



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:14 AM UTC

PDB ID : 1K8K / pdb_00001k8k
Title : Crystal Structure of Arp2/3 Complex
Authors : Robinson, R.C.; Turbedsky, K.; Kaiser, D.A.; Higgs, H.N.; Marchand, J.-B.;
Choe, S.; Pollard, T.D.
Deposited on : 2001-10-24
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

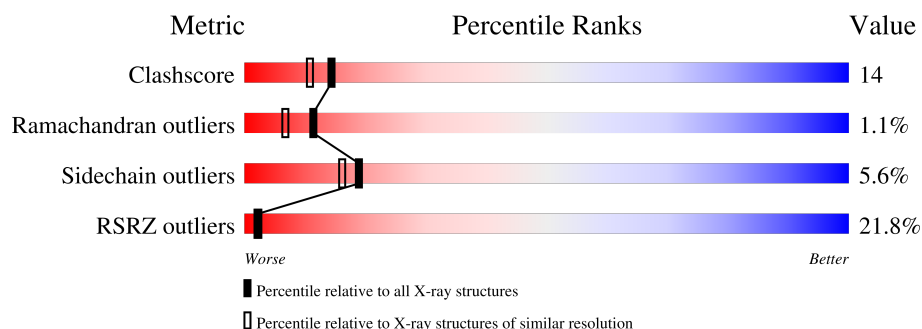
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	418	20% 78% 13% • •
2	B	394	22% 31% 14% • 52%
3	C	372	15% 74% 17% • 5%
4	D	300	6% 81% 13% • 5%
5	E	178	36% 63% 28% 7% •
6	F	168	5% 85% 12% • •
7	G	151	36% 75% 12% 5% 8%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15326 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 ACTIN-LIKE PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3212	2063	536	597	16			

- Molecule 2 is a protein called ACTIN-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1515	974	259	278	4			

- Molecule 3 is a protein called ARP2/3 COMPLEX 41 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	354	Total	C	N	O	S	0	0	0
			2757	1747	487	504	19			

- Molecule 4 is a protein called ARP2/3 COMPLEX 34 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	284	Total	C	N	O	S	0	0	0
			2291	1456	397	430	8			

- Molecule 5 is a protein called ARP2/3 COMPLEX 21 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1414	908	236	261	9			

- Molecule 6 is a protein called ARP2/3 COMPLEX 20 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1369	875	239	246	9			

- Molecule 7 is a protein called ARP2/3 COMPLEX 16 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	139	Total	C	N	O	S	0	0	0
			1058	661	185	209	3			

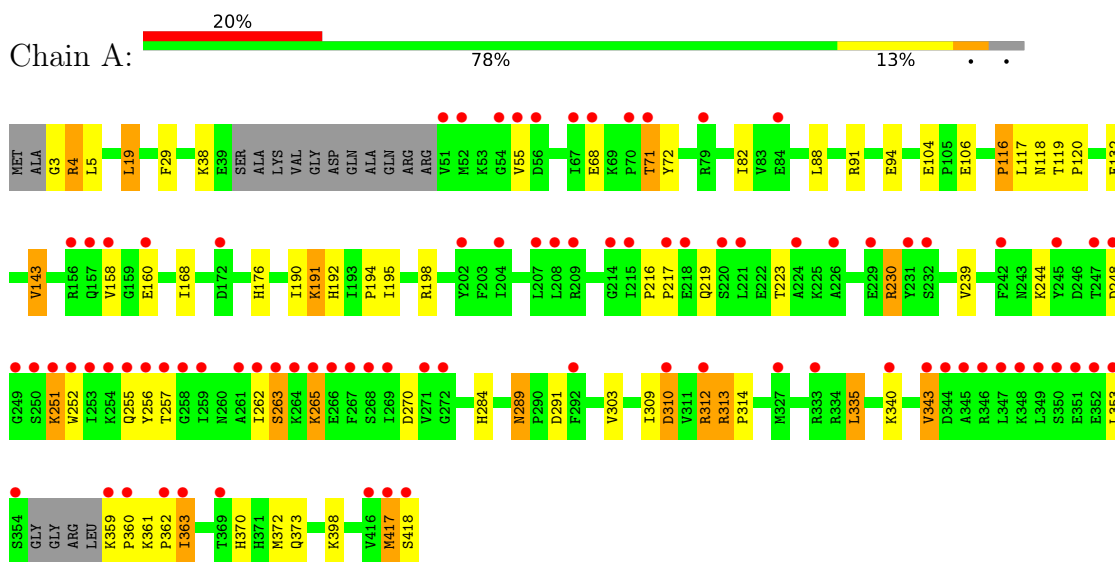
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	364	Total	O	27	0
			364	364		
8	B	209	Total	O	14	0
			209	209		
8	C	338	Total	O	30	0
			338	338		
8	D	355	Total	O	22	0
			355	355		
8	E	111	Total	O	12	0
			111	111		
8	F	230	Total	O	14	0
			230	230		
8	G	103	Total	O	9	0
			103	103		

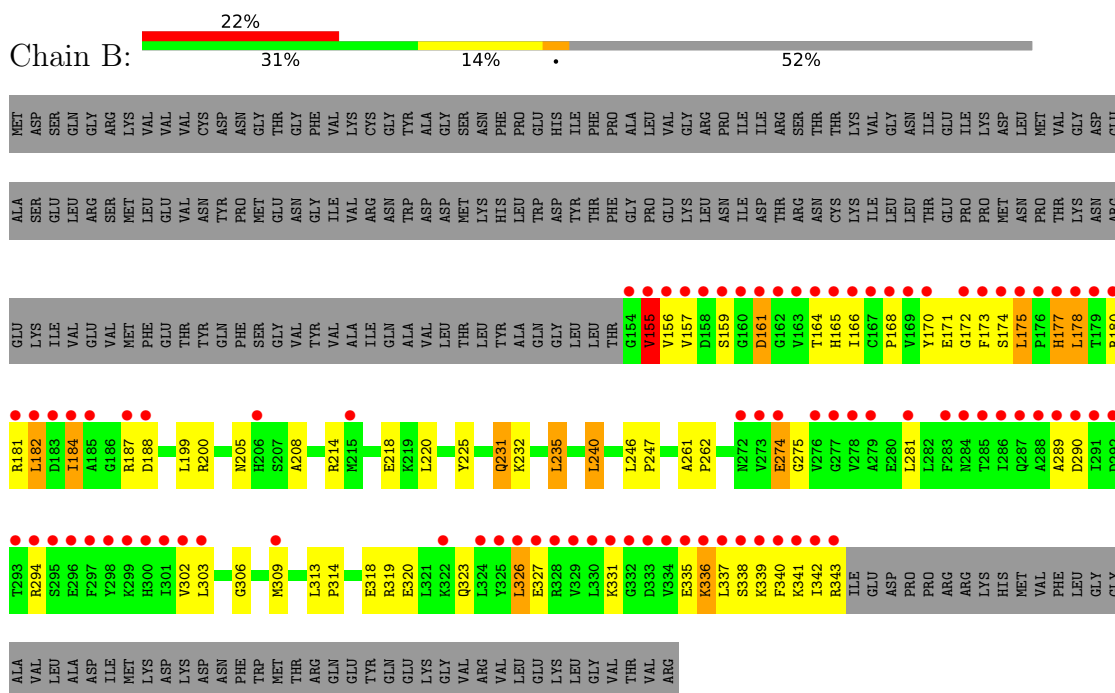
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

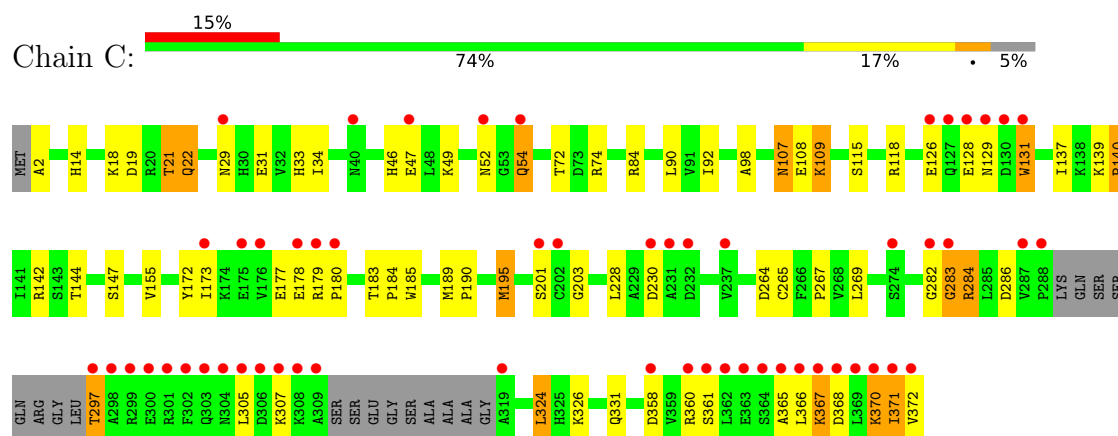
- Molecule 1: ACTIN-LIKE PROTEIN 3



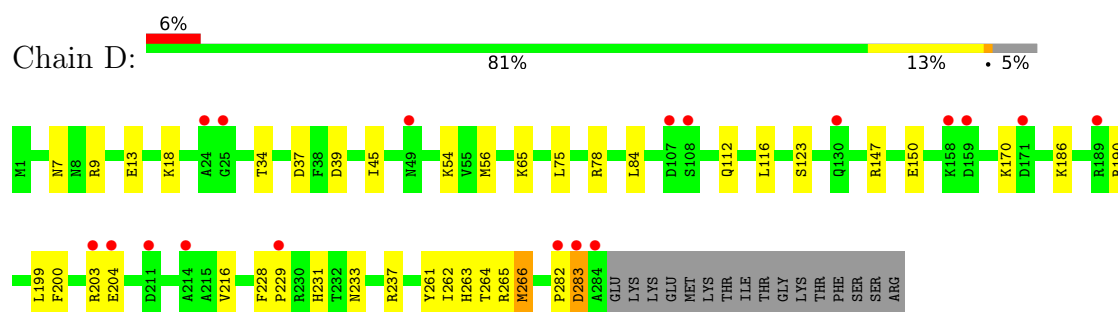
- Molecule 2: ACTIN-LIKE PROTEIN 2



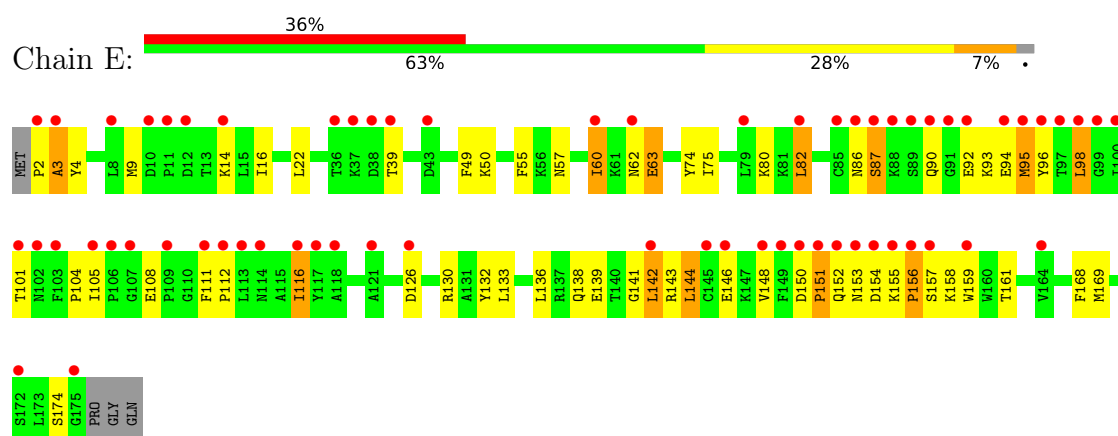
- Molecule 3: ARP2/3 COMPLEX 41 KDA SUBUNIT



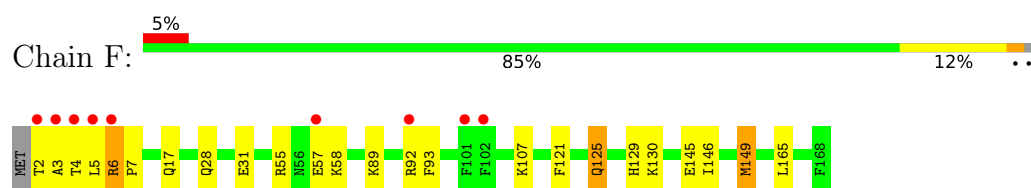
- Molecule 4: ARP2/3 COMPLEX 34 KDA SUBUNIT



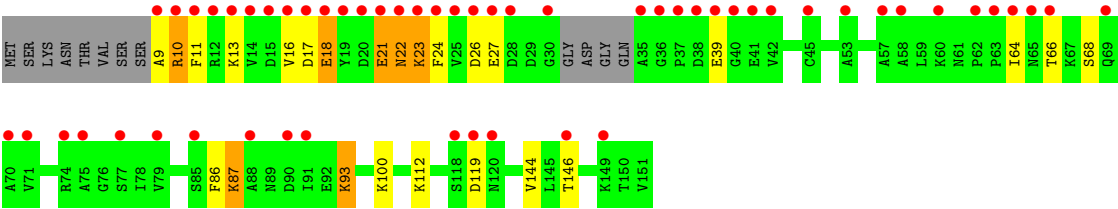
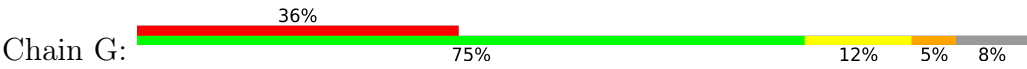
- Molecule 5: ARP2/3 COMPLEX 21 KDA SUBUNIT



- Molecule 6: ARP2/3 COMPLEX 20 KDA SUBUNIT



- Molecule 7: ARP2/3 COMPLEX 16 KDA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.71Å 130.40Å 204.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 92.1 (30.00-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.251 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	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	15326	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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

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	0.61	0/3293	0.92	3/4467 (0.1%)
2	B	0.50	0/1543	0.82	1/2084 (0.0%)
3	C	0.67	1/2826 (0.0%)	0.97	7/3832 (0.2%)
4	D	0.70	1/2340 (0.0%)	0.88	0/3160
5	E	0.48	0/1448	0.89	2/1953 (0.1%)
6	F	0.76	1/1391 (0.1%)	0.93	0/1867
7	G	0.50	0/1070	0.84	1/1441 (0.1%)
All	All	0.63	3/13911 (0.0%)	0.91	14/18804 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	266	MET	SD-CE	-10.87	1.52	1.79
3	C	195	MET	SD-CE	-9.52	1.55	1.79
6	F	149	MET	SD-CE	-8.85	1.57	1.79

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	22	GLN	OE1-CD-NE2	-9.78	112.83	122.60
3	C	54	GLN	OE1-CD-NE2	-9.75	112.85	122.60
3	C	22	GLN	CG-CD-NE2	6.65	126.37	116.40
3	C	54	GLN	CG-CD-NE2	6.63	126.34	116.40
1	A	118	ASN	N-CA-C	-6.36	100.87	110.28
1	A	373	GLN	N-CA-C	6.27	117.78	111.07
5	E	49	PHE	N-CA-C	6.16	118.50	111.11
2	B	177	HIS	N-CA-C	-5.52	101.67	109.96
5	E	174	SER	N-CA-C	-5.45	106.48	113.02
7	G	144	VAL	N-CA-C	-5.35	105.32	110.72
3	C	137	ILE	N-CA-C	-5.27	100.16	107.80
3	C	115	SER	N-CA-C	5.16	116.83	109.14
1	A	116	PRO	N-CA-C	-5.16	103.34	111.34
3	C	283	GLY	N-CA-C	5.08	125.23	113.18

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	3212	0	3163	70	0
2	B	1515	0	1548	59	0
3	C	2757	0	2713	97	0
4	D	2291	0	2257	43	0
5	E	1414	0	1416	76	0
6	F	1369	0	1410	33	0
7	G	1058	0	1065	25	0
8	A	364	0	0	13	0
8	B	209	0	0	15	0
8	C	338	0	0	38	0
8	D	355	0	0	17	0
8	E	111	0	0	4	0
8	F	230	0	0	5	0
8	G	103	0	0	8	0
All	All	15326	0	13572	383	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 14.

All (383) 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)
5:E:152:GLN:CB	5:E:155:LYS:NZ	1.85	1.38
2:B:165:HIS:CD2	2:B:181:ARG:HG2	1.58	1.37
5:E:152:GLN:HB3	5:E:155:LYS:CE	1.59	1.30
5:E:152:GLN:CB	5:E:155:LYS:CE	2.12	1.27
3:C:307:LYS:CE	8:C:568:HOH:O	1.63	1.26
5:E:152:GLN:CG	5:E:155:LYS:NZ	2.00	1.24
5:E:152:GLN:CG	5:E:155:LYS:HZ1	1.50	1.22
5:E:152:GLN:HB2	5:E:155:LYS:CD	1.71	1.21
4:D:282:PRO:O	4:D:283:ASP:CG	1.84	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:GLN:HG3	5:E:155:LYS:NZ	1.56	1.18
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.16	1.15
5:E:92:GLU:O	5:E:96:TYR:CD1	2.00	1.14
3:C:307:LYS:NZ	8:C:568:HOH:O	1.64	1.12
3:C:228:LEU:CD2	3:C:230:ASP:OD1	1.97	1.11
5:E:152:GLN:CB	5:E:155:LYS:HZ1	1.51	1.10
6:F:57:GLU:HG2	8:F:356:HOH:O	1.50	1.09
3:C:307:LYS:HE2	8:C:568:HOH:O	1.28	1.09
5:E:152:GLN:HB3	5:E:155:LYS:HE3	1.27	1.09
4:D:7:ASN:HB3	8:D:314:HOH:O	1.50	1.07
2:B:341:LYS:HD3	8:B:540:HOH:O	1.51	1.07
5:E:126:ASP:OD2	5:E:130:ARG:NH1	1.88	1.06
5:E:152:GLN:HB3	5:E:155:LYS:NZ	1.57	1.06
4:D:203:ARG:O	4:D:204:GLU:HG2	1.56	1.02
3:C:22:GLN:HG3	8:C:696:HOH:O	1.57	1.01
1:A:132:GLU:OE1	6:F:92:ARG:NH2	1.96	0.98
7:G:24:PHE:HE2	7:G:26:ASP:OD1	1.44	0.98
2:B:165:HIS:CD2	2:B:181:ARG:CG	2.47	0.97
3:C:368:ASP:O	3:C:370:LYS:NZ	1.96	0.97
1:A:38:LYS:NZ	1:A:71:THR:OG1	1.98	0.97
3:C:54:GLN:CD	8:C:641:HOH:O	2.08	0.96
1:A:398:LYS:HD3	8:A:759:HOH:O	1.66	0.95
3:C:14:HIS:H	3:C:331:GLN:HE22	1.10	0.95
7:G:18:GLU:OE1	7:G:23:LYS:NZ	1.99	0.95
2:B:165:HIS:HD2	2:B:181:ARG:HG2	0.94	0.93
5:E:152:GLN:HG3	5:E:155:LYS:HZ2	1.24	0.92
2:B:335:GLU:O	2:B:338:SER:N	2.02	0.91
7:G:24:PHE:CE2	7:G:26:ASP:OD1	2.23	0.91
5:E:152:GLN:HB3	5:E:155:LYS:HZ1	1.19	0.90
4:D:282:PRO:HD2	8:D:645:HOH:O	1.71	0.89
2:B:214:ARG:NH1	2:B:218:GLU:OE2	2.06	0.89
4:D:39:ASP:HB3	8:D:602:HOH:O	1.74	0.88
2:B:165:HIS:NE2	2:B:181:ARG:CD	2.37	0.87
3:C:228:LEU:HD21	3:C:230:ASP:OD1	1.73	0.87
5:E:152:GLN:HB2	5:E:155:LYS:CE	1.90	0.86
5:E:152:GLN:CB	5:E:155:LYS:CD	2.49	0.86
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.58	0.86
2:B:200:ARG:HD3	8:B:470:HOH:O	1.76	0.84
7:G:146:THR:HG22	7:G:146:THR:O	1.76	0.83
5:E:92:GLU:O	5:E:96:TYR:HD1	1.59	0.83
3:C:284:ARG:NH1	3:C:286:ASP:O	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:87:LYS:H	7:G:87:LYS:HD3	1.44	0.83
5:E:152:GLN:CG	5:E:155:LYS:HZ2	1.81	0.82
3:C:19:ASP:HB2	8:C:707:HOH:O	1.77	0.82
7:G:9:ALA:O	7:G:11:PHE:N	2.13	0.82
5:E:152:GLN:CB	5:E:155:LYS:HD2	2.04	0.81
3:C:367:LYS:HD3	3:C:368:ASP:N	1.95	0.81
4:D:203:ARG:O	4:D:203:ARG:HG2	1.81	0.80
2:B:177:HIS:O	2:B:178:LEU:HB2	1.79	0.80
4:D:282:PRO:O	4:D:283:ASP:OD1	2.00	0.79
5:E:152:GLN:CB	5:E:155:LYS:HZ2	1.92	0.78
2:B:205:ASN:HD22	2:B:208:ALA:H	1.33	0.77
2:B:335:GLU:O	2:B:336:LYS:C	2.29	0.76
6:F:4:THR:HG23	6:F:55:ARG:HE	1.50	0.76
1:A:359:LYS:O	1:A:359:LYS:HD3	1.85	0.76
6:F:146:ILE:HA	6:F:149:MET:HE2	1.67	0.76
3:C:189:MET:HG2	3:C:195:MET:HE3	1.68	0.76
2:B:165:HIS:NE2	2:B:181:ARG:NE	2.33	0.75
1:A:310:ASP:OD1	1:A:310:ASP:N	2.13	0.75
3:C:14:HIS:H	3:C:331:GLN:NE2	1.84	0.74
2:B:231:GLN:HG3	8:B:591:HOH:O	1.86	0.74
5:E:150:ASP:OD1	5:E:151:PRO:HD2	1.86	0.74
6:F:121:PHE:O	6:F:125:GLN:HG2	1.88	0.74
3:C:178:GLU:HB2	8:C:625:HOH:O	1.87	0.74
5:E:92:GLU:O	5:E:96:TYR:CE1	2.39	0.73
4:D:39:ASP:CB	8:D:602:HOH:O	2.31	0.73
6:F:146:ILE:HA	6:F:149:MET:CE	2.18	0.73
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.23	0.73
1:A:116:PRO:O	1:A:117:LEU:HB2	1.88	0.72
5:E:152:GLN:HB2	5:E:155:LYS:NZ	1.92	0.72
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.72	0.72
5:E:87:SER:HA	5:E:153:ASN:OD1	1.89	0.71
6:F:2:THR:OG1	6:F:3:ALA:HA	1.90	0.71
3:C:54:GLN:NE2	8:C:641:HOH:O	2.21	0.71
3:C:21:THR:HB	8:C:707:HOH:O	1.90	0.70
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.73	0.70
4:D:203:ARG:C	8:D:652:HOH:O	2.32	0.70
5:E:152:GLN:CB	5:E:155:LYS:HE3	2.04	0.70
3:C:228:LEU:HD23	3:C:230:ASP:OD1	1.89	0.69
1:A:239:VAL:HG13	5:E:4:TYR:CZ	2.28	0.69
1:A:370:HIS:HE1	8:A:616:HOH:O	1.74	0.69
2:B:165:HIS:NE2	2:B:181:ARG:HD3	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:H	6:F:28:GLN:NE2	1.90	0.68
4:D:65:LYS:HG2	8:D:479:HOH:O	1.92	0.68
4:D:282:PRO:C	4:D:283:ASP:CG	2.62	0.68
3:C:21:THR:HB	8:C:696:HOH:O	1.92	0.68
1:A:289:ASN:HD22	1:A:291:ASP:H	1.42	0.68
2:B:161:ASP:O	2:B:187:ARG:HG3	1.94	0.68
5:E:152:GLN:O	5:E:155:LYS:HG3	1.94	0.68
1:A:343:VAL:HG22	1:A:363:ILE:CD1	2.24	0.67
3:C:189:MET:HA	3:C:195:MET:HE1	1.77	0.66
5:E:86:ASN:O	5:E:87:SER:HB3	1.96	0.65
2:B:200:ARG:HD2	8:B:603:HOH:O	1.95	0.65
4:D:265:ARG:HD3	6:F:145:GLU:OE2	1.96	0.65
3:C:142:ARG:HD2	8:C:693:HOH:O	1.95	0.65
1:A:190:ILE:C	1:A:191:LYS:HD3	2.22	0.65
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.32	0.64
5:E:152:GLN:O	5:E:155:LYS:CG	2.46	0.64
3:C:2:ALA:N	8:C:705:HOH:O	2.31	0.64
1:A:176:HIS:HD2	1:A:192:HIS:HD2	1.44	0.64
7:G:9:ALA:HB3	8:G:239:HOH:O	1.95	0.64
1:A:248:ASP:OD1	1:A:251:LYS:NZ	2.30	0.64
1:A:262:ILE:O	1:A:263:SER:CB	2.45	0.64
1:A:176:HIS:HD2	1:A:192:HIS:CD2	2.16	0.63
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.79	0.63
1:A:68:GLU:HA	8:A:712:HOH:O	1.99	0.63
1:A:359:LYS:O	1:A:359:LYS:CD	2.45	0.63
2:B:335:GLU:O	2:B:337:LEU:N	2.30	0.63
3:C:118:ARG:NH2	8:C:549:HOH:O	2.25	0.63
3:C:283:GLY:O	3:C:284:ARG:HB2	1.97	0.63
1:A:3:GLY:N	8:A:771:HOH:O	2.32	0.63
5:E:9:MET:HG2	5:E:62:ASN:OD1	1.99	0.63
1:A:359:LYS:O	1:A:359:LYS:CG	2.45	0.63
2:B:214:ARG:NH1	2:B:218:GLU:CD	2.56	0.62
1:A:55:VAL:HG12	1:A:55:VAL:O	1.98	0.62
6:F:2:THR:C	8:F:397:HOH:O	2.43	0.62
6:F:130:LYS:HE2	8:F:283:HOH:O	1.98	0.62
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.82	0.62
3:C:324:LEU:HD21	8:C:705:HOH:O	1.98	0.62
1:A:343:VAL:HG22	1:A:363:ILE:HD11	1.80	0.61
5:E:90:GLN:HG2	5:E:94:GLU:OE2	2.00	0.61
7:G:66:THR:HG23	8:G:254:HOH:O	1.98	0.61
1:A:370:HIS:HD2	1:A:372:MET:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:216:VAL:HA	8:D:652:HOH:O	2.00	0.61
3:C:365:ALA:C	3:C:366:LEU:HD12	2.26	0.60
4:D:7:ASN:ND2	8:D:448:HOH:O	2.33	0.60
1:A:230:ARG:HH11	1:A:230:ARG:CB	2.15	0.60
1:A:55:VAL:O	1:A:55:VAL:CG1	2.49	0.60
1:A:289:ASN:ND2	1:A:291:ASP:H	2.00	0.60
3:C:21:THR:CB	8:C:696:HOH:O	2.49	0.60
5:E:95:MET:HA	5:E:95:MET:CE	2.32	0.60
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.32	0.59
7:G:146:THR:O	7:G:146:THR:CG2	2.46	0.59
3:C:54:GLN:OE1	8:C:641:HOH:O	2.16	0.59
2:B:231:GLN:HG3	8:B:539:HOH:O	2.02	0.59
8:A:671:HOH:O	4:D:34:THR:HG21	2.03	0.59
1:A:265:LYS:HE3	8:A:727:HOH:O	2.01	0.59
5:E:50:LYS:NZ	5:E:159:TRP:O	2.36	0.59
3:C:283:GLY:O	3:C:284:ARG:CB	2.51	0.58
4:D:9:ARG:HB3	8:D:647:HOH:O	2.03	0.58
4:D:263:HIS:HD2	4:D:266:MET:CE	2.15	0.58
2:B:181:ARG:NE	8:B:544:HOH:O	2.33	0.58
3:C:203:GLY:HA2	7:G:146:THR:HG21	1.85	0.58
3:C:371:ILE:O	3:C:372:VAL:HB	2.04	0.58
5:E:86:ASN:O	5:E:87:SER:CB	2.51	0.58
3:C:172:TYR:OH	3:C:179:ARG:HD2	2.04	0.57
3:C:21:THR:CB	8:C:707:HOH:O	2.50	0.57
3:C:142:ARG:NE	8:C:693:HOH:O	2.38	0.57
3:C:144:THR:CB	6:F:28:GLN:HE21	2.18	0.56
3:C:183:THR:HG22	3:C:185:TRP:H	1.70	0.56
4:D:186:LYS:HE3	4:D:199:LEU:HA	1.87	0.56
6:F:89:LYS:HA	6:F:92:ARG:NH1	2.19	0.56
1:A:262:ILE:O	1:A:263:SER:OG	2.18	0.56
1:A:359:LYS:N	1:A:360:PRO:HD3	2.20	0.56
5:E:150:ASP:O	5:E:152:GLN:N	2.39	0.56
4:D:170:LYS:HG2	8:D:426:HOH:O	2.05	0.56
3:C:142:ARG:CD	8:C:693:HOH:O	2.53	0.56
6:F:2:THR:OG1	6:F:3:ALA:CA	2.53	0.56
2:B:200:ARG:CD	8:B:470:HOH:O	2.42	0.55
7:G:66:THR:N	8:G:254:HOH:O	2.38	0.55
1:A:4:ARG:HD2	8:A:723:HOH:O	2.06	0.55
2:B:323:GLN:HB3	7:G:11:PHE:O	2.06	0.55
3:C:19:ASP:CB	8:C:707:HOH:O	2.46	0.55
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:LYS:HA	5:E:96:TYR:HD1	1.72	0.55
5:E:150:ASP:C	5:E:152:GLN:N	2.64	0.55
6:F:89:LYS:HA	6:F:92:ARG:HH12	1.72	0.55
3:C:107:ASN:ND2	3:C:109:LYS:H	2.05	0.55
4:D:228:PHE:H	4:D:231:HIS:HD2	1.54	0.55
3:C:178:GLU:HA	8:C:636:HOH:O	2.06	0.55
3:C:269:LEU:H	3:C:283:GLY:HA3	1.72	0.54
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.42	0.54
3:C:84:ARG:HG2	8:C:595:HOH:O	2.06	0.54
5:E:150:ASP:C	5:E:152:GLN:H	2.15	0.54
1:A:257:THR:HG23	8:A:755:HOH:O	2.06	0.54
3:C:370:LYS:HE2	3:C:370:LYS:H	1.72	0.54
4:D:203:ARG:C	4:D:204:GLU:HG2	2.31	0.54
1:A:194:PRO:C	1:A:195:ILE:HD12	2.33	0.54
3:C:107:ASN:C	3:C:107:ASN:HD22	2.15	0.54
3:C:84:ARG:HG2	3:C:84:ARG:O	2.07	0.54
5:E:152:GLN:O	5:E:155:LYS:HD2	2.08	0.54
5:E:152:GLN:CD	5:E:155:LYS:HZ1	2.13	0.54
7:G:93:LYS:NZ	7:G:93:LYS:HB3	2.23	0.54
5:E:132:TYR:CE2	5:E:136:LEU:HD11	2.43	0.54
6:F:57:GLU:HG3	6:F:58:LYS:HE3	1.90	0.53
1:A:289:ASN:HD22	1:A:289:ASN:C	2.15	0.53
7:G:21:GLU:O	7:G:22:ASN:ND2	2.41	0.53
3:C:118:ARG:NE	8:C:549:HOH:O	2.26	0.53
3:C:370:LYS:O	3:C:371:ILE:HB	2.09	0.53
1:A:230:ARG:HH11	1:A:230:ARG:HB3	1.74	0.52
3:C:54:GLN:HG3	8:C:592:HOH:O	2.09	0.52
4:D:282:PRO:O	4:D:283:ASP:OD2	2.25	0.52
3:C:21:THR:N	8:C:707:HOH:O	2.42	0.52
3:C:228:LEU:HD22	3:C:230:ASP:OD1	2.04	0.52
5:E:14:LYS:NZ	8:E:1316:HOH:O	2.42	0.52
5:E:152:GLN:O	5:E:155:LYS:CD	2.57	0.52
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.23	0.52
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.92	0.52
3:C:228:LEU:HD23	3:C:228:LEU:C	2.35	0.52
5:E:92:GLU:C	5:E:96:TYR:CD1	2.87	0.52
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.91	0.52
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.44	0.51
5:E:92:GLU:HB3	5:E:96:TYR:HE1	1.75	0.51
6:F:17:GLN:CD	8:F:348:HOH:O	2.52	0.51
1:A:340:LYS:NZ	8:A:698:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.45	0.51
7:G:100:LYS:CE	8:G:251:HOH:O	2.57	0.51
4:D:123:SER:HB3	8:D:473:HOH:O	2.11	0.51
5:E:93:LYS:NZ	8:E:1317:HOH:O	2.44	0.51
7:G:13:LYS:HD3	8:G:247:HOH:O	2.10	0.51
3:C:52:ASN:ND2	8:C:653:HOH:O	2.43	0.51
3:C:173:ILE:O	3:C:177:GLU:HG2	2.10	0.51
7:G:87:LYS:HD3	7:G:87:LYS:N	2.21	0.51
3:C:183:THR:CG2	3:C:184:PRO:HD2	2.41	0.50
1:A:68:GLU:CA	8:A:712:HOH:O	2.57	0.50
2:B:165:HIS:NE2	2:B:181:ARG:CG	2.68	0.50
1:A:4:ARG:HH11	1:A:4:ARG:HG2	1.76	0.50
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.42	0.50
3:C:367:LYS:CD	3:C:368:ASP:N	2.69	0.50
3:C:178:GLU:O	3:C:179:ARG:C	2.55	0.50
5:E:138:GLN:HG2	8:E:1268:HOH:O	2.11	0.50
6:F:4:THR:CG2	6:F:55:ARG:HE	2.22	0.50
5:E:3:ALA:N	5:E:55:PHE:CZ	2.79	0.50
1:A:343:VAL:HG22	1:A:363:ILE:HD12	1.93	0.50
1:A:361:LYS:HG2	1:A:362:PRO:HD2	1.94	0.49
3:C:189:MET:N	3:C:190:PRO:CD	2.75	0.49
2:B:155:VAL:HA	2:B:168:PRO:HA	1.94	0.49
2:B:231:GLN:HA	2:B:231:GLN:NE2	2.26	0.49
3:C:21:THR:O	3:C:21:THR:HG22	2.13	0.49
5:E:111:PHE:CD2	5:E:112:PRO:O	2.66	0.49
1:A:68:GLU:C	8:A:712:HOH:O	2.56	0.48
7:G:119:ASP:N	8:G:231:HOH:O	2.46	0.48
2:B:225:TYR:CZ	2:B:319:ARG:HD3	2.47	0.48
5:E:155:LYS:O	5:E:157:SER:N	2.46	0.48
3:C:367:LYS:HD3	3:C:367:LYS:C	2.37	0.48
3:C:144:THR:OG1	6:F:28:GLN:NE2	2.40	0.48
2:B:199:LEU:HD12	8:B:508:HOH:O	2.13	0.48
3:C:21:THR:CG2	8:C:696:HOH:O	2.62	0.48
3:C:29:ASN:OD1	3:C:31:GLU:HG3	2.12	0.48
6:F:57:GLU:HG3	6:F:58:LYS:HG2	1.94	0.48
3:C:74:ARG:CZ	6:F:31:GLU:OE2	2.61	0.48
3:C:203:GLY:HA2	8:C:475:HOH:O	2.12	0.48
3:C:360:ARG:HG2	3:C:361:SER:N	2.28	0.48
1:A:244:LYS:HD3	1:A:252:TRP:CZ2	2.48	0.48
4:D:282:PRO:C	4:D:283:ASP:OD1	2.57	0.48
5:E:95:MET:HG2	5:E:141:GLY:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:THR:HG21	6:F:5:LEU:HB3	1.95	0.48
2:B:343:ARG:C	8:B:530:HOH:O	2.56	0.47
4:D:203:ARG:O	4:D:204:GLU:CG	2.45	0.47
7:G:100:LYS:HE3	8:G:251:HOH:O	2.12	0.47
6:F:2:THR:OG1	6:F:3:ALA:C	2.56	0.47
3:C:267:PRO:HD2	3:C:286:ASP:HB2	1.95	0.47
2:B:161:ASP:OD1	2:B:161:ASP:N	2.46	0.47
3:C:118:ARG:NH1	8:C:703:HOH:O	2.48	0.47
2:B:180:ARG:HD3	8:B:583:HOH:O	2.15	0.47
3:C:264:ASP:O	3:C:265:CYS:HB2	2.15	0.47
5:E:104:PRO:HA	5:E:108:GLU:OE1	2.14	0.47
3:C:142:ARG:NH2	8:C:609:HOH:O	2.43	0.47
4:D:78:ARG:NH2	8:D:597:HOH:O	2.31	0.47
5:E:144:LEU:HD22	5:E:148:VAL:HG23	1.96	0.47
3:C:126:GLU:C	3:C:128:GLU:H	2.22	0.47
4:D:7:ASN:ND2	8:D:319:HOH:O	2.22	0.47
5:E:9:MET:SD	5:E:63:GLU:HG2	2.55	0.47
1:A:143:VAL:CG1	8:A:578:HOH:O	2.63	0.46
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.96	0.46
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.97	0.46
3:C:18:LYS:NZ	8:C:404:HOH:O	2.47	0.46
1:A:359:LYS:O	1:A:359:LYS:HG2	2.13	0.46
2:B:327:GLU:HB2	8:B:568:HOH:O	2.15	0.46
5:E:92:GLU:C	5:E:96:TYR:CE1	2.93	0.46
1:A:91:ARG:O	1:A:94:GLU:HB2	2.16	0.46
6:F:6:ARG:HB3	6:F:7:PRO:HD3	1.98	0.46
3:C:72:THR:HA	3:C:98:ALA:HB1	1.98	0.46
3:C:139:LYS:HA	3:C:140:PRO:HA	1.73	0.46
1:A:119:THR:HB	1:A:120:PRO:HD2	1.98	0.46
2:B:205:ASN:ND2	2:B:208:ALA:H	2.08	0.46
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.51	0.46
4:D:262:ILE:O	4:D:266:MET:HG3	2.16	0.45
5:E:139:GLU:O	5:E:142:LEU:HD23	2.15	0.45
7:G:9:ALA:O	7:G:10:ARG:C	2.58	0.45
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.98	0.45
2:B:235:LEU:CD2	6:F:107:LYS:HZ1	2.29	0.45
3:C:282:GLY:O	3:C:370:LYS:HE3	2.17	0.45
3:C:54:GLN:HG2	8:C:588:HOH:O	2.16	0.45
5:E:16:ILE:HG23	5:E:16:ILE:O	2.17	0.45
3:C:147:SER:HB2	8:C:699:HOH:O	2.17	0.45
7:G:10:ARG:HA	7:G:13:LYS:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:LYS:NZ	8:B:504:HOH:O	2.48	0.45
2:B:240:LEU:HB2	8:B:465:HOH:O	2.16	0.45
2:B:173:PHE:CG	2:B:174:SER:N	2.85	0.44
2:B:306:GLY:HA2	2:B:309:MET:HE2	1.99	0.44
4:D:186:LYS:NZ	4:D:200:PHE:H	2.15	0.44
2:B:318:GLU:HG3	2:B:342:ILE:HD12	1.99	0.44
3:C:21:THR:O	3:C:21:THR:CG2	2.65	0.44
4:D:237:ARG:HD3	8:D:381:HOH:O	2.16	0.44
1:A:104:GLU:OE1	1:A:106:GLU:HG3	2.16	0.44
3:C:21:THR:HG22	8:C:696:HOH:O	2.16	0.44
1:A:190:ILE:O	1:A:191:LYS:HD3	2.17	0.44
1:A:284:HIS:HE2	5:E:2:PRO:N	2.15	0.44
4:D:112:GLN:CD	8:D:592:HOH:O	2.59	0.44
6:F:121:PHE:O	6:F:125:GLN:CG	2.63	0.44
1:A:217:PRO:C	1:A:219:GLN:H	2.26	0.44
2:B:235:LEU:CD2	6:F:107:LYS:NZ	2.81	0.44
3:C:31:GLU:OE1	3:C:33:HIS:HE1	2.01	0.44
3:C:47:GLU:OE2	3:C:49:LYS:CE	2.65	0.44
4:D:75:LEU:HD23	4:D:75:LEU:C	2.42	0.44
4:D:282:PRO:O	4:D:283:ASP:CB	2.58	0.44
2:B:235:LEU:HD21	6:F:107:LYS:HZ1	1.83	0.44
5:E:93:LYS:HA	5:E:96:TYR:CD1	2.53	0.44
1:A:313:ARG:N	1:A:314:PRO:CD	2.81	0.43
3:C:107:ASN:HD22	3:C:108:GLU:N	2.15	0.43
5:E:95:MET:HG2	5:E:141:GLY:CA	2.47	0.43
3:C:203:GLY:CA	7:G:146:THR:HG21	2.48	0.43
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.18	0.43
2:B:231:GLN:NE2	2:B:231:GLN:CA	2.81	0.43
4:D:261:TYR:O	4:D:264:THR:OG1	2.33	0.43
1:A:239:VAL:CG1	5:E:4:TYR:CE2	2.98	0.43
2:B:339:LYS:CE	8:B:554:HOH:O	2.67	0.43
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.53	0.43
1:A:71:THR:HG23	1:A:72:TYR:CD1	2.54	0.43
1:A:71:THR:OG1	1:A:71:THR:O	2.37	0.43
2:B:164:THR:HB	2:B:182:LEU:HB3	2.01	0.43
5:E:95:MET:HA	5:E:95:MET:HE2	1.99	0.43
1:A:216:PRO:HB2	1:A:219:GLN:HB2	2.01	0.43
5:E:155:LYS:N	5:E:156:PRO:HD3	2.34	0.43
1:A:309:ILE:HA	1:A:312:ARG:HG3	2.01	0.42
4:D:9:ARG:O	4:D:13:GLU:HG3	2.19	0.42
1:A:313:ARG:HB2	1:A:314:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:MET:O	1:A:418:SER:HB2	2.19	0.42
3:C:19:ASP:C	8:C:707:HOH:O	2.62	0.42
2:B:331:LYS:HD3	2:B:331:LYS:C	2.44	0.42
4:D:45:ILE:HA	4:D:56:MET:O	2.19	0.42
1:A:19:LEU:HG	1:A:29:PHE:HB2	2.02	0.42
1:A:143:VAL:HG13	8:A:578:HOH:O	2.20	0.42
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.19	0.42
1:A:270:ASP:OD2	5:E:158:LYS:NZ	2.47	0.42
3:C:84:ARG:HG3	8:C:393:HOH:O	2.19	0.42
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.83	0.42
5:E:154:ASP:O	5:E:155:LYS:CG	2.67	0.42
2:B:157:VAL:HB	2:B:303:LEU:HD13	2.02	0.41
4:D:7:ASN:CG	8:D:448:HOH:O	2.63	0.41
3:C:144:THR:N	6:F:28:GLN:NE2	2.65	0.41
5:E:57:ASN:OD1	8:E:369:HOH:O	2.22	0.41
3:C:131:TRP:HE3	3:C:131:TRP:O	2.03	0.41
5:E:82:LEU:HD23	5:E:148:VAL:HG21	2.02	0.41
6:F:129:HIS:ND1	8:F:365:HOH:O	2.29	0.41
3:C:107:ASN:HD22	3:C:109:LYS:H	1.69	0.41
5:E:75:ILE:HG23	5:E:144:LEU:HD11	2.03	0.41
5:E:60:ILE:HD12	5:E:116:ILE:HG23	2.01	0.41
3:C:34:ILE:HB	3:C:46:HIS:HB2	2.01	0.41
5:E:139:GLU:O	5:E:143:ARG:HB2	2.19	0.41
7:G:100:LYS:HG2	8:G:214:HOH:O	2.20	0.41
5:E:156:PRO:O	5:E:157:SER:C	2.64	0.41
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.49	0.41
2:B:274:GLU:OE1	2:B:275:GLY:N	2.44	0.41
1:A:217:PRO:C	1:A:219:GLN:N	2.79	0.41
1:A:343:VAL:CG2	1:A:363:ILE:CD1	2.95	0.41
3:C:189:MET:N	3:C:190:PRO:HD3	2.36	0.41
4:D:233:ASN:O	4:D:237:ARG:HB2	2.20	0.41
3:C:230:ASP:OD2	8:C:437:HOH:O	2.22	0.41
3:C:297:THR:HG22	8:C:665:HOH:O	2.21	0.41
6:F:125:GLN:HE21	6:F:125:GLN:HB3	1.45	0.41
2:B:170:TYR:O	2:B:172:GLY:N	2.54	0.40
2:B:319:ARG:NH1	7:G:17:ASP:OD2	2.54	0.40
4:D:228:PHE:HB3	4:D:229:PRO:HD2	2.03	0.40
1:A:4:ARG:HD3	1:A:5:LEU:HG	2.03	0.40
2:B:232:LYS:HD2	8:B:504:HOH:O	2.21	0.40
5:E:105:ILE:HG22	5:E:133:LEU:HD23	2.03	0.40
6:F:146:ILE:HA	6:F:149:MET:HE3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:10:ARG:HA	7:G:13:LYS:HD2	2.03	0.40
1:A:176:HIS:CD2	1:A:192:HIS:HD2	2.33	0.40
3:C:201:SER:O	3:C:201:SER:OG	2.30	0.40
4:D:7:ASN:HB3	8:D:653:HOH:O	2.20	0.40
2:B:326:LEU:C	2:B:326:LEU:HD23	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/418 (94%)	377 (95%)	16 (4%)	2 (0%)	24	21
2	B	188/394 (48%)	167 (89%)	15 (8%)	6 (3%)	3	1
3	C	348/372 (94%)	328 (94%)	18 (5%)	2 (1%)	21	17
4	D	282/300 (94%)	275 (98%)	6 (2%)	1 (0%)	30	27
5	E	172/178 (97%)	160 (93%)	8 (5%)	4 (2%)	5	2
6	F	165/168 (98%)	160 (97%)	5 (3%)	0	100	100
7	G	135/151 (89%)	130 (96%)	2 (2%)	3 (2%)	5	2
All	All	1685/1981 (85%)	1597 (95%)	70 (4%)	18 (1%)	11	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ARG
2	B	155	VAL
2	B	171	GLU
2	B	336	LYS
4	D	283	ASP
5	E	3	ALA

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Mol	Chain	Res	Type
5	E	87	SER
7	G	10	ARG
7	G	22	ASN
1	A	263	SER
3	C	284	ARG
2	B	289	ALA
5	E	151	PRO
7	G	23	LYS
2	B	178	LEU
2	B	340	PHE
3	C	371	ILE
5	E	156	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	352/363 (97%)	330 (94%)	22 (6%)	16	13
2	B	165/345 (48%)	150 (91%)	15 (9%)	9	6
3	C	301/313 (96%)	288 (96%)	13 (4%)	26	25
4	D	249/264 (94%)	243 (98%)	6 (2%)	43	47
5	E	156/159 (98%)	142 (91%)	14 (9%)	9	6
6	F	154/155 (99%)	151 (98%)	3 (2%)	50	56
7	G	114/124 (92%)	103 (90%)	11 (10%)	8	5
All	All	1491/1723 (86%)	1407 (94%)	84 (6%)	19	16

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	71	THR
1	A	82	ILE
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	143	VAL
1	A	158	VAL
1	A	160	GLU
1	A	191	LYS
1	A	198	ARG
1	A	230	ARG
1	A	251	LYS
1	A	255	GLN
1	A	265	LYS
1	A	289	ASN
1	A	310	ASP
1	A	312	ARG
1	A	335	LEU
1	A	343	VAL
1	A	353	LEU
1	A	363	ILE
1	A	417	MET
2	B	155	VAL
2	B	159	SER
2	B	161	ASP
2	B	175	LEU
2	B	182	LEU
2	B	184	ILE
2	B	220	LEU
2	B	231	GLN
2	B	235	LEU
2	B	240	LEU
2	B	274	GLU
2	B	290	ASP
2	B	294	ARG
2	B	320	GLU
2	B	326	LEU
3	C	21	THR
3	C	90	LEU
3	C	92	ILE
3	C	107	ASN
3	C	109	LYS
3	C	131	TRP
3	C	140	PRO
3	C	297	THR
3	C	305	LEU
3	C	324	LEU

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Mol	Chain	Res	Type
3	C	326	LYS
3	C	367	LYS
3	C	370	LYS
4	D	18	LYS
4	D	37	ASP
4	D	54	LYS
4	D	84	LEU
4	D	116	LEU
4	D	190	ARG
5	E	22	LEU
5	E	39	THR
5	E	60	ILE
5	E	63	GLU
5	E	80	LYS
5	E	82	LEU
5	E	95	MET
5	E	98	LEU
5	E	101	THR
5	E	116	ILE
5	E	142	LEU
5	E	144	LEU
5	E	146	GLU
5	E	161	THR
6	F	6	ARG
6	F	125	GLN
6	F	165	LEU
7	G	16	VAL
7	G	18	GLU
7	G	21	GLU
7	G	27	GLU
7	G	39	GLU
7	G	64	ILE
7	G	68	SER
7	G	86	PHE
7	G	87	LYS
7	G	93	LYS
7	G	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	176	HIS
1	A	192	HIS
1	A	255	GLN
1	A	289	ASN
1	A	306	ASN
1	A	318	ASN
1	A	370	HIS
1	A	392	GLN
2	B	205	ASN
2	B	231	GLN
2	B	272	ASN
2	B	284	ASN
3	C	33	HIS
3	C	40	ASN
3	C	65	ASN
3	C	107	ASN
3	C	303	GLN
3	C	331	GLN
4	D	140	ASN
4	D	231	HIS
4	D	263	HIS
6	F	28	GLN
6	F	125	GLN
6	F	129	HIS
7	G	22	ASN
7	G	48	GLN
7	G	61	ASN
7	G	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	401/418 (95%)	0.96	84 (20%) 2 2	18, 35, 76, 97	0
2	B	190/394 (48%)	2.18	86 (45%) 0 1	22, 46, 91, 109	0
3	C	354/372 (95%)	0.95	56 (15%) 5 4	20, 30, 76, 106	0
4	D	284/300 (94%)	0.55	18 (6%) 26 24	18, 30, 44, 55	0
5	E	174/178 (97%)	1.85	64 (36%) 1 1	33, 48, 77, 80	0
6	F	167/168 (99%)	0.16	9 (5%) 31 30	18, 26, 37, 58	0
7	G	139/151 (92%)	1.98	55 (39%) 1 1	23, 47, 95, 104	0
All	All	1709/1981 (86%)	1.12	372 (21%) 2 2	18, 34, 80, 109	0

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	284	ALA	11.5
5	E	96	TYR	10.3
2	B	340	PHE	8.8
4	D	283	ASP	8.3
3	C	297	THR	8.0
3	C	230	ASP	8.0
7	G	24	PHE	7.9
3	C	372	VAL	7.9
3	C	308	LYS	7.5
2	B	181	ARG	7.4
3	C	306	ASP	7.3
2	B	154	GLY	7.2
7	G	26	ASP	7.1
5	E	155	LYS	7.1
5	E	154	ASP	6.9
2	B	336	LYS	6.9
2	B	341	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
3	C	302	PHE	6.9
2	B	342	ILE	6.7
7	G	146	THR	6.7
3	C	305	LEU	6.6
5	E	175	GLY	6.6
2	B	288	ALA	6.4
2	B	338	SER	6.4
2	B	187	ARG	6.4
2	B	179	THR	6.3
5	E	62	ASN	6.3
2	B	173	PHE	6.2
7	G	25	VAL	6.2
2	B	343	ARG	5.9
1	A	252	TRP	5.9
7	G	19	TYR	5.9
3	C	307	LYS	5.9
7	G	16	VAL	5.8
3	C	298	ALA	5.8
5	E	85	CYS	5.8
2	B	291	ILE	5.8
7	G	63	PRO	5.7
2	B	329	VAL	5.6
2	B	155	VAL	5.6
1	A	262	ILE	5.5
7	G	11	PHE	5.5
3	C	371	ILE	5.5
2	B	339	LYS	5.5
2	B	337	LEU	5.4
1	A	259	ILE	5.4
1	A	261	ALA	5.3
2	B	175	LEU	5.3
7	G	9	ALA	5.3
2	B	332	GLY	5.1
2	B	159	SER	5.0
7	G	119	ASP	5.0
5	E	151	PRO	5.0
2	B	297	PHE	4.9
7	G	12	ARG	4.9
7	G	22	ASN	4.8
5	E	150	ASP	4.8
2	B	286	ILE	4.8
1	A	354	SER	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	366	LEU	4.8
3	C	369	LEU	4.8
3	C	309	ALA	4.8
1	A	351	GLU	4.7
7	G	27	GLU	4.7
7	G	64	ILE	4.7
1	A	51	VAL	4.6
3	C	201	SER	4.6
3	C	304	ASN	4.6
2	B	324	LEU	4.6
1	A	417	MET	4.6
7	G	70	ALA	4.6
7	G	21	GLU	4.5
2	B	156	VAL	4.5
2	B	334	VAL	4.5
5	E	89	SER	4.5
2	B	330	LEU	4.5
3	C	364	SER	4.5
2	B	182	LEU	4.4
3	C	202	CYS	4.4
3	C	54	GLN	4.4
2	B	293	THR	4.4
2	B	289	ALA	4.4
2	B	169	VAL	4.4
2	B	178	LEU	4.4
2	B	295	SER	4.3
7	G	35	ALA	4.3
1	A	349	LEU	4.3
1	A	353	LEU	4.2
1	A	68	GLU	4.2
5	E	153	ASN	4.2
2	B	184	ILE	4.2
1	A	264	LYS	4.2
3	C	131	TRP	4.2
2	B	183	ASP	4.1
2	B	168	PRO	4.1
2	B	325	TYR	4.1
3	C	299	ARG	4.1
3	C	362	LEU	4.1
7	G	14	VAL	4.1
5	E	94	GLU	4.1
4	D	211	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	288	PRO	4.0
7	G	120	ASN	3.9
3	C	370	LYS	3.9
2	B	167	CYS	3.9
1	A	418	SER	3.9
2	B	326	LEU	3.9
2	B	164	THR	3.9
1	A	343	VAL	3.9
2	B	162	GLY	3.9
7	G	42	VAL	3.9
1	A	256	TYR	3.9
2	B	333	ASP	3.8
1	A	71	THR	3.8
5	E	2	PRO	3.8
2	B	272	ASN	3.8
1	A	70	PRO	3.8
2	B	163	VAL	3.8
5	E	88	LYS	3.8
3	C	301	ARG	3.8
6	F	3	ALA	3.7
1	A	160	GLU	3.7
2	B	327	GLU	3.7
1	A	214	GLY	3.7
1	A	158	VAL	3.7
2	B	177	HIS	3.7
1	A	54	GLY	3.7
2	B	335	GLU	3.6
1	A	253	ILE	3.6
7	G	20	ASP	3.6
3	C	232	ASP	3.6
2	B	170	TYR	3.6
2	B	160	GLY	3.6
2	B	166	ILE	3.6
2	B	328	ARG	3.6
2	B	157	VAL	3.5
5	E	39	THR	3.5
5	E	107	GLY	3.5
3	C	303	GLN	3.5
1	A	221	LEU	3.5
2	B	303	LEU	3.5
1	A	350	SER	3.5
5	E	38	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	300	GLU	3.5
1	A	251	LYS	3.5
2	B	276	VAL	3.5
3	C	365	ALA	3.4
1	A	348	LYS	3.4
2	B	287	GLN	3.4
5	E	112	PRO	3.4
3	C	178	GLU	3.4
5	E	91	GLY	3.4
1	A	265	LYS	3.4
3	C	287	VAL	3.4
7	G	17	ASP	3.4
7	G	28	ASP	3.4
5	E	146	GLU	3.3
3	C	127	GLN	3.3
5	E	114	ASN	3.3
7	G	23	LYS	3.3
7	G	60	LYS	3.3
6	F	2	THR	3.3
5	E	152	GLN	3.3
1	A	310	ASP	3.3
2	B	161	ASP	3.3
3	C	283	GLY	3.3
1	A	202	TYR	3.2
1	A	340	LYS	3.2
2	B	290	ASP	3.2
2	B	174	SER	3.2
2	B	296	GLU	3.2
3	C	175	GLU	3.2
7	G	41	GLU	3.2
2	B	302	VAL	3.2
1	A	215	ILE	3.2
3	C	358	ASP	3.1
1	A	247	THR	3.1
5	E	100	ILE	3.1
5	E	106	PRO	3.1
5	E	149	PHE	3.1
2	B	294	ARG	3.1
5	E	87	SER	3.1
3	C	52	ASN	3.0
3	C	176	VAL	3.0
2	B	301	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	101	THR	3.0
1	A	267	PHE	3.0
5	E	12	ASP	3.0
1	A	346	ARG	3.0
2	B	180	ARG	3.0
3	C	173	ILE	3.0
1	A	258	GLY	3.0
2	B	298	TYR	3.0
2	B	273	VAL	3.0
5	E	113	LEU	3.0
5	E	116	ILE	3.0
6	F	4	THR	3.0
2	B	300	HIS	3.0
7	G	118	SER	2.9
1	A	172	ASP	2.9
2	B	206	HIS	2.9
1	A	360	PRO	2.9
2	B	176	PRO	2.9
1	A	254	LYS	2.9
7	G	37	PRO	2.9
7	G	74	ARG	2.9
1	A	359	LYS	2.9
2	B	322	LYS	2.9
4	D	158	LYS	2.9
2	B	279	ALA	2.9
1	A	52	MET	2.9
7	G	69	GLN	2.8
5	E	121	ALA	2.8
2	B	158	ASP	2.8
5	E	103	PHE	2.8
6	F	57	GLU	2.8
1	A	347	LEU	2.8
1	A	55	VAL	2.8
7	G	79	VAL	2.8
5	E	60	ILE	2.8
6	F	101	PHE	2.8
7	G	36	GLY	2.8
4	D	107	ASP	2.7
2	B	172	GLY	2.7
1	A	257	THR	2.7
1	A	271	VAL	2.7
2	B	165	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	179	ARG	2.7
5	E	97	THR	2.7
5	E	98	LEU	2.7
5	E	11	PRO	2.7
5	E	156	PRO	2.7
1	A	255	GLN	2.7
3	C	126	GLU	2.7
7	G	39	GLU	2.7
3	C	319	ALA	2.6
5	E	92	GLU	2.6
5	E	82	LEU	2.6
7	G	66	THR	2.6
5	E	148	VAL	2.6
7	G	18	GLU	2.6
2	B	283	PHE	2.6
5	E	111	PHE	2.6
4	D	108	SER	2.6
1	A	269	ILE	2.6
3	C	282	GLY	2.6
1	A	266	GLU	2.6
4	D	24	ALA	2.6
5	E	3	ALA	2.6
1	A	363	ILE	2.6
2	B	274	GLU	2.6
2	B	277	GLY	2.6
1	A	226	ALA	2.6
1	A	352	GLU	2.5
5	E	8	LEU	2.5
5	E	159	TRP	2.5
1	A	249	GLY	2.5
2	B	292	ASP	2.5
5	E	90	GLN	2.5
2	B	331	LYS	2.5
7	G	45	CYS	2.5
3	C	130	ASP	2.5
4	D	159	ASP	2.5
4	D	204	GLU	2.5
2	B	285	THR	2.5
5	E	95	MET	2.5
4	D	25	GLY	2.5
7	G	71	VAL	2.4
1	A	231	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	117	TYR	2.4
1	A	217	PRO	2.4
3	C	180	PRO	2.4
3	C	231	ALA	2.4
1	A	79	ARG	2.4
4	D	203	ARG	2.4
7	G	85	SER	2.4
1	A	224	ALA	2.4
7	G	10	ARG	2.4
7	G	57	ALA	2.4
5	E	79	LEU	2.4
5	E	102	ASN	2.4
4	D	282	PRO	2.4
5	E	36	THR	2.4
7	G	62	PRO	2.4
1	A	218	GLU	2.3
3	C	47	GLU	2.3
1	A	248	ASP	2.3
6	F	6	ARG	2.3
1	A	220	SER	2.3
7	G	77	SER	2.3
5	E	118	ALA	2.3
7	G	65	ASN	2.3
5	E	99	GLY	2.3
1	A	56	ASP	2.3
7	G	15	ASP	2.3
2	B	215	MET	2.3
7	G	13	LYS	2.3
3	C	274	SER	2.3
1	A	204	ILE	2.3
7	G	75	ALA	2.3
1	A	333	ARG	2.3
4	D	171	ASP	2.3
3	C	367	LYS	2.3
1	A	327	MET	2.3
1	A	292	PHE	2.3
5	E	105	ILE	2.3
1	A	416	VAL	2.3
1	A	312	ARG	2.3
3	C	360	ARG	2.3
2	B	299	LYS	2.3
5	E	14	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	149	LYS	2.3
6	F	5	LEU	2.3
1	A	229	GLU	2.2
6	F	102	PHE	2.2
1	A	67	ILE	2.2
5	E	109	PRO	2.2
1	A	209	ARG	2.2
2	B	284	ASN	2.2
7	G	38	ASP	2.2
7	G	58	ALA	2.2
1	A	208	LEU	2.2
3	C	29	ASN	2.2
3	C	40	ASN	2.2
4	D	229	PRO	2.2
7	G	91	ILE	2.2
5	E	126	ASP	2.2
1	A	207	LEU	2.2
5	E	142	LEU	2.2
4	D	130	GLN	2.2
3	C	363	GLU	2.2
2	B	185	ALA	2.2
1	A	232	SER	2.2
1	A	250	SER	2.2
1	A	268	SER	2.2
5	E	37	LYS	2.2
5	E	86	ASN	2.2
1	A	362	PRO	2.1
2	B	278	VAL	2.1
7	G	30	GLY	2.1
1	A	345	ALA	2.1
3	C	361	SER	2.1
2	B	309	MET	2.1
3	C	129	ASN	2.1
1	A	84	GLU	2.1
1	A	344	ASP	2.1
7	G	88	ALA	2.1
1	A	263	SER	2.1
5	E	145	CYS	2.1
3	C	128	GLU	2.1
2	B	188	ASP	2.1
5	E	10	ASP	2.1
1	A	369	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLY	2.1
7	G	53	ALA	2.1
2	B	281	LEU	2.1
7	G	90	ASP	2.1
1	A	156	ARG	2.1
4	D	189	ARG	2.1
3	C	237	VAL	2.1
5	E	43	ASP	2.0
1	A	245	TYR	2.0
1	A	242	PHE	2.0
5	E	164	VAL	2.0
5	E	157	SER	2.0
5	E	172	SER	2.0
4	D	214	ALA	2.0
4	D	49	ASN	2.0
1	A	157	GLN	2.0
3	C	368	ASP	2.0
6	F	92	ARG	2.0
7	G	40	GLY	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 oligosaccharides 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.