



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:34 am GMT

PDB ID : 1K8K
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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

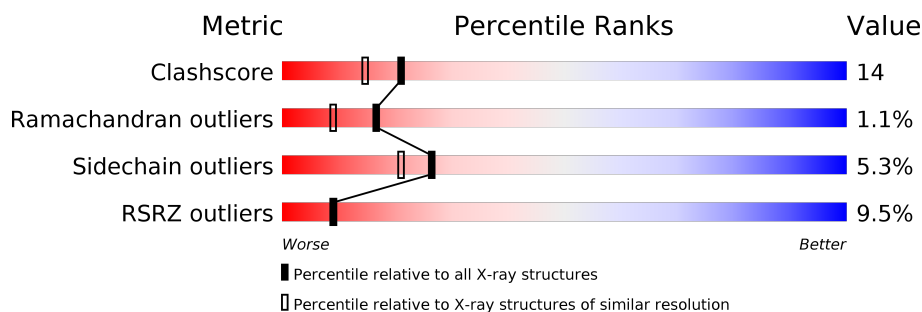
1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 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	418	<div> <div>8%</div> <div>78%</div> <div>14%</div> <div>• •</div> </div>
2	B	394	<div> <div>10%</div> <div>31%</div> <div>14%</div> <div>• •</div> <div>52%</div> </div>
3	C	372	<div> <div>8%</div> <div>74%</div> <div>18%</div> <div>• 5%</div> </div>
4	D	300	<div> <div>2%</div> <div>80%</div> <div>13%</div> <div>• 5%</div> </div>
5	E	178	<div> <div>12%</div> <div>62%</div> <div>28%</div> <div>7%</div> <div>• •</div> </div>
6	F	168	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>• •</div> </div>
7	G	151	<div> <div>17%</div> <div>75%</div> <div>11%</div> <div>5%</div> <div>8%</div> </div>

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			

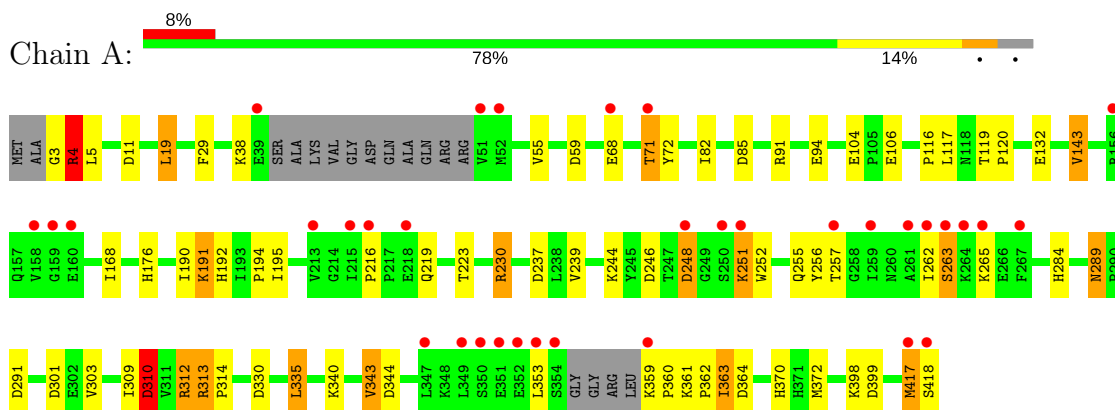
- Molecule 8 is water.

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		

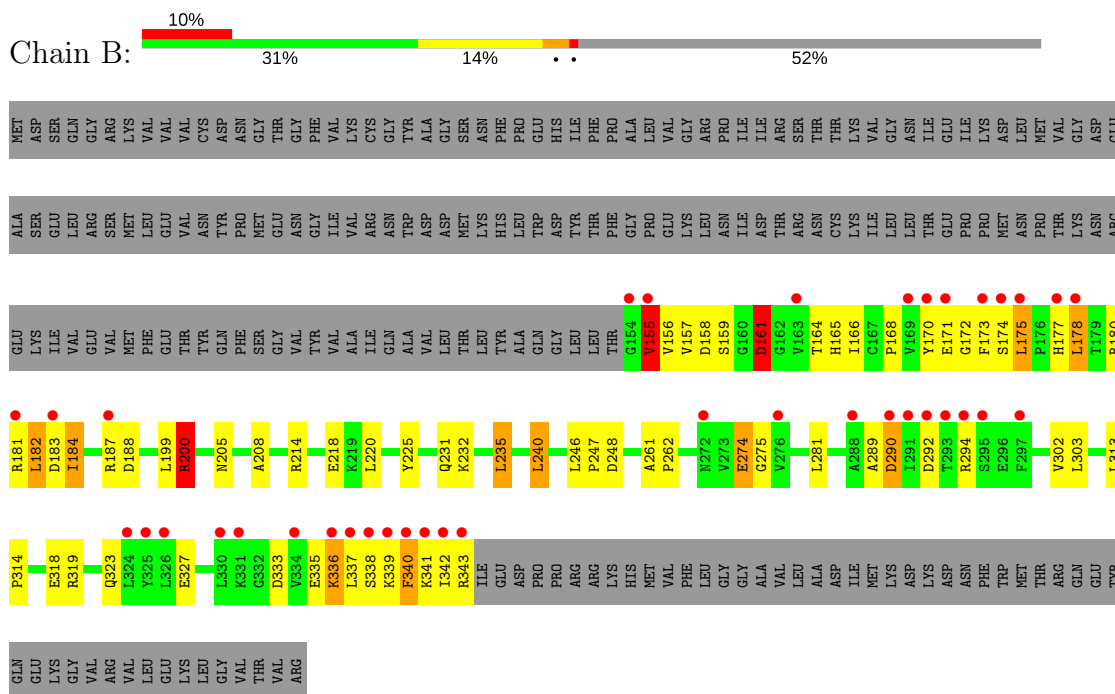
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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

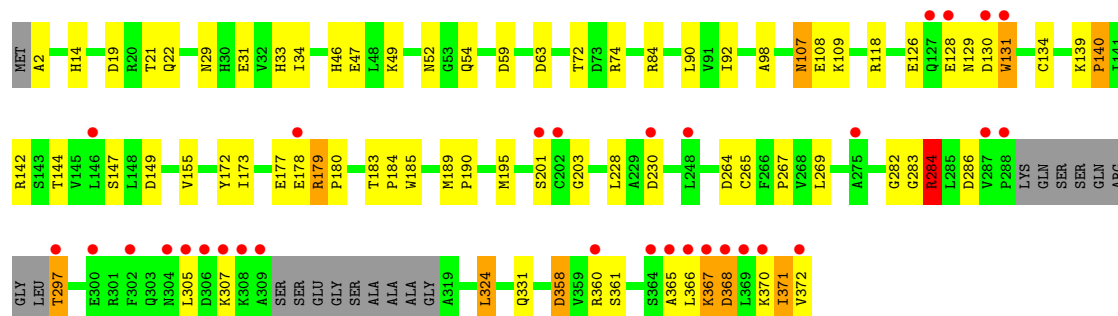


- Molecule 2: ACTIN-LIKE PROTEIN 2

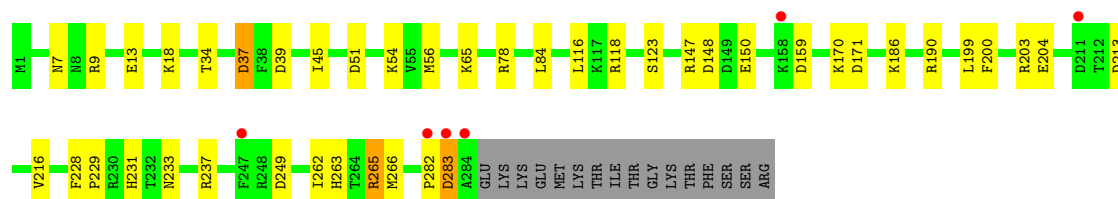
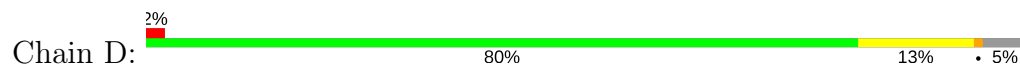


● Molecule 3: ARP2/3 COMPLEX 41 KDA SUBUNIT

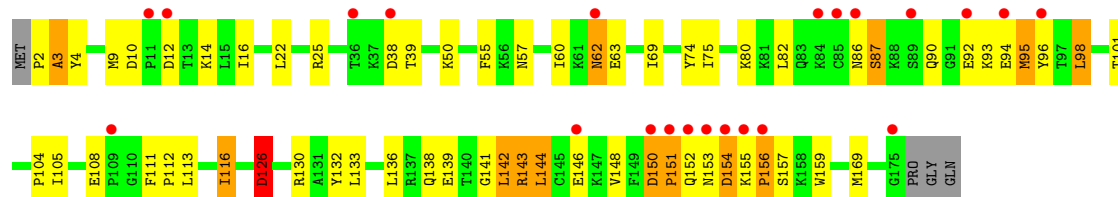




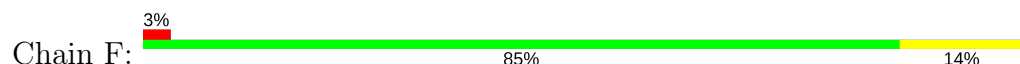
• Molecule 4: ARP2/3 COMPLEX 34 KDA SUBUNIT



• Molecule 5: ARP2/3 COMPLEX 21 KDA SUBUNIT



• Molecule 6: ARP2/3 COMPLEX 20 KDA SUBUNIT



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 41.54 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 92.1 (41.54-2.01)	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 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 49.6	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	0.94	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 [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	0.49	0/3293	0.79	13/4467 (0.3%)
2	B	0.40	0/1543	0.69	8/2084 (0.4%)
3	C	0.51	0/2826	0.79	6/3832 (0.2%)
4	D	0.53	0/2340	0.79	8/3160 (0.3%)
5	E	0.38	0/1448	0.70	5/1953 (0.3%)
6	F	0.56	0/1391	0.73	1/1867 (0.1%)
7	G	0.38	0/1070	0.73	3/1441 (0.2%)
All	All	0.48	0/13911	0.76	44/18804 (0.2%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	59	ASP	CB-CG-OD2	7.20	124.78	118.30
4	D	148	ASP	CB-CG-OD2	6.73	124.36	118.30
4	D	265	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	4	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	11	ASP	CB-CG-OD2	6.42	124.08	118.30
3	C	63	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	85	ASP	CB-CG-OD2	6.39	124.05	118.30
2	B	200	ARG	NE-CZ-NH2	-6.36	117.12	120.30
4	D	249	ASP	CB-CG-OD2	6.16	123.85	118.30
4	D	213	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	399	ASP	CB-CG-OD2	6.11	123.80	118.30
5	E	38	ASP	CB-CG-OD2	6.04	123.73	118.30
4	D	37	ASP	CB-CG-OD2	6.01	123.71	118.30
3	C	149	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	248	ASP	CB-CG-OD2	6.00	123.69	118.30
1	A	330	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	59	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	301	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	246	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	344	ASP	CB-CG-OD2	5.73	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	290	ASP	CB-CG-OD2	5.69	123.42	118.30
5	E	126	ASP	CB-CG-OD2	5.63	123.37	118.30
4	D	171	ASP	CB-CG-OD2	5.50	123.25	118.30
7	G	15	ASP	CB-CG-OD2	5.46	123.22	118.30
4	D	159	ASP	CB-CG-OD2	5.43	123.19	118.30
2	B	161	ASP	CB-CG-OD2	5.41	123.17	118.30
2	B	333	ASP	CB-CG-OD2	5.40	123.16	118.30
7	G	17	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	158	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	364	ASP	CB-CG-OD2	5.30	123.07	118.30
3	C	358	ASP	CB-CG-OD2	5.28	123.05	118.30
5	E	154	ASP	CB-CG-OD2	5.26	123.04	118.30
6	F	113	ASP	CB-CG-OD2	5.26	123.03	118.30
5	E	150	ASP	CB-CG-OD2	5.25	123.02	118.30
3	C	130	ASP	CB-CG-OD2	5.25	123.02	118.30
3	C	368	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	237	ASP	CB-CG-OD2	5.20	122.98	118.30
5	E	12	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	248	ASP	CB-CG-OD2	5.11	122.90	118.30
7	G	20	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	292	ASP	CB-CG-OD2	5.08	122.87	118.30
4	D	51	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	183	ASP	CB-CG-OD2	5.04	122.84	118.30

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	3212	0	3163	67	0
2	B	1515	0	1548	57	0
3	C	2757	0	2713	96	0
4	D	2291	0	2257	38	0
5	E	1414	0	1416	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1369	0	1410	33	0
7	G	1058	0	1065	26	0
8	A	364	0	0	13	0
8	B	209	0	0	15	0
8	C	338	0	0	36	0
8	D	355	0	0	15	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	373	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 (373) 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:HB2	5:E:155:LYS:CD	1.71	1.21
5:E:152:GLN:HG3	5:E:155:LYS:NZ	1.56	1.18
5:E:152:GLN:CG	5:E:155:LYS:HZ1	1.54	1.18
4:D:282:PRO:O	4:D:283:ASP:CG	1.84	1.16
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
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
5:E:152:GLN:CB	5:E:155:LYS:HZ1	1.56	1.05
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	1.22	0.92
3:C:54:GLN:CD	8:C:641:HOH:O	2.08	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	1.21	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:CG	5:E:155:LYS:HZ2	1.76	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
7:G:146:THR:O	7:G:146:THR:HG22	1.76	0.85
2:B:200:ARG:HD3	8:B:470:HOH:O	1.76	0.84
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
7:G:87:LYS:H	7:G:87:LYS:HD3	1.44	0.83
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
5:E:152:GLN:CB	5:E:155:LYS:HZ2	1.87	0.81
4:D:203:ARG:HG2	4:D:203:ARG:O	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
2:B:205:ASN:HD22	2:B:208:ALA:H	1.33	0.77
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
2:B:165:HIS:NE2	2:B:181:ARG:NE	2.33	0.75
1:A:310:ASP:N	1:A:310:ASP:OD1	2.13	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:335:GLU:O	2:B:336:LYS:C	2.29	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
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
6:F:146:ILE:HA	6:F:149:MET:HE2	1.74	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
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
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
4:D:203:ARG:C	8:D:652:HOH:O	2.32	0.66
6:F:129:HIS:ND1	8:F:365:HOH:O	2.29	0.65
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
3:C:189:MET:HA	3:C:195:MET:HE1	1.77	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:ALA:HB3	8:G:239:HOH:O	1.95	0.64
5:E:113:LEU:HD11	5:E:169:MET:HE3	1.80	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
3:C:189:MET:HG2	3:C:195:MET:HE3	1.80	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:CD	1:A:359:LYS:O	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
1:A:55:VAL:O	1:A:55:VAL:HG12	1.98	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
4:D:216:VAL:HA	8:D:652:HOH:O	2.00	0.61
4:D:7:ASN:ND2	8:D:448:HOH:O	2.33	0.60
1:A:230:ARG:CB	1:A:230:ARG:HH11	2.15	0.60
1:A:190:ILE:C	1:A:191:LYS:HD3	2.22	0.60
1:A:289:ASN:ND2	1:A:291:ASP:H	2.00	0.60
1:A:55:VAL:O	1:A:55:VAL:CG1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ARG:NE	8:B:544:HOH:O	2.33	0.58
2:B:214:ARG:NH1	2:B:218:GLU:CD	2.56	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
6:F:2:THR:C	8:F:397:HOH:O	2.43	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:183:THR:HG22	3:C:185:TRP:H	1.70	0.56
6:F:89:LYS:HA	6:F:92:ARG:NH1	2.19	0.56
4:D:186:LYS:HE3	4:D:199:LEU:HA	1.87	0.56
3:C:144:THR:CB	6:F:28:GLN:HE21	2.18	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:365:ALA:C	3:C:366:LEU:HD12	2.26	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
3:C:19:ASP:CB	8:C:707:HOH:O	2.46	0.55
2:B:323:GLN:HB3	7:G:11:PHE:O	2.06	0.55
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.88	0.55
5:E:93:LYS:HA	5:E:96:TYR:HD1	1.72	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
1:A:257:THR:HG23	8:A:755:HOH:O	2.06	0.54
3:C:370:LYS:H	3:C:370:LYS:HE2	1.72	0.54
3:C:84:ARG:O	3:C:84:ARG:HG2	2.07	0.54
5:E:152:GLN:O	5:E:155:LYS:HD2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:A:230:ARG:HH11	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:152:GLN:O	5:E:155:LYS:CD	2.57	0.52
5:E:95:MET:HA	5:E:95:MET:HE2	1.90	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:183:THR:HG23	3:C:184:PRO:HD2	1.91	0.52
4:D:282:PRO:O	4:D:283:ASP:CB	2.58	0.51
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
5:E:14:LYS:NZ	8:E:1316:HOH:O	2.42	0.51
1:A:340:LYS:NZ	8:A:698:HOH:O	2.43	0.51
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:173:ILE:O	3:C:177:GLU:HG2	2.10	0.51
3:C:52:ASN:ND2	8:C:653:HOH:O	2.43	0.51
7:G:87:LYS:N	7:G:87:LYS:HD3	2.21	0.51
3:C:183:THR:CG2	3:C:184:PRO:HD2	2.41	0.50
4:D:282:PRO:C	4:D:283:ASP:CG	2.62	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
5:E:150:ASP:C	5:E:152:GLN:N	2.64	0.50
1:A:4:ARG:HG2	1:A:4:ARG:HH11	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
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
5:E:150:ASP:C	5:E:152:GLN:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PRO:C	1:A:195:ILE:HD12	2.33	0.49
3:C:107:ASN:HD22	3:C:107:ASN:C	2.15	0.49
2:B:155:VAL:HA	2:B:168:PRO:HA	1.94	0.49
2:B:231:GLN:NE2	2:B:231:GLN:HA	2.26	0.49
3:C:21:THR:HG22	3:C:21:THR:O	2.13	0.49
5:E:111:PHE:CD2	5:E:112:PRO:O	2.66	0.49
1:A:289:ASN:C	1:A:289:ASN:HD22	2.15	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: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
6:F:146:ILE:HA	6:F:149:MET:HE3	1.91	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: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
3:C:74:ARG:CZ	6:F:31:GLU:OE2	2.61	0.48
1:A:244:LYS:HD3	1:A:252:TRP:CZ2	2.48	0.48
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.79	0.48
6:F:2:THR:HG21	6:F:5:LEU:HB3	1.95	0.48
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
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
3:C:228:LEU:HD23	3:C:228:LEU:C	2.35	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
2:B:180:ARG:HD3	8:B:583:HOH:O	2.15	0.47
6:F:17:GLN:CD	8:F:348:HOH:O	2.52	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
7:G:93:LYS:HB3	7:G:93:LYS:HZ3	1.79	0.47
3:C:189:MET:HG2	3:C:195:MET:CE	2.44	0.47
4:D:7:ASN:ND2	8:D:319:HOH:O	2.22	0.47
5:E:152:GLN:CD	5:E:155:LYS:HZ1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:139:LYS:HA	3:C:140:PRO:HA	1.73	0.46
3:C:72:THR:HA	3:C:98:ALA:HB1	1.98	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: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
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.98	0.45
3:C:282:GLY:O	3:C:370:LYS:HE3	2.17	0.45
3:C:178:GLU:O	3:C:179:ARG:C	2.55	0.45
3:C:54:GLN:HG2	8:C:588:HOH:O	2.16	0.45
5:E:16:ILE:O	5:E:16:ILE:HG23	2.17	0.45
3:C:147:SER:HB2	8:C:699:HOH:O	2.17	0.45
4:D:203:ARG:C	4:D:204:GLU:HG2	2.31	0.45
7:G:10:ARG:HA	7:G:13:LYS:CD	2.47	0.45
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
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:CG2	3:C:21:THR:O	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
6:F:121:PHE:O	6:F:125:GLN:CG	2.63	0.44
1:A:68:GLU:C	8:A:712:HOH:O	2.56	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
2:B:235:LEU:CD2	6:F:107:LYS:NZ	2.81	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
3:C:367:LYS:HD3	3:C:367:LYS:C	2.37	0.43
5:E:95:MET:HG2	5:E:141:GLY:CA	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CA	2:B:231:GLN:NE2	2.81	0.43
2:B:339:LYS:CE	8:B:554:HOH:O	2.67	0.43
1:A:239:VAL:CG1	5:E:4:TYR:CE2	2.98	0.43
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.53	0.43
4:D:282:PRO:C	4:D:283:ASP:OD1	2.57	0.43
5:E:95:MET:HG2	5:E:141:GLY:C	2.39	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
6:F:2:THR:OG1	6:F:3:ALA:C	2.56	0.43
1:A:216:PRO:HB2	1:A:219:GLN:HB2	2.01	0.43
2:B:343:ARG:C	8:B:530:HOH:O	2.56	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
1:A:417:MET:O	1:A:418:SER:HB2	2.19	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
3:C:126:GLU:C	3:C:128:GLU:H	2.22	0.42
3:C:84:ARG:HG3	8:C:393:HOH:O	2.19	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
5:E:57:ASN:OD1	8:E:369:HOH:O	2.22	0.41
3:C:144:THR:N	6:F:28:GLN:NE2	2.65	0.41
3:C:131:TRP:O	3:C:131:TRP:HE3	2.03	0.41
5:E:82:LEU:HD23	5:E:148:VAL:HG21	2.02	0.41
5:E:69:ILE:HG23	5:E:169:MET:HE1	2.01	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
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
7:G:9:ALA:O	7:G:10:ARG:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:228:PHE:HB3	4:D:229:PRO:HD2	2.03	0.40
2:B:319:ARG:NH1	7:G:17:ASP:OD2	2.54	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
5:E:152:GLN:HB2	5:E:155:LYS:HZ2	1.67	0.40
2:B:235:LEU:CD2	6:F:107:LYS:HZ1	2.34	0.40
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
2:B:235:LEU:HD21	6:F:107:LYS:HZ1	1.86	0.40
3:C:201:SER:OG	3:C:201:SER:O	2.30	0.40
5:E:92:GLU:C	5:E:96:TYR:CE1	2.93	0.40
2:B:235:LEU:HD23	6:F:107:LYS:HZ2	1.86	0.40
4:D:7:ASN:HB3	8:D:653:HOH:O	2.20	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%)	32 26
2	B	188/394 (48%)	167 (89%)	15 (8%)	6 (3%)	5 1
3	C	348/372 (94%)	328 (94%)	18 (5%)	2 (1%)	28 21
4	D	282/300 (94%)	275 (98%)	6 (2%)	1 (0%)	38 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	172/178 (97%)	160 (93%)	8 (5%)	4 (2%)	7	3
6	F	165/168 (98%)	160 (97%)	5 (3%)	0	100	100
7	G	135/151 (89%)	130 (96%)	2 (2%)	3 (2%)	8	3
All	All	1685/1981 (85%)	1597 (95%)	70 (4%)	18 (1%)	17	9

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
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%)	335 (95%)	17 (5%)	30	25
2	B	165/345 (48%)	151 (92%)	14 (8%)	12	7
3	C	301/313 (96%)	289 (96%)	12 (4%)	36	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	249/264 (94%)	242 (97%)	7 (3%)	49	49
5	E	156/159 (98%)	141 (90%)	15 (10%)	10	5
6	F	154/155 (99%)	150 (97%)	4 (3%)	51	52
7	G	114/124 (92%)	104 (91%)	10 (9%)	12	7
All	All	1491/1723 (86%)	1412 (95%)	79 (5%)	26	21

All (79) 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	143	VAL
1	A	191	LYS
1	A	230	ARG
1	A	251	LYS
1	A	255	GLN
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	200	ARG
2	B	220	LEU
2	B	235	LEU
2	B	240	LEU
2	B	274	GLU
2	B	290	ASP
2	B	294	ARG
2	B	340	PHE
3	C	90	LEU

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Mol	Chain	Res	Type
3	C	92	ILE
3	C	107	ASN
3	C	131	TRP
3	C	134	CYS
3	C	140	PRO
3	C	179	ARG
3	C	284	ARG
3	C	297	THR
3	C	305	LEU
3	C	324	LEU
3	C	367	LYS
4	D	18	LYS
4	D	37	ASP
4	D	54	LYS
4	D	84	LEU
4	D	116	LEU
4	D	118	ARG
4	D	190	ARG
5	E	10	ASP
5	E	22	LEU
5	E	25	ARG
5	E	39	THR
5	E	62	ASN
5	E	80	LYS
5	E	95	MET
5	E	98	LEU
5	E	101	THR
5	E	116	ILE
5	E	126	ASP
5	E	142	LEU
5	E	143	ARG
5	E	144	LEU
5	E	146	GLU
6	F	6	ARG
6	F	101	PHE
6	F	125	GLN
6	F	165	LEU
7	G	18	GLU
7	G	21	GLU
7	G	27	GLU
7	G	39	GLU
7	G	64	ILE

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Mol	Chain	Res	Type
7	G	68	SER
7	G	86	PHE
7	G	87	LYS
7	G	93	LYS
7	G	112	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	HIS
1	A	192	HIS
1	A	255	GLN
1	A	289	ASN
1	A	305	GLN
1	A	306	ASN
1	A	370	HIS
2	B	205	ASN
2	B	231	GLN
2	B	267	GLN
2	B	284	ASN
2	B	323	GLN
3	C	33	HIS
3	C	65	ASN
3	C	107	ASN
3	C	303	GLN
3	C	331	GLN
4	D	140	ASN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
6	F	28	GLN
6	F	125	GLN
6	F	154	ASN
7	G	22	ASN
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 [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	401/418 (95%)	0.49	34 (8%) 11 11	18, 35, 76, 97	0
2	B	190/394 (48%)	0.93	38 (20%) 1 1	22, 46, 91, 109	0
3	C	354/372 (95%)	0.45	31 (8%) 11 11	20, 30, 76, 106	0
4	D	284/300 (94%)	0.20	6 (2%) 64 63	18, 30, 44, 55	0
5	E	174/178 (97%)	0.71	22 (12%) 4 4	33, 48, 77, 80	0
6	F	167/168 (99%)	0.17	5 (2%) 51 51	18, 26, 37, 58	0
7	G	139/151 (92%)	0.94	26 (18%) 1 1	23, 47, 95, 104	0
All	All	1709/1981 (86%)	0.51	162 (9%) 9 9	18, 34, 80, 109	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	284	ALA	14.2
3	C	309	ALA	9.0
7	G	35	ALA	8.8
5	E	96	TYR	8.3
2	B	337	LEU	7.8
3	C	308	LYS	7.7
1	A	51	VAL	7.0
5	E	85	CYS	6.5
1	A	417	MET	6.4
3	C	372	VAL	6.1
1	A	418	SER	6.0
1	A	351	GLU	5.9
2	B	173	PHE	5.7
3	C	297	THR	5.6
2	B	336	LYS	5.6
4	D	283	ASP	5.6
5	E	154	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
3	C	307	LYS	5.4
7	G	119	ASP	5.1
5	E	175	GLY	5.1
3	C	306	ASP	5.1
2	B	341	LYS	4.9
3	C	230	ASP	4.9
5	E	151	PRO	4.8
2	B	181	ARG	4.8
2	B	343	ARG	4.8
5	E	89	SER	4.7
2	B	178	LEU	4.7
2	B	340	PHE	4.6
2	B	293	THR	4.6
7	G	28	ASP	4.6
7	G	30	GLY	4.5
4	D	211	ASP	4.5
3	C	366	LEU	4.5
7	G	27	GLU	4.5
2	B	342	ILE	4.4
5	E	155	LYS	4.4
7	G	146	THR	4.4
7	G	9	ALA	4.3
1	A	156	ARG	4.3
7	G	67	LYS	4.2
5	E	150	ASP	4.2
3	C	131	TRP	4.1
2	B	187	ARG	4.1
1	A	350	SER	4.0
2	B	292	ASP	4.0
5	E	153	ASN	4.0
3	C	127	GLN	3.9
7	G	63	PRO	3.9
1	A	347	LEU	3.9
7	G	24	PHE	3.9
1	A	359	LYS	3.9
1	A	158	VAL	3.8
2	B	339	LYS	3.7
1	A	262	ILE	3.7
3	C	367	LYS	3.7
6	F	3	ALA	3.6
7	G	120	ASN	3.6
1	A	218	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	331	LYS	3.5
7	G	10	ARG	3.5
1	A	353	LEU	3.5
5	E	62	ASN	3.5
3	C	201	SER	3.4
6	F	2	THR	3.4
1	A	354	SER	3.3
2	B	291	ILE	3.3
7	G	64	ILE	3.3
2	B	295	SER	3.3
1	A	52	MET	3.3
2	B	174	SER	3.3
1	A	352	GLU	3.2
3	C	365	ALA	3.2
2	B	170	TYR	3.2
5	E	38	ASP	3.2
5	E	156	PRO	3.2
5	E	12	ASP	3.2
3	C	369	LEU	3.2
3	C	364	SER	3.1
2	B	272	ASN	3.1
3	C	288	PRO	3.1
1	A	349	LEU	3.1
2	B	290	ASP	3.0
2	B	288	ALA	3.0
7	G	37	PRO	3.0
2	B	154	GLY	3.0
1	A	264	LYS	2.9
3	C	146	LEU	2.9
6	F	22	LEU	2.9
1	A	261	ALA	2.9
7	G	60	LYS	2.9
7	G	36	GLY	2.9
1	A	160	GLU	2.9
3	C	304	ASN	2.8
2	B	325	TYR	2.8
2	B	177	HIS	2.8
7	G	13	LYS	2.8
2	B	163	VAL	2.8
1	A	265	LYS	2.8
3	C	287	VAL	2.8
4	D	282	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
7	G	70	ALA	2.7
7	G	66	THR	2.7
3	C	248	LEU	2.7
1	A	213	VAL	2.7
3	C	130	ASP	2.7
1	A	159	GLY	2.7
2	B	326	LEU	2.7
3	C	305	LEU	2.7
2	B	276	VAL	2.7
3	C	370	LYS	2.7
3	C	300	GLU	2.6
5	E	94	GLU	2.6
7	G	26	ASP	2.6
5	E	146	GLU	2.6
5	E	86	ASN	2.6
7	G	21	GLU	2.6
2	B	183	ASP	2.6
3	C	368	ASP	2.6
2	B	338	SER	2.6
1	A	250	SER	2.5
5	E	109	PRO	2.5
1	A	248	ASP	2.5
2	B	294	ARG	2.5
7	G	29	ASP	2.5
1	A	263	SER	2.5
3	C	302	PHE	2.5
5	E	152	GLN	2.5
6	F	67	ILE	2.5
2	B	175	LEU	2.5
2	B	334	VAL	2.5
1	A	39	GLU	2.5
3	C	128	GLU	2.4
1	A	267	PHE	2.4
5	E	36	THR	2.4
2	B	155	VAL	2.4
3	C	275	ALA	2.4
1	A	215	ILE	2.4
5	E	84	LYS	2.3
7	G	19	TYR	2.3
1	A	251	LYS	2.3
1	A	216	PRO	2.3
4	D	247	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	330	LEU	2.2
2	B	297	PHE	2.2
7	G	22	ASN	2.2
7	G	149	LYS	2.2
1	A	259	ILE	2.2
1	A	71	THR	2.2
1	A	257	THR	2.2
4	D	158	LYS	2.2
7	G	65	ASN	2.2
2	B	169	VAL	2.2
5	E	11	PRO	2.2
1	A	68	GLU	2.2
2	B	324	LEU	2.2
3	C	202	CYS	2.1
5	E	92	GLU	2.1
3	C	178	GLU	2.1
6	F	25	PHE	2.1
2	B	171	GLU	2.0
3	C	360	ARG	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.