



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:17 am GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

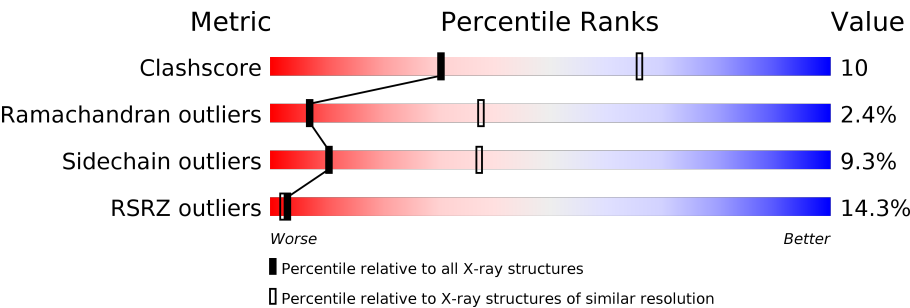
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

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	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	<div><div>7%</div><div><div></div><div>60%</div><div>19%</div><div>•</div><div>17%</div></div></div>
1	B	443	<div><div>9%</div><div><div></div><div>63%</div><div>21%</div><div>•</div><div>14%</div></div></div>
1	C	443	<div><div>6%</div><div><div></div><div>58%</div><div>21%</div><div>•</div><div>17%</div></div></div>
1	D	443	<div><div>12%</div><div><div></div><div>63%</div><div>21%</div><div>•</div><div>14%</div></div></div>
1	E	443	<div><div>17%</div><div><div></div><div>60%</div><div>20%</div><div>•</div><div>17%</div></div></div>
1	F	443	<div><div>20%</div><div><div></div><div>65%</div><div>18%</div><div>•</div><div>14%</div></div></div>
1	G	443	<div><div>11%</div><div><div></div><div>59%</div><div>20%</div><div>•</div><div>17%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	443	<div><div></div><div>14%</div><div>62%</div><div>22%</div><div>•</div><div>14%</div></div>

2 Entry composition

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			

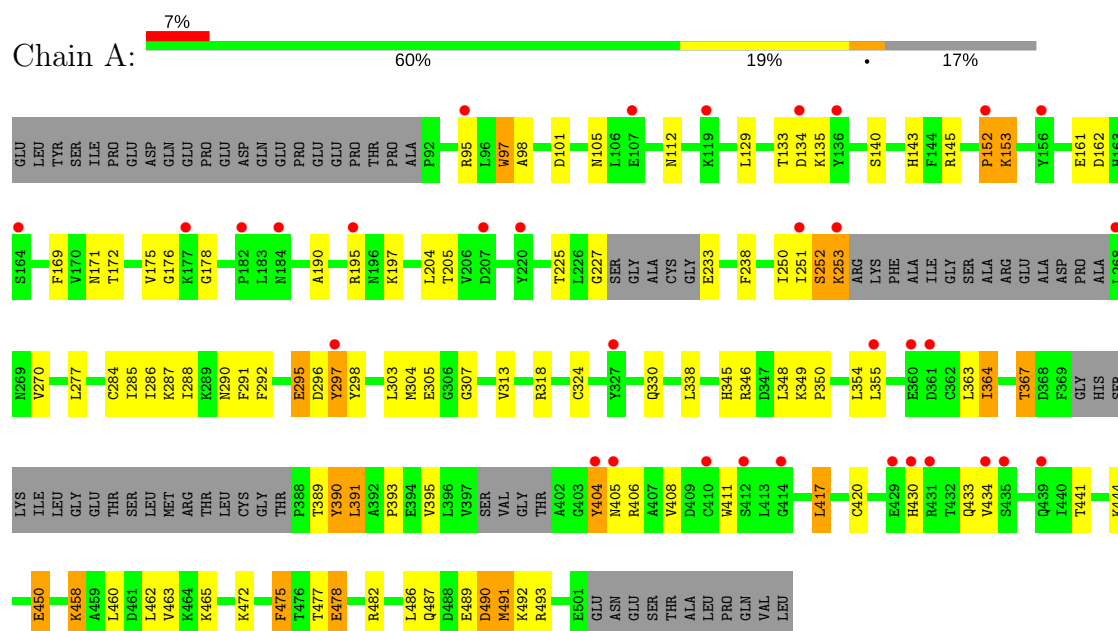
There are 8 discrepancies between the modelled and reference sequences:

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

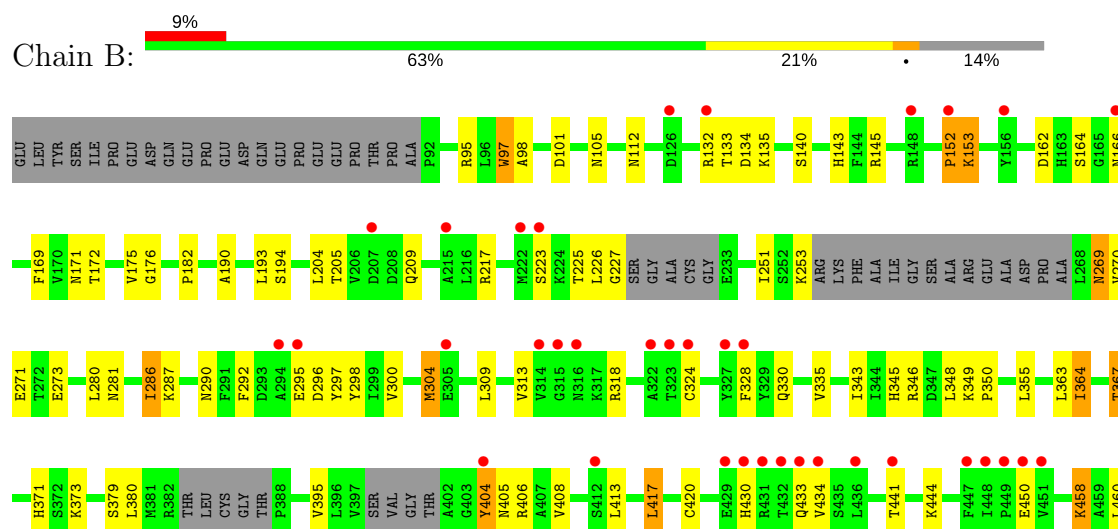
3 Residue-property plots [i](#)

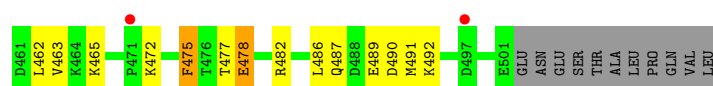
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

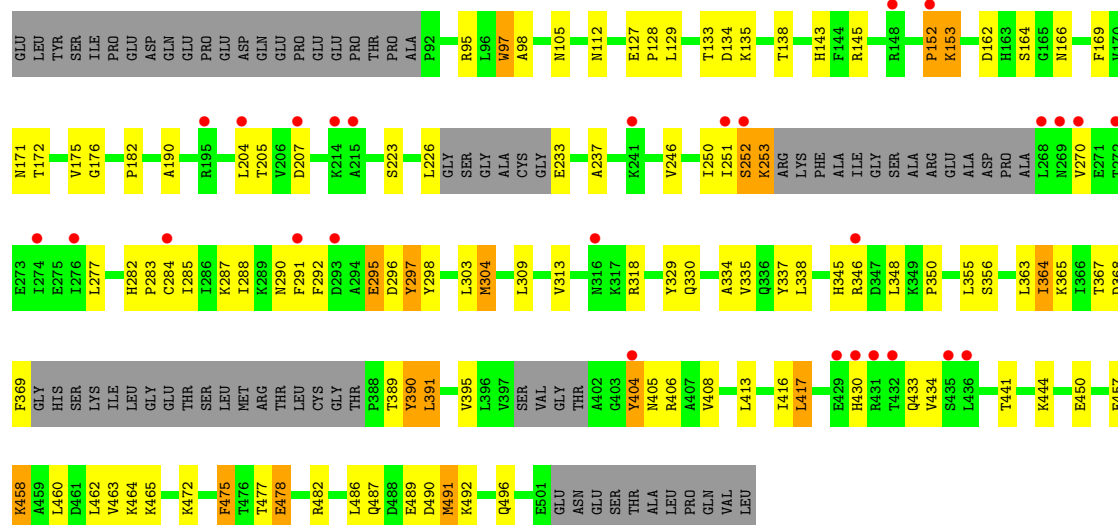


• Molecule 1: Serine/threonine-protein kinase Chk2

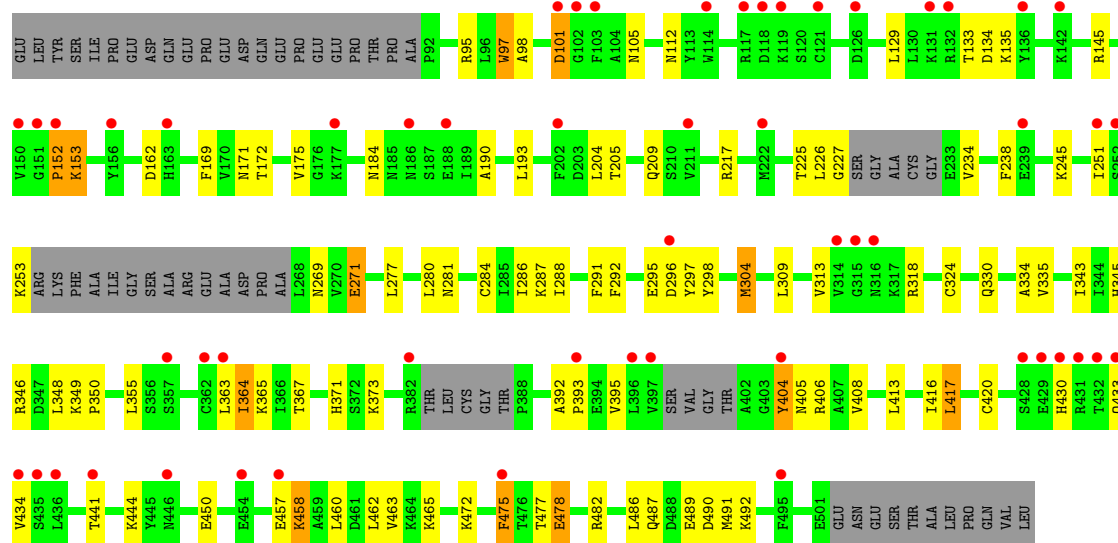




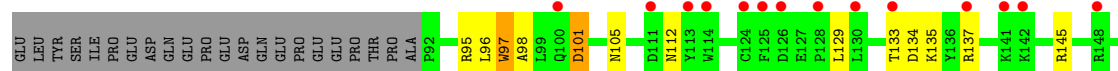
• Molecule 1: Serine/threonine-protein kinase Chk2

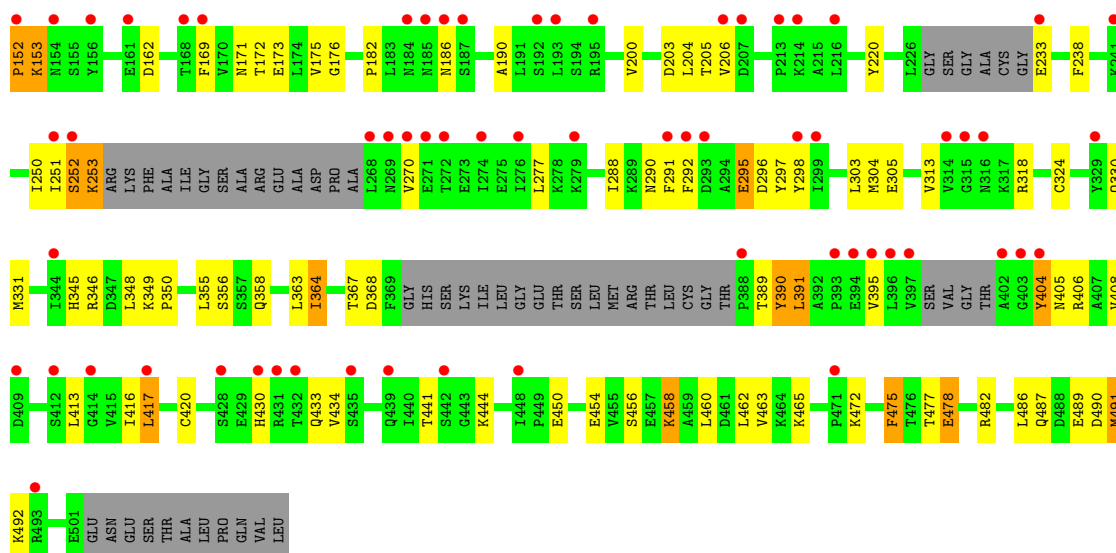


• Molecule 1: Serine/threonine-protein kinase Chk2

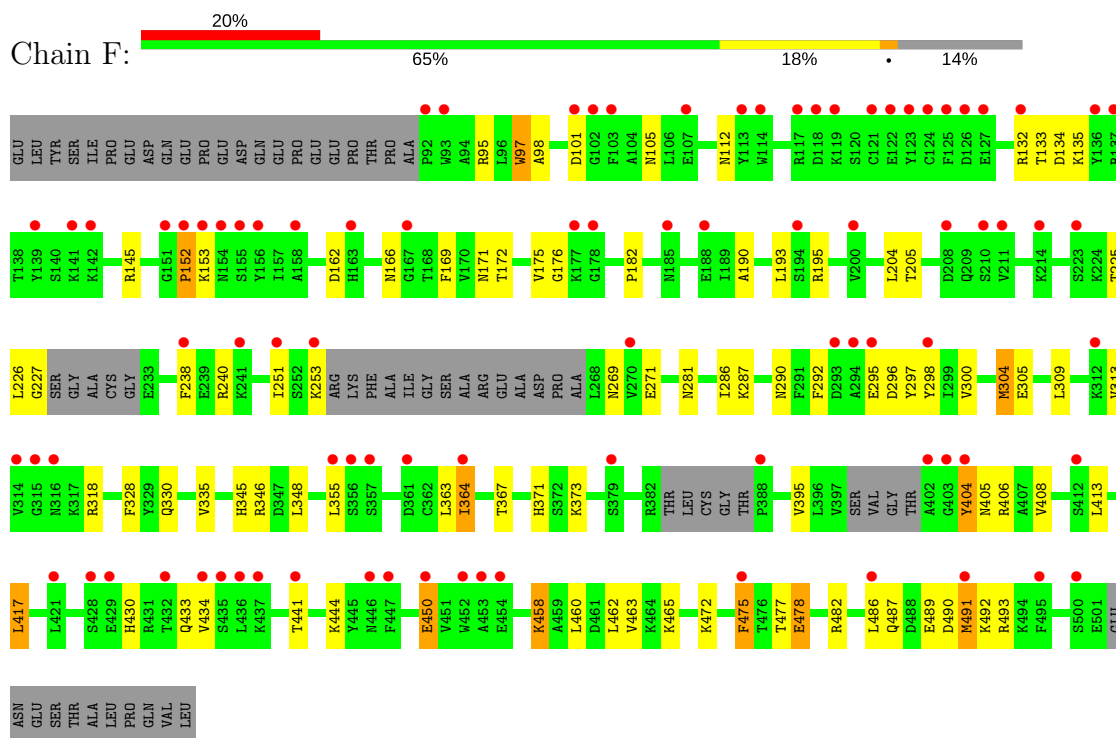


• Molecule 1: Serine/threonine-protein kinase Chk2

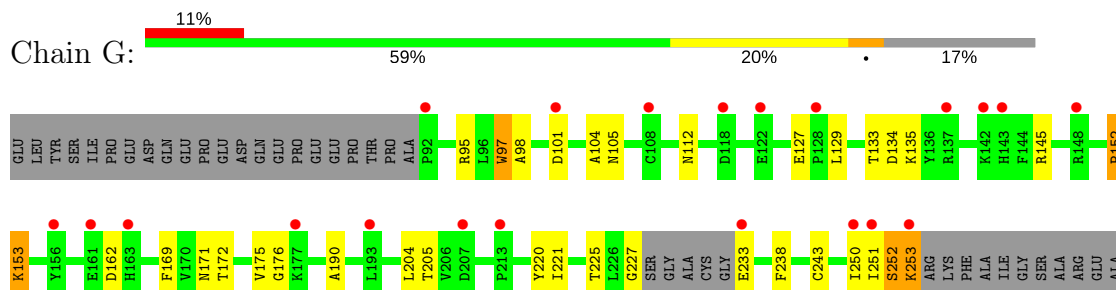


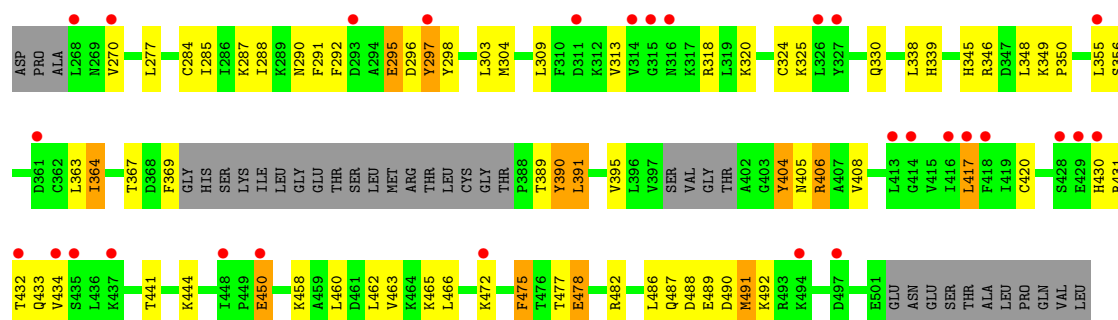


• Molecule 1: Serine/threonine-protein kinase Chk2



• Molecule 1: Serine/threonine-protein kinase Chk2





• Molecule 1: Serine/threonine-protein kinase Chk2



4 Data and refinement statistics

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) 88.8 (29.86-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.251 , 0.287 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	120.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 172.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	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(°)	Ideal(°)
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 [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	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

Continued on next page...

Continued from previous page...

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:C:98:ALA:H	1:C:105:ASN:HD22	1.30	0.79
1:B:193:LEU:HA	1:C:127:GLU:OE1	1.82	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

Continued on next page...

Continued from previous page...

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:281:ASN:HA	1:B:287:LYS:HE2	1.74	0.69
1:B:166:ASN:ND2	1:C:129:LEU:HD13	2.07	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:G:346:ARG:HG3	1:G:404:TYR:CE2	2.24	0.66
1:E:101:ASP:O	1:H:193:LEU:CD2	2.43	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

Continued on next page...

Continued from previous page...

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:O	1:C:128:PRO:HG2	1.98	0.63
1:B:166:ASN:HD21	1:C:129:LEU:CD1	2.10	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

Continued on next page...

Continued from previous page...

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:C:282:HIS:HD2	1:C:337:TYR:CD1	2.23	0.56
1:A:405:ASN:HD21	1:E:454:GLU:HB3	1.70	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

Continued on next page...

Continued from previous page...

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:HA	1:F:304:MET:CE	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:358:GLN:HE22	1:F:152:PRO:HB3	1.72	0.55
1:E:330:GLN:HE22	1:E:364:ILE:H	1.54	0.55
1:H:304:MET:CE	1:H:304:MET:HA	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:B:171:ASN:O	1:B:172:THR:HB	2.06	0.54
1:A:97:TRP:CD1	1:B:97:TRP:CE2	2.96	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

Continued on next page...

Continued from previous page...

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:HE3	1:D:304:MET:HA	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:D:330:GLN:HE22	1:D:364:ILE:H	1.57	0.52
1:A:482:ARG:NH2	1:E:458:LYS:NZ	2.58	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:C	1:C:253:LYS:HE2	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

Continued on next page...

Continued from previous page...

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:HE3	1:F:491:MET:C	2.31	0.50
1:H:350:PRO:HD3	1:H:416:ILE:HG12	1.93	0.50
1:H:346:ARG:HD2	1:H:371:HIS:O	2.12	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:489:GLU:HA	1:F:492:LYS:HB2	1.94	0.50
1:F:95:ARG:HG3	1:F:204:LEU:HD11	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: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:D:95:ARG:HG3	1:D:204:LEU:HD11	1.94	0.49
1:A:395:VAL:O	1:A:395:VAL:HG12	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:HG2	1:A:458:LYS:H	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

Continued on next page...

Continued from previous page...

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:162:ASP:HB3	1:C:176:GLY:O	2.14	0.47
1:C:95:ARG:HG3	1:C:204:LEU:HD11	1.96	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

Continued on next page...

Continued from previous page...

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:HE2	1:E:253:LYS:C	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:HE2	1:G:253:LYS:C	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:O	1:C:395:VAL:HG12	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:C	1:A:253:LYS:HE2	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:O	1:D:395:VAL:HG12	2.17	0.45
1:E:395:VAL:O	1:E:395:VAL:HG12	2.17	0.45
1:F:395:VAL:O	1:F:395:VAL:HG12	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: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:G:152:PRO:HG3	1:H:305:GLU:CG	2.45	0.45
1:A:491:MET:HE2	1:A:492:LYS:HA	1.99	0.44

Continued on next page...

Continued from previous page...

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:O	1:H:395:VAL:HG12	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: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:E:129:LEU:HD13	1:H:166:ASN:HD22	1.83	0.44
1:C:282:HIS:CG	1:C:283:PRO:HD2	2.53	0.44
1:F:162:ASP:HB2	1:F:175:VAL:HB	2.00	0.44
1:F:95:ARG:HD3	1:F:97:TRP:CZ3	2.53	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:HG2	1:H:458:LYS:H	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

Continued on next page...

Continued from previous page...

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:HG2	1:D:458:LYS:H	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:HG3	1:F:450:GLU:H	1.51	0.41
1:G:345:HIS:CG	1:G:348:LEU:HD13	2.56	0.41
1:H:450:GLU:HG3	1:H:450:GLU:H	1.51	0.41
1:H:95:ARG:HD3	1:H:97:TRP:CZ3	2.55	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

Continued on next page...

Continued from previous page...

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:HD3	1:A:287:LYS:HA	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:G:466:LEU:HA	1:G:466:LEU:HD12	1.96	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: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:HA	1:F:364:ILE:HD12	1.91	0.40
1:G:287:LYS:HD3	1:G:287:LYS:HA	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: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:E:101:ASP:C	1:H:193:LEU:HD21	2.42	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:G:320:LYS:CG	1:H:457:GLU:OE2[1_455]	1.76	0.44
1:C:166:ASN:ND2	1:C:496:GLN:OE1[1_655]	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%)	6	34
1	B	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	9	44
1	C	358/443 (81%)	326 (91%)	21 (6%)	11 (3%)	5	31
1	D	372/443 (84%)	334 (90%)	31 (8%)	7 (2%)	9	44
1	E	358/443 (81%)	327 (91%)	21 (6%)	10 (3%)	6	34
1	F	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	9	44
1	G	359/443 (81%)	328 (91%)	21 (6%)	10 (3%)	6	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	372/443 (84%)	335 (90%)	30 (8%)	7 (2%)	9	44
All	All	2922/3544 (82%)	2650 (91%)	203 (7%)	69 (2%)	7	37

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	11	39
1	B	344/395 (87%)	311 (90%)	33 (10%)	10	36
1	C	333/395 (84%)	302 (91%)	31 (9%)	10	37
1	D	344/395 (87%)	312 (91%)	32 (9%)	10	37
1	E	333/395 (84%)	303 (91%)	30 (9%)	11	39
1	F	344/395 (87%)	312 (91%)	32 (9%)	10	37
1	G	333/395 (84%)	302 (91%)	31 (9%)	10	37
1	H	344/395 (87%)	312 (91%)	32 (9%)	10	37
All	All	2708/3160 (86%)	2457 (91%)	251 (9%)	10	37

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Some 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

Continued on next page...

Continued from previous page...

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 ⓘ

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 [i](#)

There are no carbohydrates 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	369/443 (83%)	0.63	33 (8%) 10 8	118, 136, 157, 175	0
1	B	382/443 (86%)	0.57	38 (9%) 8 6	115, 136, 154, 182	0
1	C	368/443 (83%)	0.54	28 (7%) 15 11	119, 134, 158, 178	0
1	D	382/443 (86%)	0.70	54 (14%) 3 2	118, 136, 154, 182	0
1	E	368/443 (83%)	1.13	77 (20%) 1 1	118, 136, 157, 180	0
1	F	382/443 (86%)	1.05	88 (23%) 1 1	118, 137, 153, 182	0
1	G	369/443 (83%)	0.94	50 (13%) 3 3	115, 137, 156, 178	0
1	H	382/443 (86%)	0.91	62 (16%) 2 1	119, 136, 153, 181	0
All	All	3002/3544 (84%)	0.81	430 (14%) 3 2	115, 136, 156, 182	0

All (430) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	9.6
1	A	434	VAL	9.6
1	G	434	VAL	8.7
1	E	432	THR	8.3
1	E	241	LYS	6.8
1	D	314	VAL	6.8
1	H	452	TRP	6.7
1	E	126	ASP	6.6
1	F	452	TRP	6.3
1	F	102	GLY	6.3
1	E	269	ASN	6.3
1	F	475	PHE	6.2
1	G	430	HIS	6.2
1	C	431	ARG	5.9
1	E	402	ALA	5.8
1	D	429	GLU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	154	ASN	5.7
1	G	450	GLU	5.7
1	F	177	LYS	5.6
1	B	156	TYR	5.6
1	G	207	ASP	5.4
1	H	455	VAL	5.4
1	E	111	ASP	5.4
1	F	210	SER	5.3
1	F	152	PRO	5.3
1	H	451	VAL	5.3
1	H	161	GLU	5.3
1	G	268	LEU	5.3
1	C	316	ASN	5.3
1	C	268	LEU	5.2
1	B	152	PRO	5.2
1	E	293	ASP	5.1
1	F	432	THR	5.0
1	H	432	THR	5.0
1	H	251	ILE	4.9
1	E	268	LEU	4.9
1	G	108	CYS	4.9
1	E	431	ARG	4.9
1	F	158	ALA	4.9
1	G	497	ASP	4.8
1	D	428	SER	4.7
1	D	114	TRP	4.7
1	E	315	GLY	4.7
1	H	120	SER	4.7
1	H	493	ARG	4.7
1	B	471	PRO	4.7
1	E	252	SER	4.6
1	E	251	ILE	4.6
1	A	207	ASP	4.6
1	D	357	SER	4.6
1	E	142	LYS	4.5
1	H	297	TYR	4.5
1	F	124	CYS	4.5
1	F	253	LYS	4.4
1	G	429	GLU	4.4
1	D	397	VAL	4.4
1	C	269	ASN	4.4
1	F	312	LYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	295	GLU	4.4
1	H	152	PRO	4.3
1	F	126	ASP	4.3
1	H	433	GLN	4.3
1	E	272	THR	4.3
1	C	429	GLU	4.3
1	G	316	ASN	4.3
1	E	395	VAL	4.3
1	E	428	SER	4.2
1	D	316	ASN	4.2
1	B	430	HIS	4.2
1	F	315	GLY	4.2
1	E	393	PRO	4.1
1	E	213	PRO	4.1
1	F	314	VAL	4.1
1	E	404	TYR	4.1
1	H	441	THR	4.1
1	G	101	ASP	4.1
1	E	192	SER	4.0
1	E	298	TYR	4.0
1	D	142	LYS	4.0
1	D	454	GLU	4.0
1	H	361	ASP	4.0
1	B	448	ILE	4.0
1	D	435	SER	4.0
1	H	111	ASP	3.9
1	H	233	GLU	3.9
1	G	253	LYS	3.9
1	G	156	TYR	3.8
1	D	163	HIS	3.8
1	G	137	ARG	3.8
1	F	298	TYR	3.8
1	G	128	PRO	3.8
1	F	114	TRP	3.8
1	B	132	ARG	3.8
1	B	315	GLY	3.7
1	F	429	GLU	3.7
1	D	101	ASP	3.7
1	A	177	LYS	3.7
1	D	382	ARG	3.7
1	B	324	CYS	3.7
1	E	397	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	431	ARG	3.7
1	A	431	ARG	3.7
1	F	294	ALA	3.7
1	H	440	ILE	3.7
1	C	272	THR	3.7
1	F	155	SER	3.7
1	F	446	ASN	3.7
1	H	142	LYS	3.6
1	D	118	ASP	3.6
1	E	184	ASN	3.6
1	F	123	TYR	3.6
1	D	404	TYR	3.6
1	F	178	GLY	3.6
1	D	177	LYS	3.6
1	B	436	LEU	3.6
1	F	214	LYS	3.6
1	F	125	PHE	3.6
1	B	215	ALA	3.5
1	H	207	ASP	3.5
1	C	274	ILE	3.5
1	C	152	PRO	3.5
1	G	177	LYS	3.4
1	F	270	VAL	3.4
1	G	92	PRO	3.4
1	E	187	SER	3.4
1	G	122	GLU	3.4
1	G	142	LYS	3.4
1	D	156	TYR	3.4
1	F	428	SER	3.4
1	D	119	LYS	3.4
1	E	292	PHE	3.4
1	F	434	VAL	3.4
1	H	298	TYR	3.4
1	D	457	GLU	3.4
1	F	436	LEU	3.3
1	E	291	PHE	3.3
1	E	396	LEU	3.3
1	F	93	TRP	3.3
1	H	437	LYS	3.3
1	E	493	ARG	3.3
1	G	326	LEU	3.3
1	B	451	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	316	ASN	3.3
1	F	122	GLU	3.3
1	F	137	ARG	3.3
1	F	167	GLY	3.3
1	H	211	VAL	3.2
1	A	268	LEU	3.2
1	H	314	VAL	3.2
1	E	394	GLU	3.2
1	D	252	SER	3.2
1	B	432	THR	3.2
1	G	314	VAL	3.2
1	F	447	PHE	3.2
1	B	126	ASP	3.2
1	B	314	VAL	3.2
1	E	130	LEU	3.2
1	B	305	GLU	3.2
1	D	121	CYS	3.2
1	E	100	GLN	3.1
1	C	432	THR	3.1
1	E	414	GLY	3.1
1	E	156	TYR	3.1
1	C	430	HIS	3.1
1	H	414	GLY	3.1
1	F	403	GLY	3.1
1	F	495	PHE	3.1
1	D	251	ILE	3.1
1	F	388	PRO	3.1
1	H	331	MET	3.1
1	C	293	ASP	3.1
1	D	315	GLY	3.1
1	H	118	ASP	3.1
1	H	436	LEU	3.1
1	H	393	PRO	3.0
1	C	270	VAL	3.0
1	D	396	LEU	3.0
1	A	297	TYR	3.0
1	B	429	GLU	3.0
1	D	434	VAL	3.0
1	A	430	HIS	3.0
1	C	195	ARG	3.0
1	F	412	SER	3.0
1	H	117	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	107	GLU	3.0
1	C	284	CYS	3.0
1	A	404	TYR	3.0
1	H	137	ARG	3.0
1	B	447	PHE	3.0
1	B	207	ASP	3.0
1	E	409	ASP	3.0
1	A	95	ARG	3.0
1	F	356	SER	3.0
1	G	432	THR	3.0
1	E	161	GLU	3.0
1	E	125	PHE	2.9
1	D	136	TYR	2.9
1	F	119	LYS	2.9
1	E	276	ILE	2.9
1	E	299	ILE	2.9
1	H	448	ILE	2.9
1	A	119	LYS	2.9
1	E	271	GLU	2.9
1	C	215	ALA	2.9
1	G	297	TYR	2.9
1	E	279	LYS	2.9
1	A	156	TYR	2.9
1	F	402	ALA	2.9
1	F	435	SER	2.9
1	H	128	PRO	2.9
1	B	497	ASP	2.9
1	F	132	ARG	2.9
1	H	357	SER	2.9
1	B	322	ALA	2.9
1	C	404	TYR	2.9
1	G	361	ASP	2.9
1	A	164	SER	2.9
1	F	316	ASN	2.9
1	F	450	GLU	2.9
1	D	102	GLY	2.8
1	F	454	GLU	2.8
1	G	161	GLU	2.8
1	E	128	PRO	2.8
1	F	163	HIS	2.8
1	E	430	HIS	2.8
1	E	206	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	163	HIS	2.8
1	D	211	VAL	2.8
1	F	361	ASP	2.8
1	B	316	ASN	2.8
1	H	429	GLU	2.8
1	G	414	GLY	2.8
1	E	114	TRP	2.8
1	E	169	PHE	2.8
1	H	148	ARG	2.8
1	F	188	GLU	2.8
1	E	403	GLY	2.8
1	E	207	ASP	2.8
1	F	127	GLU	2.7
1	F	357	SER	2.7
1	E	185	ASN	2.7
1	A	361	ASP	2.7
1	D	430	HIS	2.7
1	H	472	LYS	2.7
1	H	220	TYR	2.7
1	B	431	ARG	2.7
1	D	117	ARG	2.7
1	D	131	LYS	2.7
1	H	305	GLU	2.7
1	G	251	ILE	2.7
1	C	207	ASP	2.7
1	F	151	GLY	2.7
1	G	233	GLU	2.7
1	E	141	LYS	2.7
1	F	437	LYS	2.7
1	G	413	LEU	2.7
1	H	430	HIS	2.7
1	E	195	ARG	2.6
1	G	428	SER	2.6
1	H	499	LEU	2.6
1	H	473	ALA	2.6
1	D	446	ASN	2.6
1	B	433	GLN	2.6
1	G	327	TYR	2.6
1	F	379	SER	2.6
1	E	137	ARG	2.6
1	E	113	TYR	2.6
1	D	103	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	358	GLN	2.6
1	D	441	THR	2.6
1	C	435	SER	2.6
1	F	194	SER	2.6
1	A	220	TYR	2.6
1	H	330	GLN	2.6
1	E	314	VAL	2.6
1	H	135	LYS	2.6
1	A	355	LEU	2.6
1	F	113	TYR	2.6
1	D	151	GLY	2.6
1	E	168	THR	2.6
1	E	214	LYS	2.6
1	G	293	ASP	2.6
1	H	252	SER	2.6
1	G	494	LYS	2.6
1	A	184	ASN	2.6
1	A	251	ILE	2.6
1	D	433	GLN	2.5
1	E	329	TYR	2.5
1	F	154	ASN	2.5
1	A	253	LYS	2.5
1	B	323	THR	2.5
1	E	412	SER	2.5
1	E	435	SER	2.5
1	H	492	LYS	2.5
1	B	412	SER	2.5
1	F	107	GLU	2.5
1	G	270	VAL	2.5
1	C	252	SER	2.5
1	F	117	ARG	2.5
1	H	119	LYS	2.5
1	F	185	ASN	2.5
1	H	146	ILE	2.5
1	D	495	PHE	2.5
1	D	436	LEU	2.5
1	E	233	GLU	2.5
1	D	152	PRO	2.5
1	C	251	ILE	2.5
1	A	414	GLY	2.4
1	F	141	LYS	2.4
1	G	193	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	434	VAL	2.4
1	E	417	LEU	2.4
1	F	156	TYR	2.4
1	G	355	LEU	2.4
1	D	188	GLU	2.4
1	F	121	CYS	2.4
1	H	315	GLY	2.4
1	A	182	PRO	2.4
1	H	380	LEU	2.4
1	E	152	PRO	2.4
1	H	328	PHE	2.4
1	E	133	THR	2.4
1	E	186	ASN	2.4
1	F	136	TYR	2.4
1	F	441	THR	2.4
1	C	241	LYS	2.4
1	F	153	LYS	2.4
1	F	364	ILE	2.4
1	B	295	GLU	2.4
1	D	150	VAL	2.3
1	H	434	VAL	2.3
1	G	437	LYS	2.3
1	E	388	PRO	2.3
1	B	328	PHE	2.3
1	F	101	ASP	2.3
1	B	404	TYR	2.3
1	G	118	ASP	2.3
1	D	296	ASP	2.3
1	A	435	SER	2.3
1	F	103	PHE	2.3
1	H	395	VAL	2.3
1	A	134	ASP	2.3
1	E	274	ILE	2.3
1	C	346	ARG	2.3
1	F	211	VAL	2.3
1	H	154	ASN	2.3
1	A	360	GLU	2.3
1	A	429	GLU	2.3
1	G	435	SER	2.3
1	D	363	LEU	2.3
1	B	222	MET	2.3
1	F	208	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	436	LEU	2.3
1	G	416	ILE	2.3
1	H	103	PHE	2.3
1	E	124	CYS	2.2
1	D	432	THR	2.2
1	E	344	ILE	2.2
1	F	142	LYS	2.2
1	F	139	TYR	2.2
1	F	486	LEU	2.2
1	C	204	LEU	2.2
1	C	276	ILE	2.2
1	D	126	ASP	2.2
1	E	471	PRO	2.2
1	G	213	PRO	2.2
1	A	327	TYR	2.2
1	B	223	SER	2.2
1	B	148	ARG	2.2
1	D	431	ARG	2.2
1	H	107	GLU	2.2
1	D	362	CYS	2.2
1	F	421	LEU	2.2
1	F	295	GLU	2.2
1	G	315	GLY	2.2
1	H	296	ASP	2.2
1	E	216	LEU	2.2
1	A	410	CYS	2.2
1	H	121	CYS	2.2
1	D	132	ARG	2.2
1	D	202	PHE	2.2
1	F	241	LYS	2.2
1	E	193	LEU	2.2
1	G	311	ASP	2.2
1	A	439	GLN	2.2
1	A	195	ARG	2.2
1	G	417	LEU	2.1
1	E	442	SER	2.1
1	G	418	PHE	2.1
1	E	448	ILE	2.1
1	G	448	ILE	2.1
1	E	439	GLN	2.1
1	B	441	THR	2.1
1	A	136	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	186	ASN	2.1
1	D	222	MET	2.1
1	F	200	VAL	2.1
1	F	355	LEU	2.1
1	F	500	SER	2.1
1	C	291	PHE	2.1
1	H	489	GLU	2.1
1	D	475	PHE	2.1
1	F	92	PRO	2.1
1	B	450	GLU	2.1
1	F	251	ILE	2.1
1	G	472	LYS	2.1
1	F	238	PHE	2.1
1	F	453	ALA	2.1
1	G	143	HIS	2.1
1	B	166	ASN	2.1
1	B	449	PRO	2.1
1	C	214	LYS	2.1
1	D	239	GLU	2.1
1	F	404	TYR	2.1
1	G	148	ARG	2.1
1	F	293	ASP	2.1
1	F	491	MET	2.1
1	B	327	TYR	2.0
1	D	393	PRO	2.0
1	G	250	ILE	2.0
1	A	412	SER	2.0
1	E	148	ARG	2.0
1	F	223	SER	2.0
1	H	404	TYR	2.0
1	E	270	VAL	2.0
1	B	294	ALA	2.0
1	H	284	CYS	2.0
1	F	118	ASP	2.0
1	A	405	ASN	2.0
1	C	148	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.