1	F	404	TYR	2.1
1	B	450	GLU	2.1
1	F	118	ASP	2.1
1	B	441	THR	2.1
1	D	132	ARG	2.1
1	D	475	PHE	2.1
1	C	276	ILE	2.1
1	G	250	ILE	2.1
1	E	193	LEU	2.1
1	G	417	LEU	2.1
1	F	453	ALA	2.1
1	F	251	ILE	2.1
1	G	143	HIS	2.1
1	B	166	ASN	2.1
1	E	448	ILE	2.1
1	F	491	MET	2.1
1	F	92	PRO	2.1
1	B	449	PRO	2.1
1	C	291	PHE	2.1
1	D	393	PRO	2.1
1	H	489	GLU	2.1
1	H	326	LEU	2.1
1	G	472	LYS	2.1
1	F	293	ASP	2.1
1	B	327	TYR	2.1
1	F	223	SER	2.1
1	E	148	ARG	2.0
1	E	429	GLU	2.0
1	C	214	LYS	2.0
1	A	405	ASN	2.0
1	C	148	ARG	2.0
1	B	435	SER	2.0
1	G	294	ALA	2.0
1	A	412	SER	2.0
1	B	294	ALA	2.0
1	F	390	TYR	2.0
1	H	284	CYS	2.0
1	B	437	LYS	2.0
1	D	155	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	130	LEU	2.0
1	A	133	THR	2.0
1	F	305	GLU	2.0
1	A	390	TYR	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.