



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 AM GMT

PDB ID : 2QMR
Title : Karyopherin beta2/transportin
Authors : Cansizoglu, A.E.; Chook, Y.M.
Deposited on : 2007-07-16
Resolution : 3.00 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

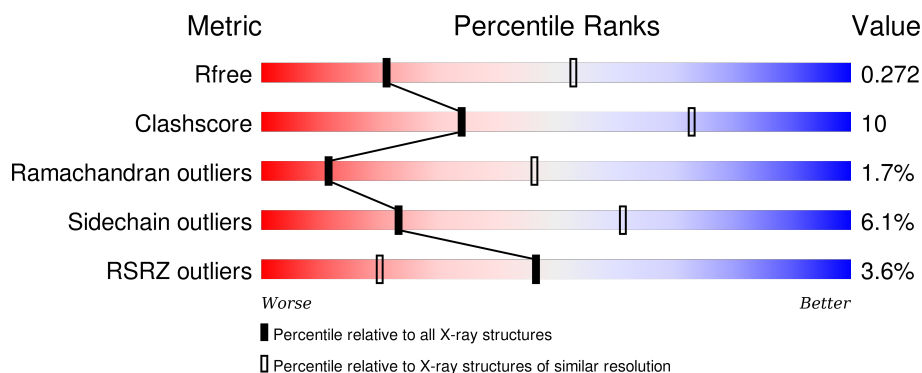
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	890	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>6%</div> </div> </div>
1	B	890	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>10%</div> </div> </div>
1	C	890	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>7%</div> </div> </div>
1	D	890	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>6%</div> </div> </div>

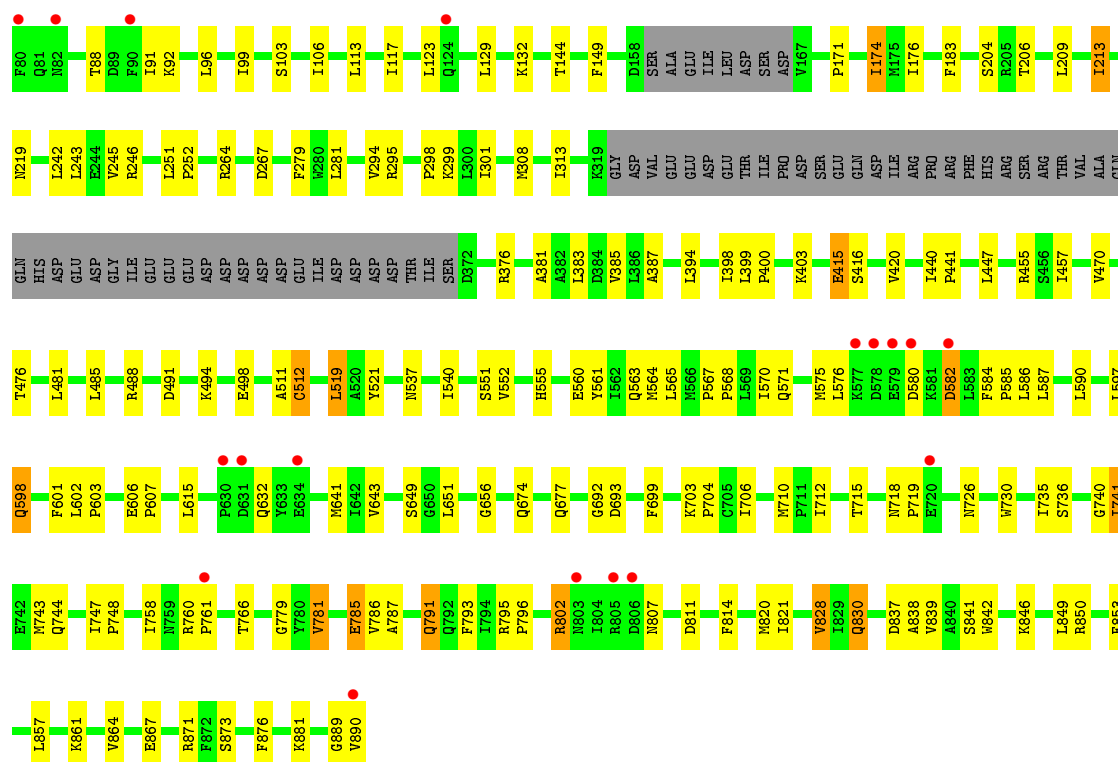
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25774 atoms, of which 0 are hydrogens and 0 are deuteriums.

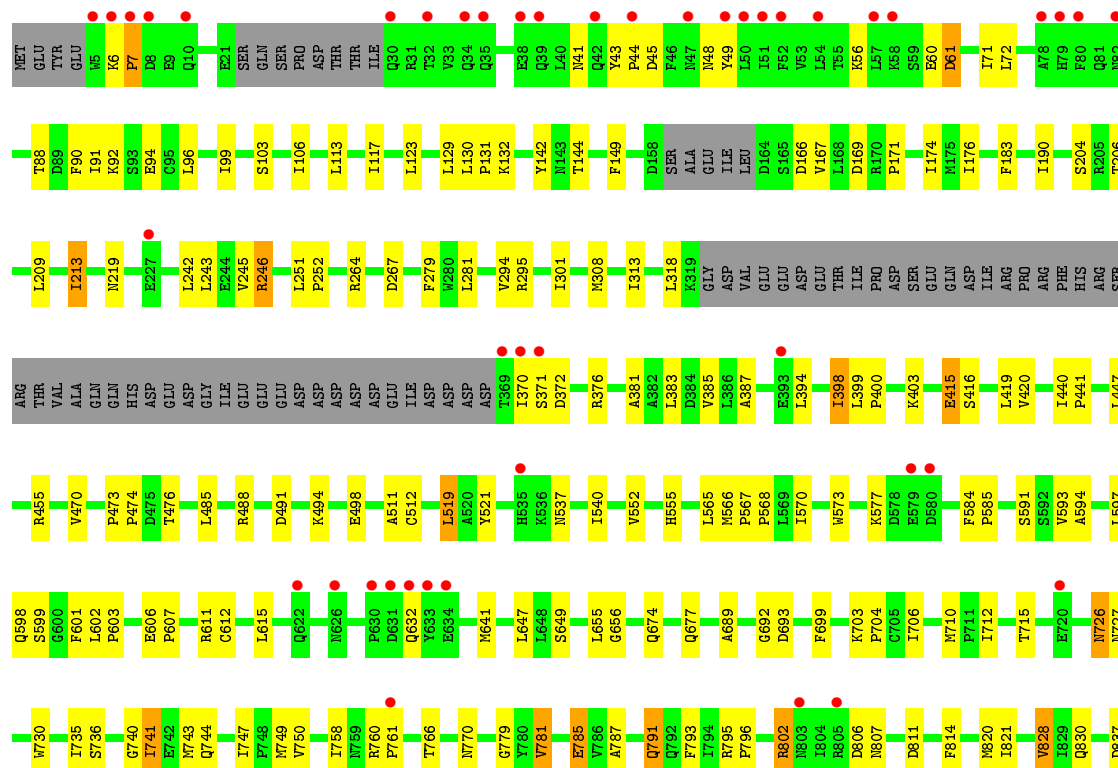
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6523	4183	1090	1199	51			
1	B	801	Total	C	N	O	S	0	0	0
			6308	4054	1051	1152	51			
1	C	824	Total	C	N	O	S	0	0	0
			6422	4122	1073	1176	51			
1	D	835	Total	C	N	O	S	0	0	0
			6521	4182	1089	1199	51			

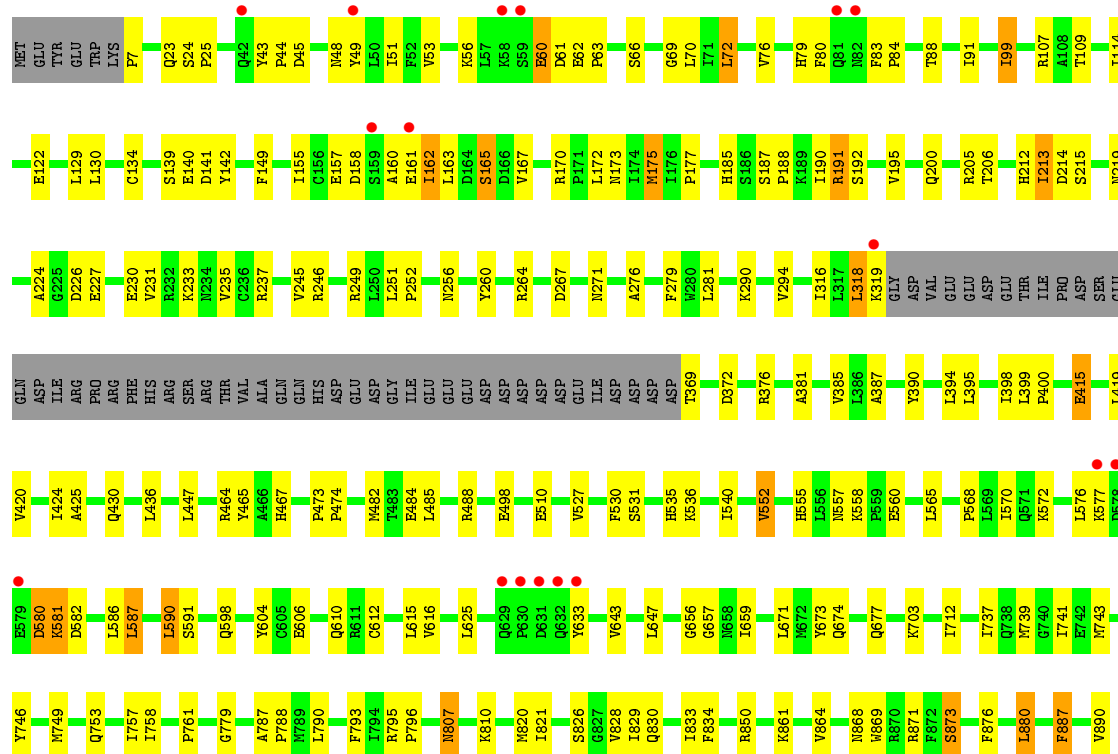


• Molecule 1: Transportin-1





● Molecule 1: Transportin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.34Å 168.89Å 140.96Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.13 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.00) 99.9 (49.13-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.286 0.247 , 0.272	Depositor DCC
R_{free} test set	6076 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 121002 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25774	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.20% 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 [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	0.41	0/6662	0.56	2/9060 (0.0%)
1	B	0.37	0/6446	0.54	0/8762
1	C	0.41	0/6559	0.55	1/8918 (0.0%)
1	D	0.40	0/6660	0.56	2/9056 (0.0%)
All	All	0.40	0/26327	0.56	5/35796 (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	A	7	PRO	N-CA-CB	6.07	110.58	103.30
1	D	7	PRO	N-CA-CB	6.03	110.53	103.30
1	D	25	PRO	N-CA-CB	6.01	110.52	103.30
1	A	25	PRO	N-CA-CB	5.90	110.38	103.30
1	C	7	PRO	N-CA-CB	5.86	110.33	103.30

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	6523	0	6459	145	0
1	B	6308	0	6296	117	0
1	C	6422	0	6345	119	0
1	D	6521	0	6462	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25774	0	25562	520	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (520) 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:60:GLU:CG	1:A:61:ASP:H	1.73	1.01
1:C:56:LYS:O	1:C:60:GLU:HB3	1.61	1.01
1:D:60:GLU:CG	1:D:61:ASP:H	1.71	1.01
1:B:56:LYS:O	1:B:60:GLU:HB3	1.64	0.98
1:D:188:PRO:HA	1:D:191:ARG:NH1	1.82	0.95
1:A:188:PRO:HA	1:A:191:ARG:NH1	1.82	0.94
1:D:177:PRO:HG3	1:D:212:HIS:CE1	2.03	0.93
1:D:587:LEU:HD22	1:D:643:VAL:HG12	1.50	0.92
1:A:177:PRO:HG3	1:A:212:HIS:CE1	2.05	0.92
1:C:873:SER:HA	1:C:876:PHE:CD2	2.04	0.91
1:B:873:SER:HA	1:B:876:PHE:CD2	2.05	0.90
1:A:821:ILE:HG12	1:A:828:VAL:HG21	1.56	0.85
1:A:49:TYR:CE1	1:A:91:ILE:HG12	2.11	0.85
1:D:49:TYR:CE1	1:D:91:ILE:HG12	2.11	0.85
1:D:134:CYS:HB3	1:D:175:MET:HE2	1.59	0.85
1:C:584:PHE:HB3	1:C:585:PRO:HD3	1.56	0.84
1:D:60:GLU:HG2	1:D:61:ASP:H	1.42	0.84
1:C:873:SER:HA	1:C:876:PHE:HD2	1.41	0.83
1:A:60:GLU:HG2	1:A:61:ASP:H	1.44	0.80
1:D:213:ILE:CD1	1:D:246:ARG:HH21	1.95	0.80
1:D:60:GLU:HG3	1:D:61:ASP:H	1.47	0.79
1:B:873:SER:HA	1:B:876:PHE:HD2	1.44	0.79
1:D:60:GLU:CG	1:D:61:ASP:N	2.45	0.79
1:D:425:ALA:HB2	1:D:465:TYR:HE1	1.46	0.78
1:B:839:VAL:HG11	1:B:853:PHE:CE2	2.19	0.78
1:A:213:ILE:CD1	1:A:246:ARG:HH21	1.97	0.77
1:A:60:GLU:HG3	1:A:61:ASP:H	1.48	0.77
1:A:793:PHE:HZ	1:A:820:MET:HE1	1.50	0.77
1:D:821:ILE:HG12	1:D:828:VAL:HG21	1.65	0.76
1:A:60:GLU:CG	1:A:61:ASP:N	2.47	0.76
1:C:839:VAL:HG11	1:C:853:PHE:CE2	2.20	0.76
1:C:814:PHE:HZ	1:C:853:PHE:HD2	1.33	0.76
1:C:785:GLU:OE1	1:C:785:GLU:HA	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:PHE:HZ	1:D:820:MET:CE	2.00	0.75
1:A:162:ILE:HG22	1:A:163:LEU:N	2.02	0.75
1:B:814:PHE:HZ	1:B:853:PHE:HD2	1.33	0.74
1:B:498:GLU:HG3	1:B:537:ASN:ND2	2.03	0.74
1:C:814:PHE:HZ	1:C:853:PHE:CD2	2.06	0.74
1:A:425:ALA:HB2	1:A:465:TYR:HE1	1.51	0.74
1:B:814:PHE:HZ	1:B:853:PHE:CD2	2.05	0.73
1:D:191:ARG:HH11	1:D:191:ARG:CG	2.02	0.73
1:D:570:ILE:HD11	1:D:604:TYR:HB3	1.71	0.73
1:C:793:PHE:HZ	1:C:820:MET:HE1	1.54	0.72
1:A:821:ILE:HG12	1:A:828:VAL:CG2	2.20	0.71
1:C:649:SER:HB2	1:C:693:ASP:OD2	1.89	0.71
1:C:470:VAL:HG22	1:C:511:ALA:HB2	1.71	0.71
1:A:793:PHE:HZ	1:A:820:MET:CE	2.04	0.71
1:A:49:TYR:CE1	1:A:72:LEU:HD21	2.26	0.70
1:C:735:ILE:HG22	1:C:743:MET:HE3	1.73	0.70
1:B:649:SER:HB2	1:B:693:ASP:OD2	1.90	0.70
1:D:162:ILE:HG22	1:D:163:LEU:H	1.56	0.70
1:A:134:CYS:HB3	1:A:175:MET:CE	2.22	0.70
1:C:793:PHE:CZ	1:C:820:MET:HE1	2.27	0.70
1:D:233:LYS:HE3	1:D:237:ARG:NH1	2.07	0.70
1:B:470:VAL:HG22	1:B:511:ALA:HB2	1.74	0.69
1:D:793:PHE:HZ	1:D:820:MET:HE3	1.58	0.69
1:A:807:ASN:ND2	1:A:810:LYS:H	1.91	0.69
1:D:49:TYR:CE1	1:D:72:LEU:HD21	2.29	0.68
1:B:567:PRO:HB2	1:B:568:PRO:HD3	1.75	0.68
1:A:49:TYR:CZ	1:A:72:LEU:HD21	2.28	0.68
1:A:673:TYR:OH	1:A:712:ILE:HD11	1.94	0.68
1:B:740:GLY:HA2	1:B:781:VAL:HG22	1.74	0.68
1:A:191:ARG:CG	1:A:191:ARG:HH11	2.07	0.68
1:B:787:ALA:HA	1:B:820:MET:HE3	1.76	0.68
1:C:599:SER:HA	1:C:655:LEU:HD23	1.75	0.67
1:C:740:GLY:HA2	1:C:781:VAL:HG22	1.75	0.67
1:A:612:CYS:O	1:A:616:VAL:HG23	1.94	0.67
1:D:673:TYR:OH	1:D:712:ILE:HD11	1.95	0.67
1:C:498:GLU:HG3	1:C:537:ASN:ND2	2.09	0.66
1:D:162:ILE:HG22	1:D:163:LEU:N	2.11	0.66
1:D:807:ASN:ND2	1:D:810:LYS:H	1.94	0.66
1:B:785:GLU:HA	1:B:785:GLU:OE1	1.94	0.65
1:A:233:LYS:HE3	1:A:237:ARG:NH1	2.10	0.65
1:A:188:PRO:CA	1:A:191:ARG:NH1	2.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:H	1:C:313:ILE:HD12	1.62	0.65
1:D:49:TYR:CZ	1:D:72:LEU:HD21	2.32	0.65
1:D:188:PRO:HA	1:D:191:ARG:HH12	1.62	0.65
1:D:185:HIS:HD2	1:D:187:SER:H	1.44	0.65
1:B:447:LEU:O	1:B:488:ARG:HD2	1.96	0.65
1:D:612:CYS:O	1:D:616:VAL:HG23	1.96	0.65
1:C:470:VAL:CG2	1:C:511:ALA:HB2	2.28	0.64
1:D:674:GLN:HA	1:D:677:GLN:HE21	1.63	0.64
1:A:162:ILE:HG22	1:A:163:LEU:H	1.60	0.64
1:D:570:ILE:CD1	1:D:604:TYR:HB3	2.28	0.64
1:A:674:GLN:HA	1:A:677:GLN:HE21	1.62	0.64
1:D:395:LEU:HA	1:D:398:ILE:HG22	1.80	0.64
1:C:447:LEU:O	1:C:488:ARG:HD2	1.98	0.64
1:D:188:PRO:HA	1:D:191:ARG:HH11	1.62	0.63
1:D:821:ILE:HG12	1:D:828:VAL:CG2	2.27	0.63
1:A:552:VAL:HG13	1:A:555:HIS:HB2	1.80	0.63
1:D:264:ARG:HB3	1:D:276:ALA:HB2	1.80	0.63
1:B:376:ARG:NH2	1:B:415:GLU:OE2	2.32	0.63
1:D:552:VAL:HG13	1:D:555:HIS:HB2	1.81	0.62
1:D:425:ALA:CB	1:D:465:TYR:HE1	2.11	0.62
1:A:264:ARG:NH1	1:A:267:ASP:OD2	2.33	0.62
1:D:191:ARG:HH11	1:D:191:ARG:HG2	1.62	0.62
1:B:601:PHE:CE2	1:B:651:LEU:HD11	2.34	0.62
1:A:188:PRO:HA	1:A:191:ARG:HH12	1.64	0.62
1:B:814:PHE:CZ	1:B:853:PHE:HD2	2.15	0.62
1:D:188:PRO:CA	1:D:191:ARG:NH1	2.61	0.62
1:C:814:PHE:CZ	1:C:853:PHE:HD2	2.15	0.62
1:B:455:ARG:NH1	1:B:491:ASP:OD2	2.31	0.62
1:A:188:PRO:CA	1:A:191:ARG:HH12	2.13	0.61
1:A:264:ARG:HB3	1:A:276:ALA:HB2	1.81	0.61
1:A:173:ASN:ND2	1:C:521:TYR:OH	2.33	0.61
1:B:313:ILE:H	1:B:313:ILE:HD12	1.65	0.61
1:A:192:SER:OG	1:A:230:GLU:HG3	2.01	0.61
1:D:795:ARG:HB2	1:D:796:PRO:HD3	1.81	0.60
1:C:400:PRO:HA	1:C:403:LYS:HE3	1.83	0.60
1:B:213:ILE:HD13	1:B:246:ARG:HE	1.65	0.60
1:A:185:HIS:HD2	1:A:187:SER:H	1.48	0.60
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.83	0.60
1:D:80:PHE:O	1:D:83:PHE:HB2	2.01	0.60
1:C:821:ILE:HG23	1:C:828:VAL:HG21	1.83	0.60
1:A:191:ARG:HH11	1:A:191:ARG:HG2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:VAL:CG2	1:B:511:ALA:HB2	2.31	0.60
1:C:455:ARG:NH1	1:C:491:ASP:OD2	2.32	0.60
1:B:740:GLY:HA2	1:B:781:VAL:CG2	2.32	0.60
1:A:570:ILE:HD11	1:A:604:TYR:HB3	1.84	0.60
1:D:192:SER:OG	1:D:230:GLU:HG3	2.01	0.59
1:D:213:ILE:HD11	1:D:246:ARG:HH21	1.67	0.59
1:B:521:TYR:OH	1:D:173:ASN:ND2	2.35	0.59
1:A:425:ALA:CB	1:A:465:TYR:HE1	2.15	0.59
1:A:290:LYS:O	1:A:294:VAL:HG23	2.02	0.59
1:C:567:PRO:HB2	1:C:568:PRO:HD3	1.85	0.59
1:D:142:TYR:HE1	1:D:190:ILE:HD12	1.67	0.59
1:B:793:PHE:HZ	1:B:820:MET:CE	2.15	0.59
1:A:231:VAL:O	1:A:235:VAL:HG23	2.02	0.59
1:D:861:LYS:HD2	1:D:890:VAL:HG13	1.83	0.59
1:A:80:PHE:O	1:A:83:PHE:HB2	2.03	0.59
1:B:821:ILE:HG23	1:B:828:VAL:HG21	1.83	0.59
1:A:188:PRO:HA	1:A:191:ARG:HH11	1.62	0.59
1:B:873:SER:HA	1:B:876:PHE:CE2	2.36	0.59
1:D:62:GLU:N	1:D:63:PRO:HD2	2.17	0.59
1:D:188:PRO:CA	1:D:191:ARG:HH12	2.15	0.59
1:C:873:SER:HA	1:C:876:PHE:CE2	2.37	0.59
1:D:213:ILE:HD12	1:D:249:ARG:HG3	1.84	0.58
1:B:565:LEU:O	1:B:568:PRO:HD2	2.03	0.58
1:C:49:TYR:CE2	1:C:72:LEU:HD21	2.38	0.58
1:B:308:MET:HE3	1:B:383:LEU:HD22	1.85	0.58
1:A:142:TYR:CE1	1:A:190:ILE:HD12	2.38	0.58
1:D:290:LYS:O	1:D:294:VAL:HG23	2.03	0.58
1:C:91:ILE:HG23	1:C:92:LYS:N	2.19	0.58
1:A:864:VAL:HG22	1:A:868:ASN:CB	2.34	0.58
1:B:793:PHE:CZ	1:B:820:MET:HE1	2.38	0.58
1:C:308:MET:HE3	1:C:383:LEU:HD22	1.84	0.58
1:A:793:PHE:O	1:A:796:PRO:HD2	2.03	0.58
1:B:49:TYR:CE2	1:B:72:LEU:HD21	2.39	0.58
1:D:436:LEU:HD21	1:D:465:TYR:CE2	2.38	0.57
1:C:740:GLY:HA2	1:C:781:VAL:CG2	2.34	0.57
1:B:213:ILE:HG21	1:B:246:ARG:HD3	1.86	0.57
1:B:91:ILE:HG23	1:B:92:LYS:N	2.18	0.57
1:D:587:LEU:HD22	1:D:643:VAL:CG1	2.30	0.57
1:B:793:PHE:HZ	1:B:820:MET:HE1	1.67	0.57
1:C:103:SER:HB3	1:C:106:ILE:HD12	1.86	0.57
1:C:793:PHE:HZ	1:C:820:MET:CE	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:LEU:HD11	1:B:586:LEU:HD23	1.87	0.57
1:C:213:ILE:HG21	1:C:246:ARG:HD3	1.85	0.57
1:C:381:ALA:O	1:C:385:VAL:HG23	2.05	0.57
1:C:519:LEU:HD11	1:C:552:VAL:HG21	1.85	0.57
1:D:251:LEU:HB3	1:D:252:PRO:HD3	1.87	0.57
1:C:243:LEU:HD22	1:C:279:PHE:CE1	2.40	0.57
1:B:779:GLY:HA3	1:B:820:MET:SD	2.45	0.56
1:D:134:CYS:HB3	1:D:175:MET:CE	2.34	0.56
1:C:213:ILE:HD13	1:C:246:ARG:HE	1.71	0.56
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.87	0.56
1:B:802:ARG:HA	1:B:842:TRP:CD1	2.40	0.56
1:C:96:LEU:HD13	1:C:132:LYS:HG2	1.87	0.56
1:C:376:ARG:NH2	1:C:415:GLU:OE2	2.39	0.56
1:A:60:GLU:HG3	1:A:61:ASP:N	2.18	0.56
1:B:400:PRO:HA	1:B:403:LYS:HE3	1.87	0.56
1:C:48:ASN:HD22	1:C:72:LEU:HD13	1.71	0.56
1:A:150:GLY:HA2	1:A:193:HIS:CE1	2.41	0.56
1:A:214:ASP:OD1	1:A:249:ARG:HD2	2.06	0.56
1:C:552:VAL:HG13	1:C:555:HIS:HB2	1.88	0.56
1:C:802:ARG:HA	1:C:842:TRP:CD1	2.40	0.56
1:C:735:ILE:HG22	1:C:743:MET:CE	2.35	0.56
1:A:524:ASP:OD1	1:A:564:MET:HE1	2.06	0.56
1:A:62:GLU:N	1:A:63:PRO:HD2	2.20	0.56
1:A:795:ARG:HB2	1:A:796:PRO:HD3	1.86	0.55
1:A:527:VAL:O	1:A:530:PHE:HB2	2.07	0.55
1:B:552:VAL:HG13	1:B:555:HIS:HB2	1.87	0.55
1:A:861:LYS:HD2	1:A:890:VAL:HG13	1.89	0.55
1:A:438:GLU:OE1	1:B:299:LYS:NZ	2.36	0.55
1:A:49:TYR:OH	1:A:91:ILE:HG23	2.07	0.55
1:B:103:SER:HB3	1:B:106:ILE:HD12	1.89	0.55
1:A:864:VAL:HG22	1:A:868:ASN:HB2	1.89	0.54
1:B:49:TYR:CZ	1:B:72:LEU:HD21	2.43	0.54
1:A:45:ASP:HA	1:A:48:ASN:HB2	1.89	0.54
1:D:758:ILE:HG12	1:D:796:PRO:HB2	1.89	0.54
1:D:864:VAL:HG22	1:D:868:ASN:CB	2.37	0.54
1:A:215:SER:O	1:A:219:ASN:ND2	2.40	0.54
1:A:779:GLY:HA3	1:A:820:MET:SD	2.48	0.54
1:D:49:TYR:OH	1:D:91:ILE:HG23	2.07	0.54
1:A:793:PHE:CZ	1:A:820:MET:HE1	2.37	0.54
1:A:142:TYR:HE1	1:A:190:ILE:HD12	1.72	0.54
1:C:779:GLY:HA3	1:C:820:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:OE1	1:A:193:HIS:ND1	2.37	0.54
1:D:264:ARG:NH1	1:D:267:ASP:OD2	2.38	0.53
1:A:582:ASP:O	1:A:585:PRO:HD2	2.08	0.53
1:D:425:ALA:CB	1:D:465:TYR:CE1	2.90	0.53
1:A:130:LEU:HD21	1:A:155:ILE:HG21	1.90	0.53
1:C:594:ALA:HA	1:C:601:PHE:CD1	2.43	0.53
1:C:264:ARG:NH1	1:C:267:ASP:OD2	2.41	0.53
1:C:853:PHE:HE1	1:C:857:LEU:HD11	1.73	0.53
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.89	0.53
1:A:826:SER:HA	1:A:829:ILE:HD12	1.90	0.53
1:C:584:PHE:HB3	1:C:585:PRO:CD	2.35	0.53
1:D:214:ASP:OD1	1:D:249:ARG:HD2	2.09	0.53
1:A:625:LEU:HB3	1:A:633:TYR:CD1	2.43	0.53
1:B:498:GLU:HG3	1:B:537:ASN:HD22	1.72	0.53
1:A:134:CYS:HB3	1:A:175:MET:HE2	1.90	0.53
1:B:519:LEU:HD11	1:B:552:VAL:HG21	1.89	0.53
1:C:606:GLU:HB3	1:C:607:PRO:HD3	1.91	0.53
1:C:183:PHE:HD1	1:C:219:ASN:HB3	1.74	0.52
1:D:447:LEU:O	1:D:488:ARG:HD2	2.09	0.52
1:D:45:ASP:HA	1:D:48:ASN:HB2	1.90	0.52
1:D:134:CYS:CB	1:D:175:MET:HE2	2.37	0.52
1:B:601:PHE:HE2	1:B:651:LEU:HD11	1.74	0.52
1:D:264:ARG:O	1:D:267:ASP:HB2	2.09	0.52
1:C:674:GLN:HA	1:C:677:GLN:HE21	1.74	0.52
1:B:183:PHE:HD1	1:B:219:ASN:HB3	1.75	0.52
1:B:597:LEU:O	1:B:598:GLN:C	2.48	0.52
1:B:853:PHE:HE1	1:B:857:LEU:HD11	1.75	0.52
1:C:49:TYR:CZ	1:C:72:LEU:HD21	2.44	0.52
1:D:703:LYS:HE3	1:D:739:MET:HE1	1.92	0.52
1:A:447:LEU:HD23	1:A:484:GLU:HB3	1.92	0.51
1:D:793:PHE:O	1:D:796:PRO:HD2	2.09	0.51
1:C:308:MET:HE1	1:C:383:LEU:HB2	1.92	0.51
1:C:318:LEU:HD21	1:C:370:ILE:HB	1.91	0.51
1:D:793:PHE:CZ	1:D:820:MET:HE3	2.44	0.51
1:D:130:LEU:HD21	1:D:155:ILE:HG21	1.91	0.51
1:B:674:GLN:HA	1:B:677:GLN:HE21	1.76	0.51
1:D:245:VAL:HG12	1:D:246:ARG:HG2	1.91	0.51
1:C:787:ALA:HA	1:C:820:MET:HE3	1.93	0.51
1:A:436:LEU:HD21	1:A:465:TYR:CE2	2.44	0.51
1:D:60:GLU:HG3	1:D:61:ASP:N	2.17	0.51
1:B:96:LEU:HD13	1:B:132:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:HD22	1:B:279:PHE:CE1	2.45	0.51
1:D:625:LEU:HB3	1:D:633:TYR:CD1	2.45	0.51
1:A:318:LEU:O	1:A:319:LYS:HB2	2.11	0.51
1:D:826:SER:HA	1:D:829:ILE:HD12	1.91	0.51
1:C:573:TRP:HZ2	1:C:611:ARG:HB3	1.76	0.51
1:D:60:GLU:HG2	1:D:61:ASP:N	2.18	0.51
1:A:425:ALA:CB	1:A:465:TYR:CE1	2.94	0.51
1:A:403:LYS:HE3	1:B:299:LYS:HE3	1.92	0.51
1:D:376:ARG:NH2	1:D:415:GLU:OE2	2.43	0.51
1:B:838:ALA:O	1:B:842:TRP:HB2	2.10	0.51
1:B:91:ILE:CG2	1:B:92:LYS:N	2.75	0.50
1:A:703:LYS:HE3	1:A:739:MET:HE1	1.93	0.50
1:C:251:LEU:HB3	1:C:252:PRO:HD3	1.92	0.50
1:C:91:ILE:CG2	1:C:92:LYS:N	2.74	0.50
1:C:440:ILE:HB	1:C:441:PRO:HD3	1.92	0.50
1:A:577:LYS:O	1:A:579:GLU:N	2.44	0.50
1:C:88:THR:O	1:C:91:ILE:HG22	2.12	0.50
1:D:318:LEU:O	1:D:319:LYS:HB2	2.11	0.50
1:B:301:ILE:HG21	1:B:398:ILE:HG12	1.92	0.50
1:D:165:SER:C	1:D:167:VAL:H	2.15	0.50
1:D:753:GLN:O	1:D:757:ILE:HG13	2.12	0.50
1:A:69:GLY:HA2	1:A:72:LEU:HD23	1.93	0.50
1:D:69:GLY:HA2	1:D:72:LEU:HD23	1.93	0.50
1:A:213:ILE:HD12	1:A:249:ARG:HG3	1.92	0.50
1:C:498:GLU:HG3	1:C:537:ASN:HD22	1.74	0.50
1:A:264:ARG:O	1:A:267:ASP:HB2	2.12	0.50
1:B:113:LEU:O	1:B:117:ILE:HD12	2.12	0.50
1:A:565:LEU:O	1:A:568:PRO:HD2	2.12	0.50
1:A:758:ILE:HG12	1:A:796:PRO:HB2	1.93	0.49
1:A:162:ILE:CG2	1:A:163:LEU:N	2.73	0.49
1:C:308:MET:HE1	1:C:383:LEU:CB	2.42	0.49
1:B:381:ALA:O	1:B:385:VAL:HG23	2.12	0.49
1:D:779:GLY:HA3	1:D:820:MET:SD	2.52	0.49
1:B:699:PHE:CE1	1:B:706:ILE:HD11	2.47	0.49
1:B:440:ILE:HB	1:B:441:PRO:HD3	1.93	0.49
1:B:560:GLU:O	1:B:564:MET:HG2	2.12	0.49
1:D:464:ARG:C	1:D:465:TYR:HD1	2.15	0.49
1:B:176:ILE:HD13	1:B:209:LEU:HB2	1.93	0.49
1:D:436:LEU:HD21	1:D:465:TYR:CD2	2.47	0.49
1:D:577:LYS:O	1:D:580:ASP:HB2	2.13	0.49
1:B:606:GLU:HB3	1:B:607:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD11	1:A:246:ARG:HH21	1.73	0.49
1:B:846:LYS:O	1:B:850:ARG:HB2	2.11	0.49
1:B:735:ILE:HG22	1:B:743:MET:HE3	1.94	0.49
1:D:591:SER:HA	1:D:647:LEU:HD13	1.95	0.49
1:A:795:ARG:HD3	1:A:834:PHE:HE2	1.78	0.49
1:C:176:ILE:HD13	1:C:209:LEU:HB2	1.95	0.49
1:B:48:ASN:HD22	1:B:72:LEU:HD13	1.77	0.49
1:C:183:PHE:CD1	1:C:219:ASN:HB3	2.48	0.49
1:A:447:LEU:O	1:A:488:ARG:HD2	2.12	0.49
1:A:464:ARG:C	1:A:465:TYR:HD1	2.16	0.48
1:B:692:GLY:HA3	1:B:730:TRP:CZ3	2.47	0.48
1:D:498:GLU:HG2	1:D:540:ILE:HD12	1.95	0.48
1:A:376:ARG:NH2	1:A:415:GLU:OE2	2.45	0.48
1:B:264:ARG:NH1	1:B:267:ASP:OD2	2.44	0.48
1:B:43:TYR:N	1:B:44:PRO:CD	2.77	0.48
1:D:557:ASN:C	1:D:558:LYS:HG2	2.33	0.48
1:C:308:MET:CE	1:C:383:LEU:HD22	2.44	0.48
1:D:565:LEU:O	1:D:568:PRO:HD2	2.14	0.48
1:B:786:VAL:HG12	1:B:820:MET:HE1	1.95	0.48
1:C:806:ASP:HB3	1:C:846:LYS:HE3	1.94	0.48
1:A:224:ALA:HB1	1:A:260:TYR:CE1	2.49	0.48
1:C:43:TYR:N	1:C:44:PRO:CD	2.76	0.48
1:A:753:GLN:O	1:A:757:ILE:HG13	2.13	0.48
1:A:498:GLU:HG2	1:A:540:ILE:HD12	1.96	0.48
1:D:864:VAL:HG22	1:D:868:ASN:HB2	1.96	0.48
1:D:99:ILE:HG13	1:D:114:ILE:CD1	2.44	0.48
1:B:183:PHE:CD1	1:B:219:ASN:HB3	2.48	0.48
1:D:807:ASN:HD22	1:D:810:LYS:H	1.62	0.47
1:A:850:ARG:HH11	1:A:887:PHE:HE2	1.61	0.47
1:B:735:ILE:HG22	1:B:743:MET:CE	2.44	0.47
1:D:586:LEU:O	1:D:590:LEU:HB2	2.14	0.47
1:A:435:TYR:CE2	1:B:298:PRO:HG2	2.49	0.47
1:B:795:ARG:HB2	1:B:796:PRO:HD3	1.95	0.47
1:B:251:LEU:HB3	1:B:252:PRO:HD3	1.95	0.47
1:C:570:ILE:O	1:C:573:TRP:HB3	2.14	0.47
1:D:376:ARG:NH2	1:D:419:LEU:HD22	2.30	0.47
1:C:113:LEU:O	1:C:117:ILE:HD12	2.15	0.47
1:D:213:ILE:HD13	1:D:246:ARG:HE	1.80	0.47
1:B:387:ALA:HA	1:B:394:LEU:HD22	1.97	0.47
1:B:582:ASP:O	1:B:585:PRO:HD2	2.14	0.47
1:C:699:PHE:CE1	1:C:706:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ALA:HA	1:C:394:LEU:HD22	1.96	0.47
1:D:795:ARG:HD3	1:D:834:PHE:HE2	1.80	0.47
1:A:376:ARG:NH2	1:A:419:LEU:HD22	2.29	0.47
1:C:873:SER:CA	1:C:876:PHE:HD2	2.20	0.46
1:C:49:TYR:CZ	1:C:91:ILE:HG13	2.50	0.46
1:B:308:MET:CE	1:B:383:LEU:HD22	2.44	0.46
1:C:692:GLY:HA3	1:C:730:TRP:CZ3	2.50	0.46
1:A:530:PHE:HD2	1:A:568:PRO:HB2	1.80	0.46
1:C:264:ARG:O	1:C:267:ASP:HB2	2.14	0.46
1:C:795:ARG:HB2	1:C:796:PRO:HD3	1.96	0.46
1:B:743:MET:HE2	1:B:743:MET:HB2	1.82	0.46
1:C:846:LYS:O	1:C:850:ARG:HB2	2.14	0.46
1:D:215:SER:O	1:D:219:ASN:ND2	2.46	0.46
1:C:889:GLY:O	1:C:890:VAL:HG23	2.16	0.46
1:A:70:LEU:HG	1:A:109:THR:HG23	1.98	0.46
1:D:231:VAL:O	1:D:235:VAL:HG23	2.16	0.46
1:A:99:ILE:HG13	1:A:114:ILE:CD1	2.45	0.46
1:B:488:ARG:NE	1:B:488:ARG:HA	2.31	0.46
1:D:43:TYR:N	1:D:44:PRO:CD	2.79	0.46
1:A:60:GLU:O	1:A:61:ASP:HB3	2.16	0.45
1:C:488:ARG:NE	1:C:488:ARG:HA	2.30	0.45
1:A:597:LEU:O	1:A:598:GLN:C	2.55	0.45
1:A:49:TYR:CE1	1:A:72:LEU:CD2	2.97	0.45
1:B:88:THR:O	1:B:91:ILE:HG22	2.15	0.45
1:C:602:LEU:HB3	1:C:603:PRO:HD3	1.98	0.45
1:A:587:LEU:HD23	1:A:647:LEU:HD23	1.99	0.45
1:D:142:TYR:CE1	1:D:190:ILE:CD1	2.99	0.45
1:A:76:VAL:O	1:A:80:PHE:HB2	2.16	0.45
1:B:416:SER:O	1:B:420:VAL:HG23	2.16	0.45
1:D:224:ALA:HB1	1:D:260:TYR:CE1	2.51	0.45
1:A:213:ILE:H	1:A:213:ILE:HG12	1.57	0.45
1:C:741:ILE:H	1:C:741:ILE:HG13	1.34	0.45
1:B:587:LEU:HD13	1:B:643:VAL:HG12	1.98	0.45
1:C:597:LEU:O	1:C:599:SER:N	2.50	0.45
1:A:584:PHE:HB2	1:A:640:PHE:HE1	1.82	0.45
1:D:467:HIS:HA	1:D:510:GLU:HG2	1.97	0.45
1:D:233:LYS:HE3	1:D:237:ARG:HH12	1.78	0.45
1:C:591:SER:HA	1:C:647:LEU:HD13	1.98	0.45
1:D:581:LYS:HA	1:D:581:LYS:HD2	1.77	0.45
1:A:60:GLU:HG2	1:A:61:ASP:N	2.19	0.45
1:C:60:GLU:O	1:C:61:ASP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:HA	1:A:319:LYS:HE3	1.99	0.45
1:A:387:ALA:HA	1:A:394:LEU:HD22	1.99	0.45
1:C:760:ARG:HA	1:C:761:PRO:HD3	1.82	0.45
1:D:793:PHE:HZ	1:D:820:MET:HE1	1.76	0.45
1:B:60:GLU:O	1:B:61:ASP:C	2.55	0.45
1:B:699:PHE:HE1	1:B:706:ILE:HD11	1.81	0.45
1:D:230:GLU:OE2	1:D:233:LYS:NZ	2.34	0.44
1:C:498:GLU:HG2	1:C:540:ILE:HD12	1.99	0.44
1:C:301:ILE:HG21	1:C:398:ILE:HG12	1.99	0.44
1:D:527:VAL:O	1:D:530:PHE:HB2	2.17	0.44
1:D:213:ILE:HG12	1:D:213:ILE:H	1.61	0.44
1:B:498:GLU:HG2	1:B:540:ILE:HD12	2.00	0.44
1:A:542:TYR:HE1	1:A:586:LEU:HB2	1.82	0.44
1:D:746:TYR:HD2	1:D:749:MET:HE3	1.82	0.44
1:A:57:LEU:HA	1:A:60:GLU:HB2	1.99	0.44
1:D:60:GLU:O	1:D:61:ASP:HB3	2.16	0.44
1:C:838:ALA:O	1:C:842:TRP:HB2	2.16	0.44
1:A:861:LYS:HG3	1:A:869:TRP:CG	2.53	0.44
1:A:649:SER:HB2	1:A:693:ASP:OD2	2.16	0.44
1:B:741:ILE:HG13	1:B:741:ILE:H	1.35	0.44
1:B:873:SER:CA	1:B:876:PHE:HD2	2.22	0.44
1:D:657:GLY:H	1:D:659:ILE:HG22	1.82	0.44
1:A:467:HIS:HA	1:A:510:GLU:HG2	1.98	0.44
1:A:43:TYR:N	1:A:44:PRO:CD	2.81	0.44
1:C:791:GLN:H	1:C:791:GLN:HG3	1.56	0.44
1:A:134:CYS:CB	1:A:175:MET:CE	2.95	0.44
1:D:294:VAL:HG22	1:D:390:TYR:HE2	1.83	0.44
1:D:70:LEU:HG	1:D:109:THR:HG23	1.99	0.44
1:D:316:ILE:HA	1:D:319:LYS:HE3	1.99	0.44
1:A:191:ARG:O	1:A:195:VAL:HG23	2.18	0.43
1:D:173:ASN:OD1	1:D:173:ASN:O	2.36	0.43
1:B:308:MET:HE1	1:B:383:LEU:HB2	2.00	0.43
1:C:736:SER:HA	1:C:743:MET:CE	2.49	0.43
1:D:530:PHE:CD2	1:D:568:PRO:HB2	2.53	0.43
1:B:602:LEU:HB3	1:B:603:PRO:HD3	1.99	0.43
1:B:48:ASN:HA	1:B:51:ILE:HD12	2.01	0.43
1:C:566:MET:HE1	1:C:593:VAL:HG11	2.00	0.43
1:B:512:CYS:HB3	1:B:551:SER:O	2.18	0.43
1:B:174:ILE:H	1:B:174:ILE:HG13	1.62	0.43
1:C:473:PRO:HA	1:C:474:PRO:HD3	1.82	0.43
1:C:399:LEU:O	1:C:403:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:HG3	1:D:200:GLN:NE2	2.32	0.43
1:A:743:MET:HE2	1:A:743:MET:HA	1.99	0.43
1:C:749:MET:HG3	1:C:750:VAL:HG23	2.00	0.43
1:D:88:THR:O	1:D:91:ILE:HB	2.19	0.43
1:B:567:PRO:CB	1:B:568:PRO:HD3	2.47	0.43
1:D:850:ARG:HH11	1:D:887:PHE:HE2	1.65	0.43
1:D:482:MET:HE2	1:D:482:MET:HB3	1.79	0.43
1:D:376:ARG:CZ	1:D:419:LEU:HD22	2.49	0.43
1:D:572:LYS:O	1:D:576:LEU:HG	2.18	0.43
1:C:242:LEU:O	1:C:245:VAL:O	2.36	0.43
1:A:49:TYR:CZ	1:A:91:ILE:HG23	2.53	0.43
1:A:213:ILE:HD13	1:A:246:ARG:HE	1.83	0.43
1:B:519:LEU:HD23	1:B:561:TYR:CE1	2.53	0.43
1:D:205:ARG:HG2	1:D:245:VAL:HG13	2.00	0.43
1:D:861:LYS:HG3	1:D:869:TRP:CG	2.53	0.43
1:C:699:PHE:HE1	1:C:706:ILE:HD11	1.83	0.43
1:C:593:VAL:HG12	1:C:593:VAL:O	2.19	0.43
1:B:242:LEU:O	1:B:245:VAL:O	2.37	0.43
1:B:703:LYS:HB3	1:B:704:PRO:HD3	2.01	0.43
1:D:876:PHE:HB3	1:D:880:LEU:HB3	2.00	0.43
1:A:706:ILE:HD12	1:A:706:ILE:HA	1.94	0.43
1:A:236:CYS:O	1:A:240:VAL:HG23	2.19	0.43
1:D:625:LEU:HD22	1:D:633:TYR:CE1	2.53	0.43
1:B:736:SER:HA	1:B:743:MET:HE3	2.00	0.43
1:C:758:ILE:HG12	1:C:796:PRO:HB2	2.01	0.43
1:D:172:LEU:HD13	1:D:206:THR:HG21	2.01	0.43
1:D:399:LEU:N	1:D:400:PRO:HD2	2.34	0.43
1:B:49:TYR:CZ	1:B:91:ILE:HG13	2.54	0.43
1:A:530:PHE:HD1	1:A:541:LEU:HD21	1.83	0.43
1:C:416:SER:O	1:C:420:VAL:HG23	2.19	0.42
1:A:746:TYR:HD2	1:A:749:MET:HE3	1.83	0.42
1:B:744:GLN:HA	1:B:747:ILE:HD12	2.01	0.42
1:B:457:ILE:HA	1:B:457:ILE:HD12	1.91	0.42
1:A:56:LYS:O	1:A:60:GLU:HA	2.19	0.42
1:A:205:ARG:HG2	1:A:245:VAL:HG13	2.00	0.42
1:C:130:LEU:HB2	1:C:131:PRO:HD3	2.01	0.42
1:C:744:GLN:HA	1:C:747:ILE:HD12	2.01	0.42
1:D:191:ARG:CG	1:D:191:ARG:NH1	2.72	0.42
1:D:49:TYR:CZ	1:D:91:ILE:HG23	2.55	0.42
1:C:295:ARG:H	1:C:295:ARG:HG2	1.52	0.42
1:A:876:PHE:HB3	1:A:880:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:565:LEU:O	1:C:568:PRO:HD2	2.20	0.42
1:C:49:TYR:OH	1:C:91:ILE:HG13	2.19	0.42
1:A:436:LEU:N	1:A:437:PRO:CD	2.83	0.42
1:D:873:SER:HA	1:D:876:PHE:CD1	2.55	0.42
1:B:718:ASN:HA	1:B:719:PRO:HD3	1.78	0.42
1:D:425:ALA:HB2	1:D:465:TYR:CE1	2.37	0.42
1:D:473:PRO:HA	1:D:474:PRO:HD3	1.87	0.42
1:D:76:VAL:O	1:D:80:PHE:HB2	2.19	0.42
1:B:861:LYS:O	1:B:864:VAL:HG12	2.20	0.42
1:D:191:ARG:O	1:D:195:VAL:HG23	2.19	0.42
1:B:399:LEU:O	1:B:403:LYS:HG2	2.19	0.42
1:A:48:ASN:HA	1:A:51:ILE:HD12	2.00	0.42
1:B:264:ARG:O	1:B:267:ASP:HB2	2.20	0.42
1:B:889:GLY:O	1:B:890:VAL:HG23	2.19	0.42
1:B:481:LEU:O	1:B:485:LEU:HB2	2.20	0.42
1:A:294:VAL:HG22	1:A:390:TYR:HE2	1.85	0.42
1:C:376:ARG:NH2	1:C:419:LEU:HD22	2.35	0.42
1:A:38:GLU:C	1:A:40:LEU:H	2.23	0.42
1:B:567:PRO:HB2	1:B:568:PRO:CD	2.47	0.42
1:D:387:ALA:HA	1:D:394:LEU:HD22	2.01	0.42
1:A:88:THR:O	1:A:91:ILE:HB	2.19	0.41
1:A:512:CYS:HA	1:A:551:SER:HB3	2.02	0.41
1:B:760:ARG:HA	1:B:761:PRO:HD3	1.83	0.41
1:C:726:ASN:HD21	1:C:770:ASN:HD22	1.68	0.41
1:D:673:TYR:CZ	1:D:712:ILE:HD11	2.55	0.41
1:B:706:ILE:HG23	1:B:710:MET:HG2	2.01	0.41
1:B:811:ASP:OD2	1:B:849:LEU:HD11	2.20	0.41
1:C:811:ASP:OD2	1:C:849:LEU:HD11	2.20	0.41
1:A:673:TYR:CZ	1:A:712:ILE:HD11	2.55	0.41
1:A:473:PRO:HA	1:A:474:PRO:HD3	1.85	0.41
1:B:791:GLN:HG3	1:B:791:GLN:H	1.59	0.41
1:A:606:GLU:HB3	1:A:607:PRO:HD3	2.02	0.41
1:C:706:ILE:HG23	1:C:710:MET:HG2	2.03	0.41
1:A:591:SER:HA	1:A:647:LEU:HD13	2.02	0.41
1:C:90:PHE:CE1	1:C:94:GLU:HG3	2.55	0.41
1:A:787:ALA:HB3	1:A:788:PRO:HD3	2.02	0.41
1:D:142:TYR:CE1	1:D:190:ILE:HD12	2.51	0.41
1:B:519:LEU:HD21	1:B:552:VAL:HG11	2.03	0.41
1:D:420:VAL:O	1:D:424:ILE:HG12	2.20	0.41
1:C:71:ILE:HG13	1:C:71:ILE:H	1.76	0.41
1:B:498:GLU:HG3	1:B:537:ASN:HD21	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:TRP:CZ2	1:C:611:ARG:HB3	2.54	0.41
1:B:830:GLN:HE21	1:B:830:GLN:HA	1.84	0.41
1:A:807:ASN:HD21	1:A:810:LYS:H	1.68	0.41
1:D:276:ALA:O	1:D:279:PHE:HB3	2.20	0.41
1:A:276:ALA:O	1:A:279:PHE:HB3	2.21	0.41
1:A:173:ASN:OD1	1:A:173:ASN:O	2.39	0.41
1:B:308:MET:HE1	1:B:383:LEU:CB	2.50	0.41
1:D:83:PHE:HA	1:D:84:PRO:HD3	1.96	0.41
1:D:447:LEU:HD23	1:D:484:GLU:HB3	2.03	0.41
1:D:48:ASN:HA	1:D:51:ILE:HD12	2.02	0.41
1:B:758:ILE:HG12	1:B:796:PRO:HB2	2.03	0.41
1:C:726:ASN:HA	1:C:726:ASN:HD22	1.76	0.41
1:C:142:TYR:CE1	1:C:190:ILE:HD12	2.55	0.41
1:D:185:HIS:HD2	1:D:187:SER:N	2.13	0.41
1:B:521:TYR:CZ	1:D:173:ASN:ND2	2.89	0.41
1:A:864:VAL:HG22	1:A:868:ASN:HB3	2.02	0.41
1:B:747:ILE:N	1:B:748:PRO:CD	2.84	0.41
1:A:873:SER:HA	1:A:876:PHE:CD1	2.56	0.41
1:C:703:LYS:HB3	1:C:704:PRO:HD3	2.03	0.41
1:D:436:LEU:CD2	1:D:465:TYR:CD2	3.04	0.40
1:D:864:VAL:HG22	1:D:868:ASN:HB3	2.02	0.40
1:D:787:ALA:HB3	1:D:788:PRO:HD3	2.03	0.40
1:C:567:PRO:CB	1:C:568:PRO:HD3	2.50	0.40
1:A:787:ALA:O	1:A:790:LEU:HB2	2.22	0.40
1:D:739:MET:HG3	1:D:743:MET:CE	2.51	0.40
1:A:376:ARG:CZ	1:A:419:LEU:HD22	2.50	0.40
1:C:90:PHE:HE1	1:C:94:GLU:HG3	1.87	0.40
1:C:689:ALA:HB2	1:C:727:ASN:ND2	2.36	0.40
1:A:740:GLY:HA2	1:A:781:VAL:HG22	2.04	0.40
1:A:233:LYS:HE2	1:A:233:LYS:HB3	1.94	0.40
1:D:185:HIS:CD2	1:D:187:SER:H	2.32	0.40
1:C:447:LEU:O	1:C:455:ARG:HG2	2.22	0.40
1:A:861:LYS:HE3	1:A:869:TRP:CD1	2.56	0.40
1:D:381:ALA:O	1:D:385:VAL:HG23	2.21	0.40
1:C:821:ILE:HG12	1:C:828:VAL:HG21	2.04	0.40
1:A:485:LEU:HA	1:A:485:LEU:HD12	1.94	0.40

There are no symmetry-related clashes.

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	831/890 (93%)	758 (91%)	56 (7%)	17 (2%)	9	41
1	B	795/890 (89%)	736 (93%)	49 (6%)	10 (1%)	15	53
1	C	816/890 (92%)	739 (91%)	63 (8%)	14 (2%)	11	46
1	D	831/890 (93%)	766 (92%)	50 (6%)	15 (2%)	11	45
All	All	3273/3560 (92%)	2999 (92%)	218 (7%)	56 (2%)	11	46

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	SER
1	A	60	GLU
1	A	122	GLU
1	A	535	HIS
1	A	578	ASP
1	A	598	GLN
1	B	580	ASP
1	C	7	PRO
1	C	372	ASP
1	C	598	GLN
1	D	23	GLN
1	D	24	SER
1	D	60	GLU
1	D	122	GLU
1	D	535	HIS
1	A	41	ASN
1	A	158	ASP
1	A	160	ALA
1	A	656	GLY
1	B	123	LEU
1	B	294	VAL

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Mol	Chain	Res	Type
1	B	575	MET
1	B	598	GLN
1	B	656	GLY
1	C	171	PRO
1	C	656	GLY
1	D	160	ALA
1	D	162	ILE
1	D	598	GLN
1	D	656	GLY
1	A	140	GLU
1	A	761	PRO
1	B	41	ASN
1	B	61	ASP
1	B	171	PRO
1	C	41	ASN
1	C	61	ASP
1	C	123	LEU
1	C	169	ASP
1	D	158	ASP
1	D	165	SER
1	A	56	LYS
1	A	162	ILE
1	C	166	ASP
1	C	512	CYS
1	D	56	LYS
1	D	140	GLU
1	D	761	PRO
1	A	39	GLN
1	A	139	SER
1	D	139	SER
1	B	512	CYS
1	C	294	VAL
1	C	167	VAL
1	C	6	LYS

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	712/802 (89%)	667 (94%)	45 (6%)	22	60
1	B	696/802 (87%)	655 (94%)	41 (6%)	24	63
1	C	697/802 (87%)	658 (94%)	39 (6%)	26	65
1	D	712/802 (89%)	664 (93%)	48 (7%)	20	57
All	All	2817/3208 (88%)	2644 (94%)	173 (6%)	23	61

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	53	VAL
1	A	66	SER
1	A	72	LEU
1	A	83	PHE
1	A	99	ILE
1	A	107	ARG
1	A	113	LEU
1	A	129	LEU
1	A	141	ASP
1	A	149	PHE
1	A	161	GLU
1	A	166	ASP
1	A	170	ARG
1	A	175	MET
1	A	191	ARG
1	A	213	ILE
1	A	226	ASP
1	A	227	GLU
1	A	256	ASN
1	A	271	ASN
1	A	318	LEU
1	A	415	GLU
1	A	430	GLN
1	A	485	LEU
1	A	535	HIS
1	A	552	VAL
1	A	579	GLU
1	A	582	ASP
1	A	606	GLU
1	A	610	GLN
1	A	615	LEU
1	A	671	LEU

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Mol	Chain	Res	Type
1	A	737	ILE
1	A	741	ILE
1	A	781	VAL
1	A	790	LEU
1	A	806	ASP
1	A	807	ASN
1	A	830	GLN
1	A	833	ILE
1	A	871	ARG
1	A	873	SER
1	A	880	LEU
1	A	887	PHE
1	B	45	ASP
1	B	99	ILE
1	B	129	LEU
1	B	144	THR
1	B	149	PHE
1	B	174	ILE
1	B	204	SER
1	B	206	THR
1	B	213	ILE
1	B	281	LEU
1	B	295	ARG
1	B	415	GLU
1	B	476	THR
1	B	494	LYS
1	B	519	LEU
1	B	563	GLN
1	B	570	ILE
1	B	571	GLN
1	B	582	ASP
1	B	584	PHE
1	B	590	LEU
1	B	615	LEU
1	B	632	GLN
1	B	641	MET
1	B	712	ILE
1	B	715	THR
1	B	726	ASN
1	B	741	ILE
1	B	766	THR
1	B	781	VAL

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Mol	Chain	Res	Type
1	B	785	GLU
1	B	791	GLN
1	B	802	ARG
1	B	807	ASN
1	B	828	VAL
1	B	830	GLN
1	B	837	ASP
1	B	841	SER
1	B	867	GLU
1	B	871	ARG
1	B	881	LYS
1	C	45	ASP
1	C	99	ILE
1	C	129	LEU
1	C	144	THR
1	C	149	PHE
1	C	174	ILE
1	C	204	SER
1	C	206	THR
1	C	213	ILE
1	C	246	ARG
1	C	281	LEU
1	C	371	SER
1	C	398	ILE
1	C	415	GLU
1	C	476	THR
1	C	485	LEU
1	C	494	LYS
1	C	519	LEU
1	C	577	LYS
1	C	612	CYS
1	C	615	LEU
1	C	632	GLN
1	C	641	MET
1	C	712	ILE
1	C	715	THR
1	C	726	ASN
1	C	741	ILE
1	C	766	THR
1	C	781	VAL
1	C	785	GLU
1	C	791	GLN

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Mol	Chain	Res	Type
1	C	802	ARG
1	C	807	ASN
1	C	828	VAL
1	C	830	GLN
1	C	837	ASP
1	C	841	SER
1	C	846	LYS
1	C	871	ARG
1	D	53	VAL
1	D	66	SER
1	D	72	LEU
1	D	79	HIS
1	D	99	ILE
1	D	107	ARG
1	D	129	LEU
1	D	141	ASP
1	D	149	PHE
1	D	161	GLU
1	D	170	ARG
1	D	175	MET
1	D	191	ARG
1	D	213	ILE
1	D	226	ASP
1	D	227	GLU
1	D	256	ASN
1	D	271	ASN
1	D	281	LEU
1	D	318	LEU
1	D	369	THR
1	D	372	ASP
1	D	415	GLU
1	D	430	GLN
1	D	485	LEU
1	D	531	SER
1	D	536	LYS
1	D	552	VAL
1	D	560	GLU
1	D	580	ASP
1	D	581	LYS
1	D	582	ASP
1	D	587	LEU
1	D	590	LEU

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Mol	Chain	Res	Type
1	D	606	GLU
1	D	610	GLN
1	D	615	LEU
1	D	671	LEU
1	D	737	ILE
1	D	741	ILE
1	D	790	LEU
1	D	807	ASN
1	D	830	GLN
1	D	833	ILE
1	D	871	ARG
1	D	873	SER
1	D	880	LEU
1	D	887	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	173	ASN
1	A	185	HIS
1	A	212	HIS
1	A	617	GLN
1	A	677	GLN
1	A	807	ASN
1	A	824	ASN
1	B	397	HIS
1	B	442	HIS
1	B	497	GLN
1	B	537	ASN
1	B	617	GLN
1	B	632	GLN
1	B	677	GLN
1	B	726	ASN
1	B	830	GLN
1	C	48	ASN
1	C	442	HIS
1	C	497	GLN
1	C	535	HIS
1	C	537	ASN
1	C	617	GLN
1	C	632	GLN

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Mol	Chain	Res	Type
1	C	677	GLN
1	C	726	ASN
1	C	830	GLN
1	D	125	ASN
1	D	173	ASN
1	D	185	HIS
1	D	212	HIS
1	D	617	GLN
1	D	677	GLN
1	D	792	GLN
1	D	807	ASN
1	D	824	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	835/890 (93%)	0.11	25 (2%)	54	25	41, 67, 117, 128	0
1	B	801/890 (90%)	0.19	30 (3%)	45	19	37, 69, 122, 161	0
1	C	824/890 (92%)	0.28	45 (5%)	29	11	44, 76, 149, 163	0
1	D	835/890 (93%)	0.05	17 (2%)	68	39	41, 65, 101, 116	0
All	All	3295/3560 (92%)	0.16	117 (3%)	46	20	37, 69, 121, 163	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	TRP	7.2
1	B	57	LEU	6.1
1	C	7	PRO	6.1
1	B	50	LEU	4.4
1	B	630	PRO	4.1
1	C	803	ASN	4.1
1	D	161	GLU	4.0
1	C	8	ASP	3.9
1	C	631	ASP	3.9
1	C	82	ASN	3.8
1	C	57	LEU	3.8
1	C	50	LEU	3.7
1	B	32	THR	3.7
1	A	59	SER	3.7
1	B	805	ARG	3.7
1	A	82	ASN	3.7
1	A	163	LEU	3.6
1	D	82	ASN	3.6
1	C	370	ILE	3.6
1	D	58	LYS	3.5
1	B	579	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	34	GLN	3.4
1	A	58	LYS	3.2
1	C	58	LYS	3.2
1	A	55	THR	3.2
1	A	81	GLN	3.2
1	B	582	ASP	3.2
1	D	631	ASP	3.1
1	C	80	PHE	3.1
1	A	49	TYR	3.0
1	D	42	GLN	3.0
1	A	631	ASP	3.0
1	B	578	ASP	3.0
1	C	369	THR	3.0
1	D	49	TYR	2.9
1	C	47	ASN	2.9
1	C	371	SER	2.9
1	A	577	LYS	2.9
1	D	319	LYS	2.9
1	B	82	ASN	2.9
1	C	32	THR	2.9
1	D	629	GLN	2.8
1	A	633	TYR	2.8
1	C	848	ASP	2.8
1	C	579	GLU	2.8
1	D	579	GLU	2.8
1	B	577	LYS	2.8
1	A	870	ARG	2.7
1	C	49	TYR	2.7
1	B	80	PHE	2.7
1	C	51	ILE	2.7
1	B	124	GLN	2.7
1	C	626	ASN	2.7
1	C	580	ASP	2.6
1	B	720	GLU	2.6
1	B	71	ILE	2.6
1	C	44	PRO	2.6
1	B	634	GLU	2.6
1	C	10	GLN	2.6
1	D	81	GLN	2.5
1	C	227	GLU	2.5
1	B	49	TYR	2.5
1	C	720	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	54	LEU	2.5
1	C	805	ARG	2.5
1	C	38	GLU	2.4
1	A	42	GLN	2.4
1	B	58	LYS	2.4
1	C	79	HIS	2.4
1	A	875	GLN	2.4
1	B	761	PRO	2.3
1	B	803	ASN	2.3
1	B	631	ASP	2.3
1	C	39	GLN	2.3
1	B	41	ASN	2.3
1	A	634	GLU	2.3
1	D	577	LYS	2.3
1	C	633	TYR	2.3
1	D	630	PRO	2.3
1	B	890	VAL	2.3
1	B	42	GLN	2.3
1	C	6	LYS	2.3
1	D	578	ASP	2.2
1	A	79	HIS	2.2
1	C	393	GLU	2.2
1	B	806	ASP	2.2
1	C	632	GLN	2.2
1	B	39	GLN	2.2
1	A	860	PHE	2.2
1	A	227	GLU	2.2
1	A	319	LYS	2.2
1	A	80	PHE	2.2
1	A	85	ASN	2.2
1	C	35	GLN	2.1
1	C	535	HIS	2.1
1	C	78	ALA	2.1
1	D	59	SER	2.1
1	C	42	GLN	2.1
1	C	622	GLN	2.1
1	B	90	PHE	2.1
1	D	159	SER	2.1
1	D	632	GLN	2.1
1	A	51	ILE	2.1
1	C	634	GLU	2.1
1	A	632	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	30	GLN	2.1
1	B	52	PHE	2.1
1	C	52	PHE	2.1
1	D	633	TYR	2.1
1	B	580	ASP	2.1
1	B	47	ASN	2.1
1	A	52	PHE	2.0
1	B	54	LEU	2.0
1	C	54	LEU	2.0
1	C	630	PRO	2.0
1	C	761	PRO	2.0
1	A	578	ASP	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.