



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:24 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

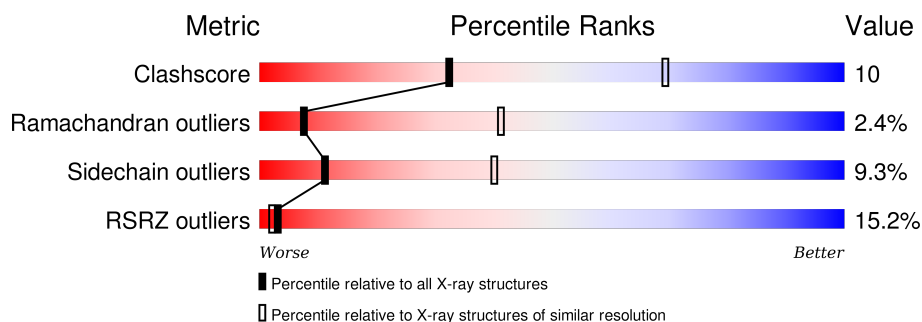
1 Overall quality at a glance

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	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (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>8%</div> <div>60% 19% 17%</div> </div>
1	B	443	<div> <div>9%</div> <div>63% 21% 14%</div> </div>
1	C	443	<div> <div>7%</div> <div>58% 21% 17%</div> </div>
1	D	443	<div> <div>13%</div> <div>63% 21% 14%</div> </div>
1	E	443	<div> <div>18%</div> <div>60% 20% 17%</div> </div>
1	F	443	<div> <div>21%</div> <div>65% 18% 14%</div> </div>
1	G	443	<div> <div>12%</div> <div>59% 20% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	443	<div><div></div><div>15%</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.

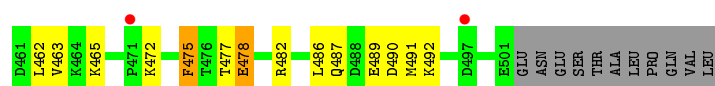
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein kinase Chk2.

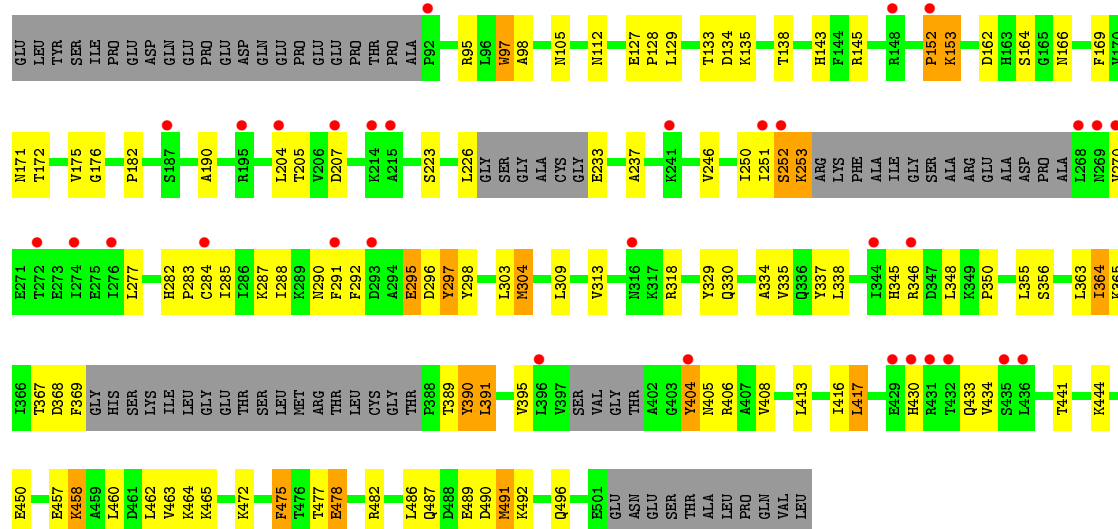
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			3022	1952	504	553	13			
1	B	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	C	368	Total	C	N	O	S	0	0	0
			3018	1950	503	552	13			
1	D	382	Total	C	N	O	S	0	0	0
			3120	2012	523	571	14			
1	E	368	Total	C	N	O	S	0	0	0
	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

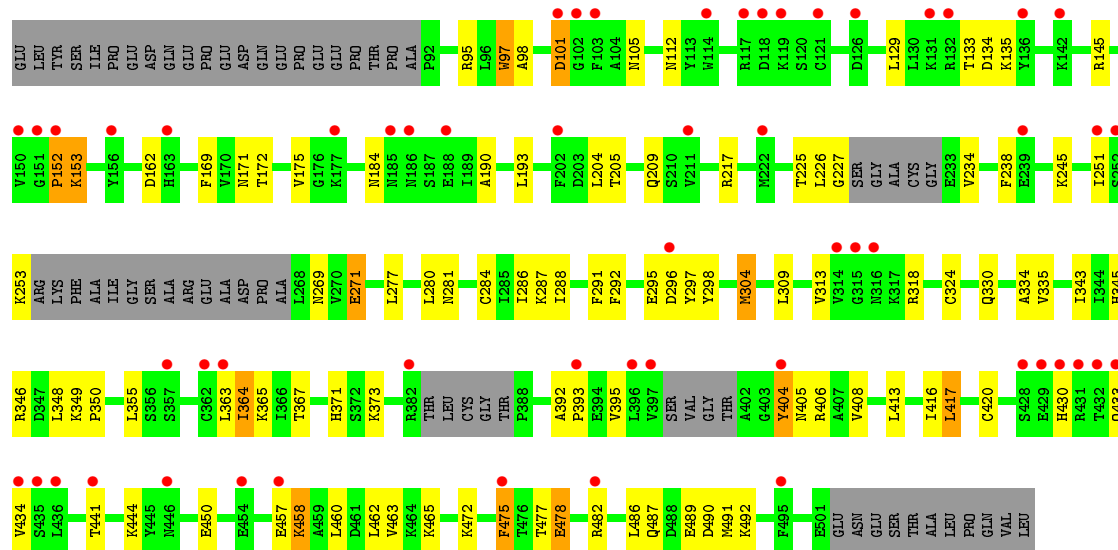
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ARG	LYS	engineered	UNP O96017
B	249	ARG	LYS	engineered	UNP O96017
C	249	ARG	LYS	engineered	UNP O96017
D	249	ARG	LYS	engineered	UNP O96017
E	249	ARG	LYS	engineered	UNP O96017
F	249	ARG	LYS	engineered	UNP O96017
G	249	ARG	LYS	engineered	UNP O96017
H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



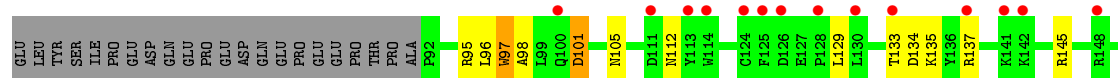
• Molecule 1: Serine/threonine-protein kinase Chk2

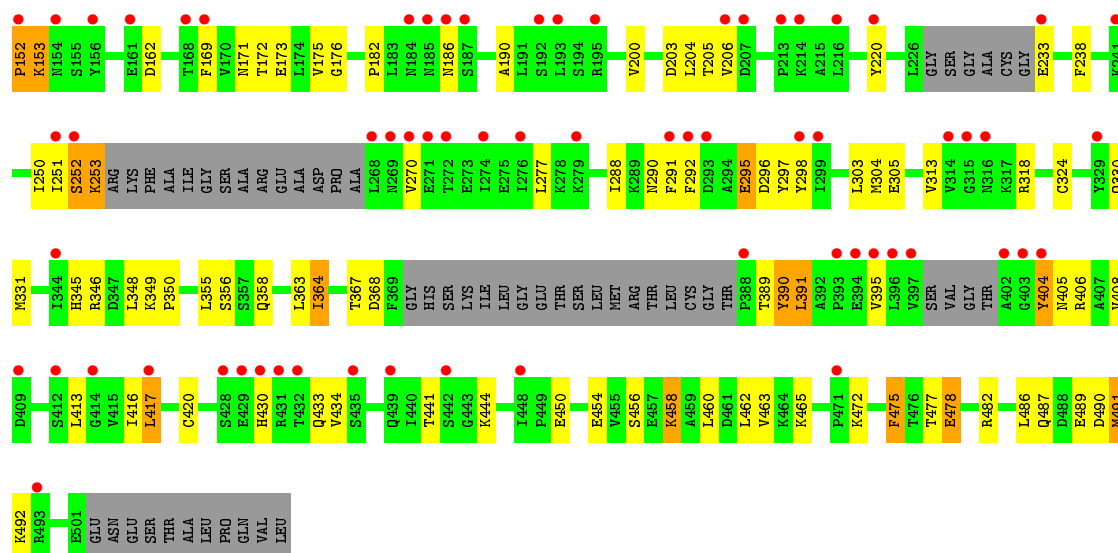


• Molecule 1: Serine/threonine-protein kinase Chk2

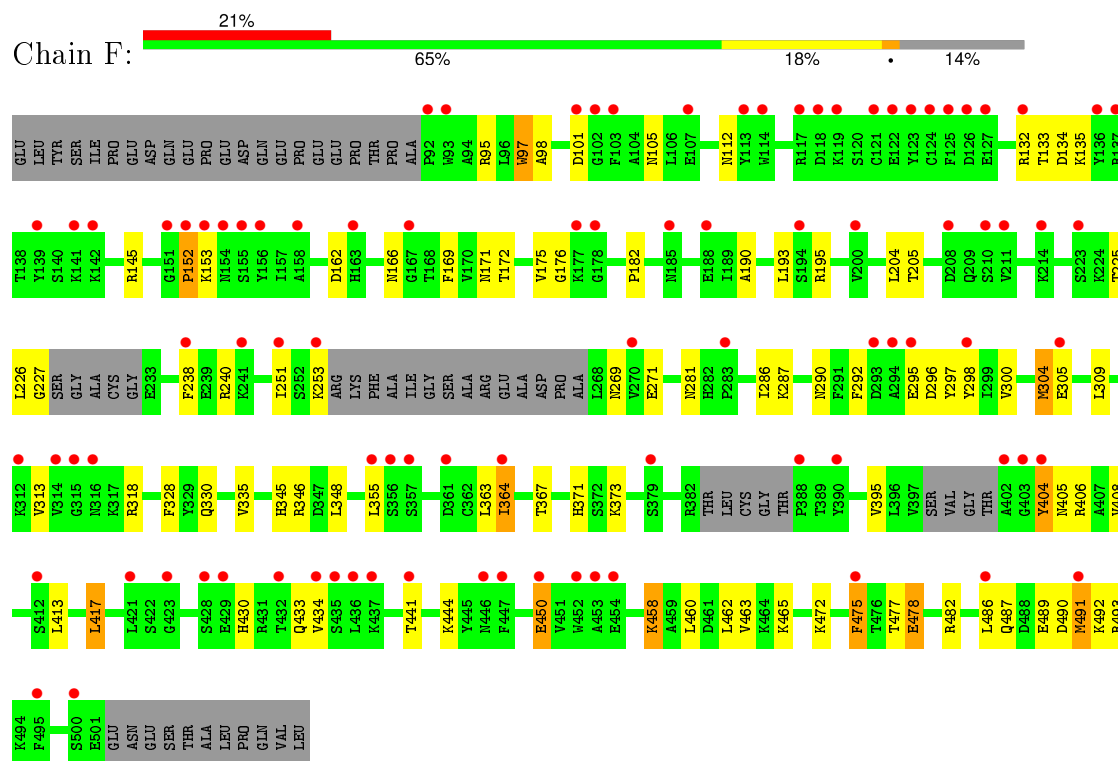


• Molecule 1: Serine/threonine-protein kinase Chk2

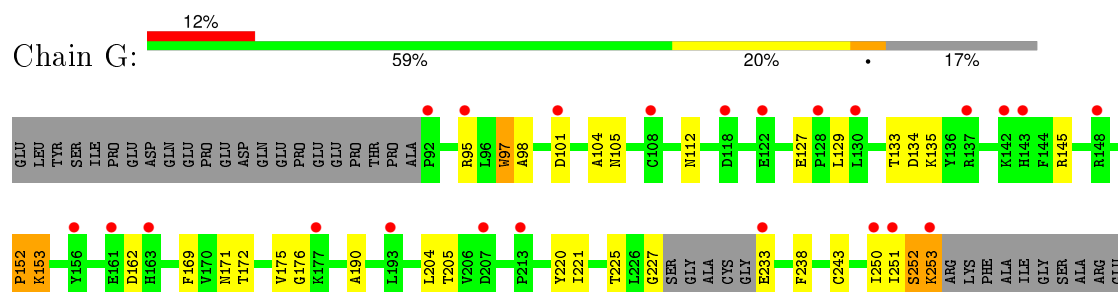




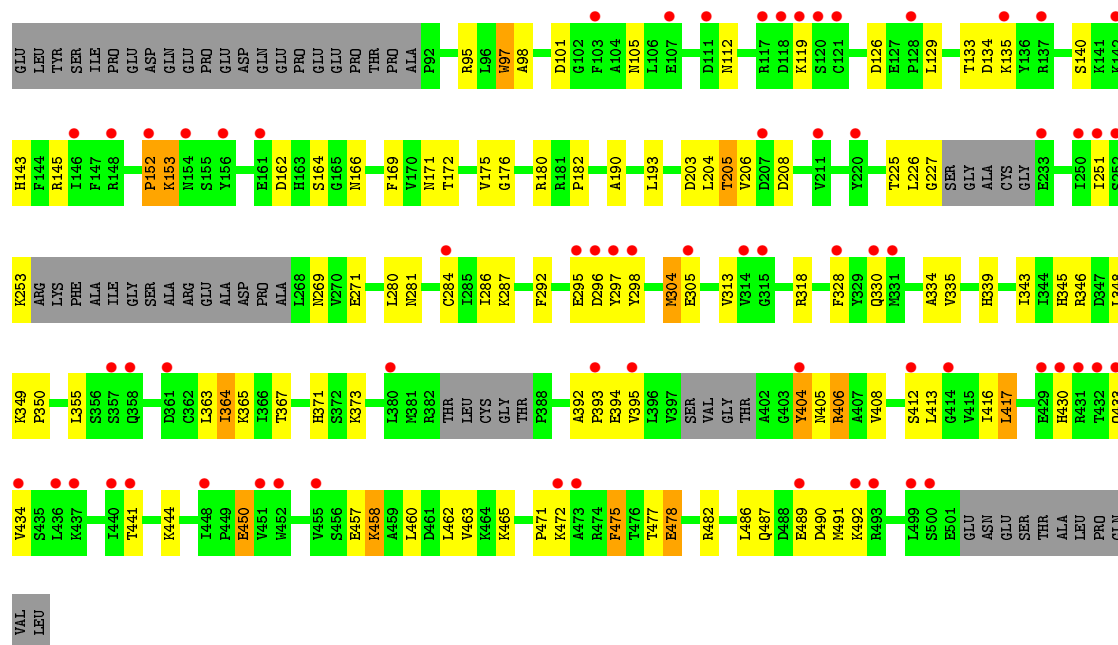
• Molecule 1: Serine/threonine-protein kinase Chk2



• 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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60982 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	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

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:G:346:ARG:HG3	1:G:404:TYR:HE2	1.33	0.93
1:E:478:GLU:HB2	1:E:482:ARG:HH12	1.32	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: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:D:98:ALA:H	1:D:105:ASN:HD22	1.30	0.77
1:B:269:ASN:ND2	1:B:380:LEU:HD13	2.00	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:D:112:ASN:ND2	1:D:145:ARG:HH11	1.90	0.69
1:B:281:ASN:HA	1:B:287:LYS:HE2	1.74	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:G:169:PHE:HB2	1:G:190:ALA:HB3	1.75	0.68
1:D:281:ASN:HA	1:D:287:LYS:HE2	1.74	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:E:292:PHE:HB2	1:E:298:TYR:HB2	1.77	0.66
1:B:225:THR:HG22	1:B:227:GLY:H	1.60	0.66
1:E:478:GLU:HB2	1:E:482:ARG:NH1	2.09	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:101:ASP:O	1:H:193:LEU:CD2	2.43	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:A:292:PHE:HB2	1:A:298:TYR:HB2	1.78	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:F:169:PHE:HB2	1:F:190:ALA:HB3	1.78	0.64
1:B:169:PHE:HB2	1:B: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:H:346:ARG:HG3	1:H:404:TYR:CE2	2.25	0.64
1:H:330:GLN:NE2	1:H:364:ILE:H	1.96	0.64
1:E:305:GLU:O	1:F:152:PRO:CG	2.46	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:G:405:ASN:O	1:G:408:VAL:HG12	1.99	0.63
1:E:304:MET:HE3	1:E:356:SER:HA	1.78	0.63
1:B:465:LYS:HD3	1:B:475:PHE:CE1	2.34	0.63
1:G:277:LEU:CB	1:G:288:ILE:HD12	2.29	0.62
1:F:405:ASN:O	1:F:408:VAL:HG12	1.99	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:H:478:GLU:HB2	1:H:482:ARG:NH1	2.11	0.62
1:C:478:GLU:HB2	1:C:482:ARG:NH1	2.11	0.62
1:D:405:ASN:O	1:D:408:VAL:HG12	1.99	0.62
1:F:330:GLN:NE2	1:F:364:ILE:H	1.97	0.61
1:C:330:GLN:NE2	1:C:364:ILE:H	1.99	0.61
1:A:277:LEU:CB	1:A:288:ILE:HD12	2.30	0.61
1:G:152:PRO:HG3	1:H:305:GLU:HG3	1.81	0.61
1:B:405:ASN:O	1:B:408:VAL:HG12	2.00	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:H:335:VAL:HG21	1:H:413:LEU:HD11	1.81	0.61
1:H:280:LEU:HD21	1:H:343:ILE:HD12	1.83	0.61
1:D:330:GLN:NE2	1:D:364:ILE:H	1.99	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:B:269:ASN:ND2	1:B:380:LEU:CD1	2.63	0.60
1:A:465:LYS:HD3	1:A:475:PHE:CE1	2.36	0.60
1:F:465:LYS:HD3	1:F:475:PHE:CE1	2.36	0.60
1:D:465:LYS:HD3	1:D:475:PHE:CE1	2.36	0.60
1:A:129:LEU:CD2	1:D:193:LEU:CG	2.79	0.60
1:H:465:LYS:HD3	1:H:475:PHE:CE1	2.36	0.60
1:C:465:LYS:HD3	1:C: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:B:166:ASN:ND2	1:C:129:LEU:CB	2.63	0.56
1:A:225:THR:HG22	1:A:227:GLY:H	1.69	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:H:330:GLN:HE22	1:H:363:LEU:HA	1.70	0.56
1:G:330:GLN:HE22	1:G:364:ILE:H	1.53	0.56
1:C:282:HIS:HD2	1:C:337:TYR:CD1	2.23	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: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: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:D:355:LEU:HD22	1:D:364:ILE:HD11	1.88	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:H:304:MET:SD	1:H:365:LYS:HD2	2.47	0.55
1:D:280:LEU:HD21	1:D:343:ILE:HD12	1.89	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:B:346:ARG:NH1	1:B:371:HIS:ND1	2.55	0.54
1:A:296:ASP:O	1:A:297:TYR:HB2	2.06	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:F:133:THR:O	1:F:135:LYS:N	2.36	0.54
1:C:296:ASP:O	1:C:297:TYR:HB2	2.08	0.54
1:G:225:THR:HG22	1:G:227:GLY:N	2.19	0.54
1:A:389:THR:O	1:A:391:LEU:N	2.40	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:F:292:PHE:HB2	1:F:298:TYR:HB2	1.90	0.53
1:D:292:PHE:HB2	1:D:298:TYR:HB2	1.90	0.53
1:B:273:GLU:OE2	1:B:380:LEU:N	2.41	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:C:171:ASN:O	1:C:172:THR:HB	2.09	0.53
1:A:133:THR:O	1:A:135:LYS:N	2.35	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: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:E:346:ARG:CG	1:E:404:TYR:HE2	2.11	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:F:330:GLN:HE22	1:F:364:ILE:H	1.55	0.52
1:G:152:PRO:HD2	1:G:153:LYS:HZ2	1.74	0.52
1:E:296:ASP:O	1:E:297:TYR:HB2	2.08	0.52
1:A:171:ASN:O	1:A:172:THR:HB	2.09	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:H:95:ARG:HD3	1:H:97:TRP:HZ3	1.74	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: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:482:ARG:NH2	1:E:458:LYS:NZ	2.58	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: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:E:171:ASN:O	1:E:172:THR:HB	2.10	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:G:478:GLU:HB2	1:G:482:ARG:NH1	2.18	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:C:253:LYS:C	1:C:253:LYS:HE2	2.31	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:F:195:ARG:HG3	1:G:104:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HG13	1:A:367:THR:HG23	1.94	0.50
1:H:296:ASP:O	1:H:297:TYR:HB2	2.10	0.50
1:G:489:GLU:HA	1:G:492:LYS:HB2	1.93	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: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:G:277:LEU:CB	1:G:288:ILE:CD1	2.89	0.50
1:D:296:ASP:O	1:D:297:TYR:HB2	2.11	0.50
1:G:95:ARG:HG3	1:G:204:LEU:HD11	1.94	0.50
1:E:133:THR:O	1:E:135:LYS:N	2.38	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:D:171:ASN:O	1:D:172:THR:HB	2.10	0.50
1:D:284:CYS:HB3	1:D:334:ALA:HB2	1.94	0.49
1:C:284:CYS:CB	1:C:334:ALA:HB2	2.42	0.49
1:E:417:LEU:HD13	1:E:463:VAL:HG22	1.94	0.49
1:H:328:PHE:CD1	1:H:417:LEU:HG	2.47	0.49
1:B:292:PHE:HB2	1:B:298:TYR:HB2	1.93	0.49
1:A:489:GLU:HA	1:A:492:LYS:HB2	1.94	0.49
1:D:417:LEU:HD13	1:D:463:VAL:HG22	1.94	0.49
1:A:417:LEU:HD13	1:A:463:VAL:HG22	1.94	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:489:GLU:HA	1:D:492:LYS:HB2	1.95	0.49
1:D:350:PRO:HD3	1:D:416:ILE:HG12	1.94	0.49
1:F:166:ASN:HD21	1:G:129:LEU:HD13	1.77	0.49
1:A:395:VAL:O	1:A:395:VAL:HG12	2.12	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:B:95:ARG:HG3	1:B:204:LEU:HD11	1.94	0.49
1:A:417:LEU:HD13	1:A:463:VAL:CG2	2.43	0.49
1:F:346:ARG:HD2	1:F:371:HIS:O	2.13	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:A:458:LYS:HG2	1:A:458:LYS:H	1.47	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:G:284:CYS:HA	1:G:364:ILE:O	2.13	0.48
1:E:417:LEU:HD13	1:E:463:VAL:CG2	2.43	0.48
1:H:489:GLU:HA	1:H:492:LYS:HB2	1.95	0.48
1:E:489:GLU:HA	1:E:492:LYS:HB2	1.94	0.48
1:B:417:LEU:HD13	1:B:463:VAL:HG22	1.96	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: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: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: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:G:112:ASN:HD21	1:G:145:ARG:HH11	1.61	0.47
1:C:95:ARG:HG3	1:C:204:LEU:HD11	1.96	0.47
1:H:417:LEU:HD13	1:H:463:VAL:HG22	1.95	0.47
1:C:162:ASP:HB3	1:C:176:GLY:O	2.14	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:F:132:ARG:HH11	1:H:129:LEU:HB2	1.79	0.47
1:D:457:GLU:OE2	1:H:119:LYS:CD	2.51	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:E:152:PRO:HG3	1:F:305:GLU:HG3	1.96	0.47
1:B:458:LYS:HG2	1:B:458:LYS:H	1.47	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:H:203:ASP:HB3	1:H:206:VAL:CG2	2.45	0.46
1:F:458:LYS:H	1:F:458:LYS:HG2	1.47	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:417:LEU:HD13	1:G:463:VAL:HG22	1.96	0.46
1:G:253:LYS:HE2	1:G:253:LYS:C	2.36	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:F:112:ASN:HD21	1:F:145:ARG:HH11	1.62	0.45
1:C:304:MET:HE2	1:C:356:SER:HB3	1.96	0.45
1:A:152:PRO:HD2	1:A:153:LYS:HZ2	1.81	0.45
1:E:112:ASN:HD21	1:E:145:ARG:HH11	1.64	0.45
1:A:162:ASP:HB2	1:A:175:VAL:HB	1.98	0.45
1:E:345:HIS:CG	1:E:348:LEU:HD13	2.51	0.45
1:F:328:PHE:CD1	1:F:417:LEU:HG	2.50	0.45
1:B:345:HIS:CG	1:B:348:LEU:HD13	2.51	0.45
1:G:304:MET:CE	1:G:356:SER:HA	2.46	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:A:345:HIS:CG	1:A:348:LEU:HD13	2.52	0.45
1:A:253:LYS:C	1:A:253:LYS:HE2	2.37	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:G:221:ILE:HG21	1:H:182:PRO:HG2	1.99	0.45
1:G:152:PRO:HG3	1:H:305:GLU:CG	2.45	0.45
1:G:417:LEU:HD13	1:G:463:VAL:CG2	2.46	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: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:457:GLU:HG3	1:H:126:ASP:OD2	2.18	0.44
1:D:284:CYS:HB2	1:D:334:ALA:HB2	2.00	0.44
1:E:129:LEU:HD13	1:H:166:ASN:HD22	1.83	0.44
1:G:491:MET:HE2	1:G:492:LYS:HA	1.99	0.44
1:E:491:MET:HE2	1:E:492:LYS:HA	2.00	0.44
1:F:95:ARG:HD3	1:F:97:TRP:CZ3	2.53	0.44
1:C:282:HIS:CG	1:C:283:PRO:HD2	2.53	0.44
1:G:233:GLU:HG3	1:G:250:ILE:HB	2.00	0.44
1:F:162:ASP:HB2	1:F:175:VAL: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:B:132:ARG:HG3	1:D:101:ASP:OD1	2.18	0.43
1:A:225:THR:HG22	1:A:227:GLY:N	2.32	0.43
1:C:95:ARG:HD3	1:C:97:TRP:CZ3	2.51	0.43
1:D:304:MET:SD	1:D:365:LYS:HD2	2.59	0.43
1:A:393:PRO:HD3	1:A:411:TRP:CD2	2.54	0.43
1:C:282:HIS:CD2	1:C:337:TYR:HB2	2.53	0.43
1:A:162:ASP:HB3	1:A:176:GLY:O	2.18	0.43
1:C:282:HIS:HD2	1:C:337:TYR:CG	2.36	0.43
1:C:162:ASP:HB2	1:C:175:VAL:HB	2.01	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:H:458:LYS:HG2	1:H:458:LYS:H	1.47	0.43
1:F:193:LEU:HD23	1:G:127:GLU:OE1	2.19	0.43
1:A:304:MET:HB2	1:A:354:LEU:HD13	2.00	0.43
1:A:285:ILE:HD11	1:A:338:LEU:HG	2.01	0.43
1:E:186:ASN:OD1	1:F:204:LEU:HD22	2.19	0.42
1:G:152:PRO:CG	1:H:305:GLU:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:HB2	1:A:350:PRO:HD2	2.01	0.42
1:G:339:HIS:CG	1:G:406:ARG:HD2	2.54	0.42
1:C:152:PRO:HD2	1:C:153:LYS:HZ2	1.82	0.42
1:A:233:GLU:HG3	1:A:250:ILE:HB	2.01	0.42
1:H:345:HIS:CG	1:H:348:LEU:HD13	2.54	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: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:C:233:GLU:HG3	1:C:250:ILE:HB	2.01	0.42
1:A:290:ASN:OD1	1:A:291:PHE:N	2.52	0.42
1:E:305:GLU:O	1:F:152:PRO:HB2	2.19	0.42
1:A:393:PRO:HD3	1:A:411:TRP:CE2	2.54	0.42
1:E:324:CYS:SG	1:E:420:CYS:HB3	2.60	0.42
1:A:450:GLU:H	1:A:450:GLU:HG3	1.49	0.42
1:H:162:ASP:HB2	1:H:175:VAL:HB	2.00	0.42
1:B:328:PHE:CD1	1:B:417:LEU:HG	2.55	0.42
1:C:491:MET:HE2	1:C:492:LYS:HA	2.02	0.42
1:C:458:LYS:H	1:C:458:LYS:HG2	1.43	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:G:290:ASN:OD1	1:G:291:PHE:N	2.53	0.41
1:D:271:GLU:HG2	1:D:291:PHE:CE2	2.55	0.41
1:C:282:HIS:CD2	1:C:337:TYR:CB	3.02	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:H:95:ARG:HD3	1:H:97:TRP:CZ3	2.55	0.41
1:G:345:HIS:CG	1:G:348:LEU:HD13	2.56	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:H:450:GLU:HG3	1:H:450:GLU:H	1.51	0.41
1:H:346:ARG:NH1	1:H:371:HIS:ND1	2.68	0.41
1:B:194:SER:H	1:C:127:GLU:CD	2.24	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:B:290:ASN:HB3	1:B:300:VAL:HB	2.03	0.41
1:H:225:THR:HG22	1:H:227:GLY:H	1.85	0.41
1:E:331:MET:CE	1:E:413:LEU:HD22	2.50	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:220:TYR:HA	1:E:238:PHE:O	2.21	0.41
1:C:491:MET:HE3	1:C:491:MET:O	2.19	0.41
1:A:140:SER:HB2	1:A:143:HIS:HA	2.02	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:E:305:GLU:O	1:F:152:PRO:CB	2.69	0.41
1:C:253:LYS:H	1:C:253:LYS:HG3	1.73	0.41
1:G:466:LEU:HA	1:G:466:LEU:HD12	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:D:238:PHE:CE2	1:D:245:LYS:HG2	2.56	0.40
1:C:284:CYS:HB2	1:C:334:ALA:HB2	2.02	0.40
1:B:335:VAL:HG21	1:B:413:LEU:HD11	2.01	0.40
1:G:431:ARG:HB3	1:G:432:THR:H	1.77	0.40
1:C:237:ALA:HB3	1:C:246:VAL:HG23	2.03	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:E:129:LEU:HD13	1:H:166:ASN:ND2	2.37	0.40
1:A:112:ASN:HD21	1:A:145:ARG:HH11	1.65	0.40
1:D:392:ALA:HA	1:D:393:PRO:HD3	1.95	0.40
1:F:364:ILE:HD12	1:F:364:ILE:HA	1.91	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: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:F:132:ARG:HH11	1:H:129:LEU:HD13	1.86	0.40
1:E:101:ASP:C	1:H:193:LEU:HD21	2.42	0.40
1:B:364:ILE:HD12	1:B:364:ILE:HA	1.90	0.40
1:D:392:ALA:HB2	1:D:408:VAL:HG23	2.03	0.40
1:C:329:TYR:CE1	1:C:492:LYS:HE2	2.57	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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	37
1	B	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	10	48
1	C	358/443 (81%)	326 (91%)	21 (6%)	11 (3%)	5	34
1	D	372/443 (84%)	334 (90%)	31 (8%)	7 (2%)	10	48
1	E	358/443 (81%)	327 (91%)	21 (6%)	10 (3%)	6	37
1	F	372/443 (84%)	337 (91%)	28 (8%)	7 (2%)	10	48
1	G	359/443 (81%)	328 (91%)	21 (6%)	10 (3%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	372/443 (84%)	335 (90%)	30 (8%)	7 (2%)	10	48
All	All	2922/3544 (82%)	2650 (91%)	203 (7%)	69 (2%)	7	41

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 ⓘ

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%)	12	42
1	B	344/395 (87%)	311 (90%)	33 (10%)	10	38
1	C	333/395 (84%)	302 (91%)	31 (9%)	11	40
1	D	344/395 (87%)	312 (91%)	32 (9%)	11	40
1	E	333/395 (84%)	303 (91%)	30 (9%)	12	42
1	F	344/395 (87%)	312 (91%)	32 (9%)	11	40
1	G	333/395 (84%)	302 (91%)	31 (9%)	11	40
1	H	344/395 (87%)	312 (91%)	32 (9%)	11	40
All	All	2708/3160 (86%)	2457 (91%)	251 (9%)	11	40

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

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

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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 ⓘ

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%)	0.67	36 (9%) 10 7	118, 136, 157, 175	0
1	B	382/443 (86%)	0.61	40 (10%) 8 6	115, 136, 154, 182	0
1	C	368/443 (83%)	0.58	32 (8%) 13 8	119, 134, 158, 178	0
1	D	382/443 (86%)	0.74	56 (14%) 3 2	118, 136, 154, 182	0
1	E	368/443 (83%)	1.18	79 (21%) 1 1	118, 136, 157, 180	0
1	F	382/443 (86%)	1.10	92 (24%) 1 1	118, 137, 153, 182	0
1	G	369/443 (83%)	0.98	55 (14%) 3 2	115, 137, 156, 178	0
1	H	382/443 (86%)	0.95	66 (17%) 2 1	119, 136, 153, 181	0
All	All	3002/3544 (84%)	0.85	456 (15%) 3 2	115, 136, 156, 182	0

All (456) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	9.9
1	A	434	VAL	9.8
1	G	434	VAL	9.0
1	E	432	THR	8.6
1	E	241	LYS	7.0
1	D	314	VAL	6.9
1	H	452	TRP	6.9
1	E	126	ASP	6.7
1	F	452	TRP	6.6
1	F	475	PHE	6.4
1	F	102	GLY	6.4
1	E	269	ASN	6.4
1	G	430	HIS	6.3
1	C	431	ARG	6.1
1	E	402	ALA	6.0
1	D	429	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	G	450	GLU	5.8
1	B	156	TYR	5.8
1	E	154	ASN	5.8
1	F	177	LYS	5.8
1	G	207	ASP	5.5
1	H	455	VAL	5.5
1	F	210	SER	5.5
1	E	111	ASP	5.5
1	F	152	PRO	5.5
1	G	268	LEU	5.4
1	H	451	VAL	5.4
1	C	268	LEU	5.4
1	H	161	GLU	5.4
1	B	152	PRO	5.4
1	C	316	ASN	5.4
1	E	293	ASP	5.2
1	F	432	THR	5.2
1	H	432	THR	5.1
1	E	268	LEU	5.1
1	G	108	CYS	5.1
1	H	251	ILE	5.1
1	E	431	ARG	5.0
1	F	158	ALA	5.0
1	D	114	TRP	4.9
1	G	497	ASP	4.9
1	D	428	SER	4.9
1	E	315	GLY	4.9
1	H	493	ARG	4.9
1	H	120	SER	4.8
1	B	471	PRO	4.8
1	E	252	SER	4.7
1	D	357	SER	4.7
1	A	207	ASP	4.7
1	E	251	ILE	4.7
1	H	297	TYR	4.7
1	E	142	LYS	4.6
1	F	124	CYS	4.6
1	F	253	LYS	4.6
1	D	397	VAL	4.5
1	G	429	GLU	4.5
1	F	312	LYS	4.5
1	H	152	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	269	ASN	4.5
1	H	295	GLU	4.5
1	F	126	ASP	4.4
1	H	433	GLN	4.4
1	E	272	THR	4.4
1	E	395	VAL	4.4
1	C	429	GLU	4.4
1	E	428	SER	4.4
1	G	316	ASN	4.3
1	D	316	ASN	4.3
1	F	315	GLY	4.3
1	B	430	HIS	4.3
1	E	404	TYR	4.3
1	E	393	PRO	4.2
1	E	213	PRO	4.2
1	H	441	THR	4.2
1	E	298	TYR	4.2
1	F	314	VAL	4.2
1	G	101	ASP	4.2
1	E	192	SER	4.1
1	D	142	LYS	4.1
1	D	454	GLU	4.1
1	H	361	ASP	4.1
1	D	435	SER	4.1
1	B	448	ILE	4.0
1	G	156	TYR	4.0
1	G	253	LYS	4.0
1	H	111	ASP	4.0
1	F	298	TYR	4.0
1	H	233	GLU	4.0
1	G	137	ARG	4.0
1	F	114	TRP	3.9
1	B	132	ARG	3.9
1	G	128	PRO	3.9
1	D	163	HIS	3.9
1	D	382	ARG	3.9
1	H	431	ARG	3.9
1	B	315	GLY	3.9
1	A	431	ARG	3.8
1	B	324	CYS	3.8
1	A	177	LYS	3.8
1	D	101	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	429	GLU	3.8
1	E	397	VAL	3.8
1	F	123	TYR	3.8
1	F	294	ALA	3.8
1	D	404	TYR	3.8
1	C	272	THR	3.8
1	F	155	SER	3.8
1	H	440	ILE	3.8
1	H	142	LYS	3.8
1	D	118	ASP	3.7
1	F	446	ASN	3.7
1	F	178	GLY	3.7
1	E	184	ASN	3.7
1	D	177	LYS	3.7
1	B	436	LEU	3.7
1	F	214	LYS	3.7
1	F	125	PHE	3.7
1	B	215	ALA	3.6
1	H	207	ASP	3.6
1	C	152	PRO	3.6
1	C	274	ILE	3.6
1	D	156	TYR	3.5
1	G	177	LYS	3.5
1	G	92	PRO	3.5
1	E	187	SER	3.5
1	F	270	VAL	3.5
1	H	298	TYR	3.5
1	G	142	LYS	3.5
1	G	122	GLU	3.5
1	F	428	SER	3.5
1	D	119	LYS	3.5
1	E	292	PHE	3.5
1	F	436	LEU	3.5
1	F	434	VAL	3.5
1	D	457	GLU	3.4
1	E	291	PHE	3.4
1	F	93	TRP	3.4
1	E	396	LEU	3.4
1	E	493	ARG	3.4
1	F	137	ARG	3.4
1	G	326	LEU	3.4
1	H	437	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	451	VAL	3.4
1	F	167	GLY	3.4
1	F	122	GLU	3.4
1	A	268	LEU	3.3
1	E	316	ASN	3.3
1	H	211	VAL	3.3
1	H	314	VAL	3.3
1	B	432	THR	3.3
1	E	394	GLU	3.3
1	D	252	SER	3.3
1	G	314	VAL	3.3
1	F	447	PHE	3.3
1	E	130	LEU	3.3
1	E	156	TYR	3.3
1	B	314	VAL	3.3
1	D	121	CYS	3.3
1	B	126	ASP	3.3
1	C	432	THR	3.2
1	B	305	GLU	3.2
1	E	414	GLY	3.2
1	H	331	MET	3.2
1	E	100	GLN	3.2
1	F	495	PHE	3.2
1	H	414	GLY	3.2
1	F	403	GLY	3.2
1	F	388	PRO	3.2
1	A	297	TYR	3.2
1	C	430	HIS	3.2
1	C	293	ASP	3.2
1	D	251	ILE	3.2
1	D	315	GLY	3.2
1	H	393	PRO	3.2
1	H	436	LEU	3.2
1	H	118	ASP	3.1
1	D	396	LEU	3.1
1	C	270	VAL	3.1
1	A	404	TYR	3.1
1	C	195	ARG	3.1
1	H	117	ARG	3.1
1	D	434	VAL	3.1
1	B	429	GLU	3.1
1	H	137	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	284	CYS	3.1
1	F	412	SER	3.1
1	B	447	PHE	3.1
1	A	95	ARG	3.1
1	A	107	GLU	3.1
1	D	136	TYR	3.1
1	A	430	HIS	3.1
1	B	207	ASP	3.1
1	E	409	ASP	3.1
1	G	432	THR	3.0
1	E	125	PHE	3.0
1	F	356	SER	3.0
1	G	297	TYR	3.0
1	E	161	GLU	3.0
1	F	119	LYS	3.0
1	A	119	LYS	3.0
1	A	156	TYR	3.0
1	E	279	LYS	3.0
1	C	404	TYR	3.0
1	E	271	GLU	3.0
1	C	215	ALA	3.0
1	E	276	ILE	3.0
1	E	299	ILE	3.0
1	F	132	ARG	3.0
1	H	448	ILE	3.0
1	H	128	PRO	3.0
1	F	435	SER	3.0
1	F	402	ALA	3.0
1	H	357	SER	3.0
1	B	497	ASP	3.0
1	A	164	SER	2.9
1	G	361	ASP	2.9
1	B	322	ALA	2.9
1	F	450	GLU	2.9
1	D	102	GLY	2.9
1	E	128	PRO	2.9
1	F	316	ASN	2.9
1	F	454	GLU	2.9
1	G	161	GLU	2.9
1	H	148	ARG	2.9
1	E	206	VAL	2.9
1	F	163	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	114	TRP	2.9
1	D	211	VAL	2.9
1	E	430	HIS	2.9
1	E	169	PHE	2.9
1	F	361	ASP	2.9
1	G	414	GLY	2.9
1	H	429	GLU	2.9
1	G	163	HIS	2.9
1	H	220	TYR	2.8
1	E	403	GLY	2.8
1	B	316	ASN	2.8
1	F	188	GLU	2.8
1	E	207	ASP	2.8
1	F	357	SER	2.8
1	F	127	GLU	2.8
1	B	431	ARG	2.8
1	A	361	ASP	2.8
1	D	117	ARG	2.8
1	H	472	LYS	2.8
1	E	185	ASN	2.8
1	D	131	LYS	2.8
1	H	305	GLU	2.8
1	D	430	HIS	2.8
1	C	207	ASP	2.8
1	F	151	GLY	2.8
1	E	141	LYS	2.8
1	F	437	LYS	2.8
1	G	251	ILE	2.8
1	G	233	GLU	2.8
1	E	195	ARG	2.8
1	G	413	LEU	2.7
1	G	327	TYR	2.7
1	E	113	TYR	2.7
1	H	499	LEU	2.7
1	E	137	ARG	2.7
1	G	428	SER	2.7
1	A	220	TYR	2.7
1	H	430	HIS	2.7
1	H	473	ALA	2.7
1	D	103	PHE	2.7
1	F	379	SER	2.7
1	F	113	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	441	THR	2.7
1	B	433	GLN	2.7
1	D	446	ASN	2.7
1	C	435	SER	2.7
1	F	194	SER	2.7
1	H	358	GLN	2.7
1	E	329	TYR	2.7
1	A	355	LEU	2.7
1	H	135	LYS	2.7
1	E	168	THR	2.7
1	E	314	VAL	2.7
1	D	151	GLY	2.7
1	H	330	GLN	2.7
1	E	214	LYS	2.6
1	G	494	LYS	2.6
1	H	252	SER	2.6
1	G	293	ASP	2.6
1	B	323	THR	2.6
1	A	253	LYS	2.6
1	E	412	SER	2.6
1	E	435	SER	2.6
1	F	117	ARG	2.6
1	A	184	ASN	2.6
1	D	433	GLN	2.6
1	A	251	ILE	2.6
1	H	492	LYS	2.6
1	B	412	SER	2.6
1	F	154	ASN	2.6
1	G	270	VAL	2.6
1	C	252	SER	2.6
1	F	107	GLU	2.6
1	H	119	LYS	2.6
1	D	495	PHE	2.6
1	F	185	ASN	2.6
1	F	156	TYR	2.6
1	D	436	LEU	2.5
1	H	146	ILE	2.5
1	D	152	PRO	2.5
1	E	233	GLU	2.5
1	G	193	LEU	2.5
1	F	141	LYS	2.5
1	A	414	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	417	LEU	2.5
1	F	121	CYS	2.5
1	B	434	VAL	2.5
1	G	355	LEU	2.5
1	C	251	ILE	2.5
1	D	188	GLU	2.5
1	H	315	GLY	2.5
1	A	182	PRO	2.5
1	F	136	TYR	2.5
1	H	380	LEU	2.5
1	E	152	PRO	2.5
1	H	328	PHE	2.5
1	E	133	THR	2.5
1	F	441	THR	2.5
1	C	241	LYS	2.5
1	F	153	LYS	2.5
1	B	404	TYR	2.4
1	E	186	ASN	2.4
1	E	388	PRO	2.4
1	B	295	GLU	2.4
1	G	437	LYS	2.4
1	B	328	PHE	2.4
1	D	150	VAL	2.4
1	H	434	VAL	2.4
1	F	364	ILE	2.4
1	F	101	ASP	2.4
1	C	346	ARG	2.4
1	G	118	ASP	2.4
1	F	103	PHE	2.4
1	A	435	SER	2.4
1	D	296	ASP	2.4
1	H	395	VAL	2.4
1	A	134	ASP	2.4
1	B	222	MET	2.4
1	F	211	VAL	2.4
1	D	363	LEU	2.4
1	E	274	ILE	2.4
1	G	435	SER	2.4
1	A	360	GLU	2.4
1	A	429	GLU	2.4
1	F	139	TYR	2.4
1	H	154	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	436	LEU	2.3
1	F	208	ASP	2.3
1	E	124	CYS	2.3
1	H	103	PHE	2.3
1	A	327	TYR	2.3
1	D	432	THR	2.3
1	F	142	LYS	2.3
1	F	486	LEU	2.3
1	G	416	ILE	2.3
1	B	148	ARG	2.3
1	D	431	ARG	2.3
1	C	204	LEU	2.3
1	E	471	PRO	2.3
1	G	213	PRO	2.3
1	D	362	CYS	2.3
1	D	126	ASP	2.3
1	E	344	ILE	2.3
1	B	223	SER	2.3
1	H	107	GLU	2.3
1	D	132	ARG	2.3
1	C	276	ILE	2.3
1	F	421	LEU	2.3
1	A	410	CYS	2.3
1	H	121	CYS	2.3
1	E	216	LEU	2.3
1	G	315	GLY	2.3
1	F	295	GLU	2.3
1	H	296	ASP	2.3
1	D	202	PHE	2.3
1	F	241	LYS	2.3
1	A	195	ARG	2.3
1	E	193	LEU	2.3
1	G	311	ASP	2.2
1	A	136	TYR	2.2
1	G	417	LEU	2.2
1	G	418	PHE	2.2
1	A	439	GLN	2.2
1	E	442	SER	2.2
1	D	222	MET	2.2
1	B	441	THR	2.2
1	E	448	ILE	2.2
1	G	448	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	439	GLN	2.2
1	C	291	PHE	2.2
1	F	355	LEU	2.2
1	F	200	VAL	2.2
1	F	500	SER	2.2
1	D	186	ASN	2.2
1	F	92	PRO	2.2
1	D	475	PHE	2.2
1	F	404	TYR	2.2
1	H	489	GLU	2.2
1	F	238	PHE	2.2
1	G	472	LYS	2.2
1	B	450	GLU	2.2
1	G	148	ARG	2.2
1	B	327	TYR	2.1
1	F	491	MET	2.1
1	B	449	PRO	2.1
1	F	251	ILE	2.1
1	C	214	LYS	2.1
1	H	404	TYR	2.1
1	E	148	ARG	2.1
1	F	453	ALA	2.1
1	D	239	GLU	2.1
1	D	393	PRO	2.1
1	B	166	ASN	2.1
1	G	143	HIS	2.1
1	F	293	ASP	2.1
1	A	412	SER	2.1
1	F	223	SER	2.1
1	E	270	VAL	2.1
1	C	148	ARG	2.1
1	G	250	ILE	2.1
1	H	284	CYS	2.1
1	B	294	ALA	2.1
1	F	118	ASP	2.1
1	A	108	CYS	2.1
1	D	482	ARG	2.1
1	F	423	GLY	2.1
1	A	117	ARG	2.1
1	H	156	TYR	2.1
1	E	429	GLU	2.1
1	C	187	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	405	ASN	2.1
1	D	185	ASN	2.0
1	E	220	TYR	2.0
1	F	305	GLU	2.0
1	G	443	GLY	2.0
1	C	92	PRO	2.0
1	G	299	ILE	2.0
1	H	250	ILE	2.0
1	B	417	LEU	2.0
1	H	500	SER	2.0
1	F	390	TYR	2.0
1	F	283	PRO	2.0
1	G	130	LEU	2.0
1	B	435	SER	2.0
1	H	412	SER	2.0
1	A	133	THR	2.0
1	G	95	ARG	2.0
1	C	344	ILE	2.0
1	C	396	LEU	2.0
1	G	328	PHE	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 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.