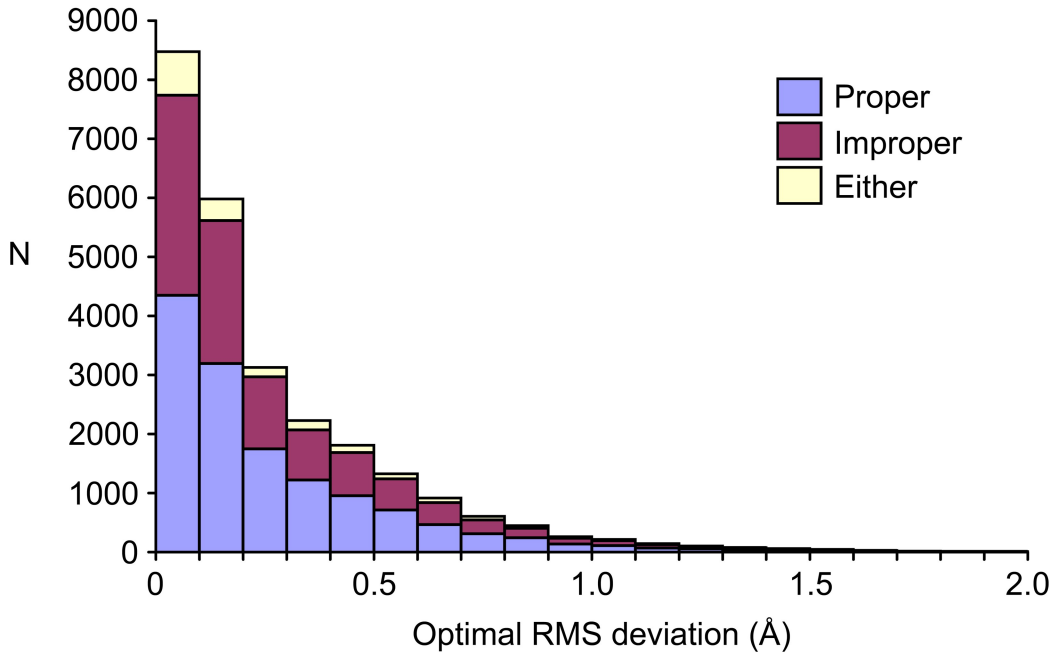
S1. Binned Distributions of RMS Values

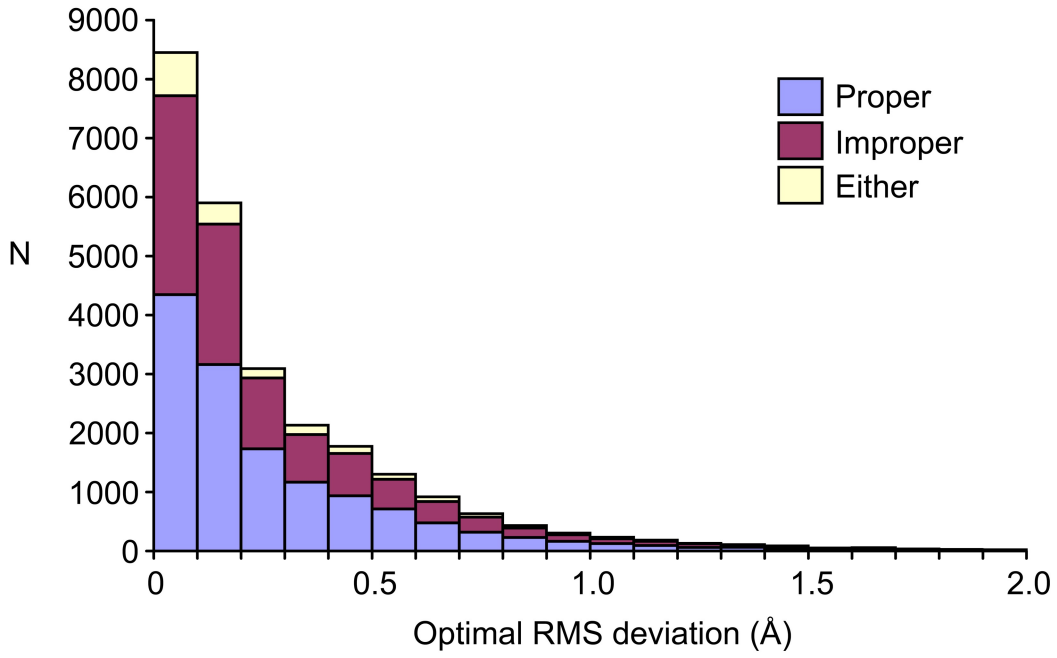
(a) Unconstrained (25926 matches):

RMS Range	Proper	Improper	Either	TOTAL	RMS Range	Proper	Improper	Either	TOTAL
0.00–0.10	4350	3389	737	8476	2.00–2.10	7	1	2	10
0.10–0.20	3194	2420	368	5982	2.10–2.20	1	2	0	3
0.20–0.30	1746	1222	160	3128	2.20–2.30	3	0	1	4
0.30–0.40	1220	848	160	2228	2.30–2.40	0	1	1	2
0.40–0.50	954	730	124	1808	2.40–2.50	0	0	1	1
0.50–0.60	712	527	87	1326	2.50–2.60	0	0	2	2
0.60–0.70	466	373	77	916	2.60–2.70	0	0	0	0
0.70–0.80	311	234	61	606	2.70–2.80	0	0	0	0
0.80–0.90	242	161	45	448	2.80–2.90	0	0	1	1
0.90–1.00	137	96	29	262	2.90–3.00	0	2	0	2
1.00–1.10	108	84	24	216	3.00–3.10	1	0	0	1
1.10–1.20	68	58	17	143	3.10–3.20	0	0	0	0
1.20–1.30	54	43	5	102	3.20–3.30	0	0	0	0
1.30–1.40	47	28	5	80	3.30–3.40	0	0	0	0
1.40–1.50	23	25	12	60	3.40–3.50	0	0	0	0
1.50–1.60	27	12	6	45	3.50–3.60	0	0	0	0
1.60–1.70	16	12	3	31	3.60–3.70	0	1	0	1
1.70–1.80	7	5	3	15	3.70–3.80	0	0	0	0
1.80–1.90	7	2	4	13	3.80–3.90	0	0	1	1
1.90–2.00	7	3	3	13	3.90–4.00	0	0	0	0



(b) Constrained by atom type (25926 matches):

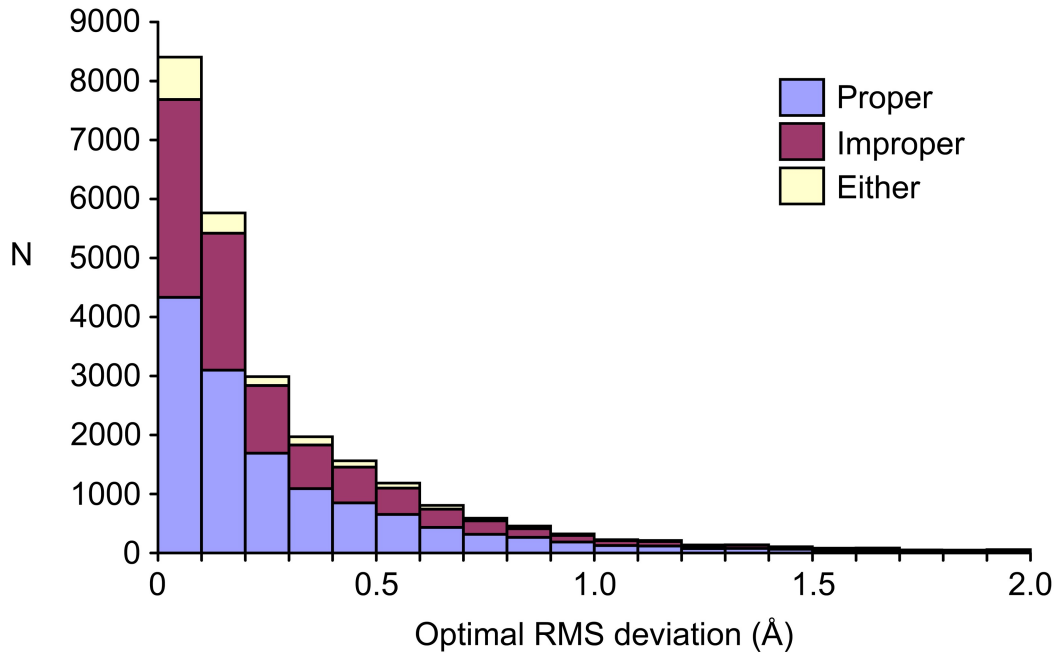
RMS Range	Proper	Improper	Either	TOTAL	RMS Range	Proper	Improper	Either	TOTAL
0.00–0.10	4347	3372	731	8450	2.20–2.30	4	2	1	7
0.10–0.20	3161	2379	361	5901	2.30–2.40	8	3	2	13
0.20–0.30	1730	1202	160	3092	2.40–2.50	0	0	0	0
0.30–0.40	1168	805	159	2132	2.50–2.60	1	1	1	3
0.40–0.50	936	716	120	1772	2.60–2.70	0	0	0	0
0.50–0.60	713	504	87	1304	2.70–2.80	0	0	0	0
0.60–0.70	475	364	79	918	2.80–2.90	0	0	0	0
0.70–0.80	317	256	60	633	2.90–3.00	0	0	1	1
0.80–0.90	228	162	42	432	3.00–3.10	0	0	1	1
0.90–1.00	164	110	30	304	3.10–3.20	0	0	1	1
1.00–1.10	125	83	25	233	3.20–3.30	1	0	0	1
1.10–1.20	93	69	23	185	3.30–3.40	0	0	1	1
1.20–1.30	60	63	7	130	3.40–3.50	0	0	0	0
1.30–1.40	63	41	4	108	3.50–3.60	0	0	0	0
1.40–1.50	37	37	12	86	3.60–3.70	1	1	0	2
1.50–1.60	27	15	11	53	3.70–3.80	0	0	0	0
1.60–1.70	27	22	9	58	3.80–3.90	0	0	0	0
1.70–1.80	10	19	5	34	3.90–4.00	0	0	0	0
1.80–1.90	15	10	1	26	4.00–4.10	0	0	0	0
1.90–2.00	8	9	4	21	4.10–4.20	0	0	1	1
2.00–2.10	5	4	3	12	4.20–4.30	1	0	0	1
2.10–2.20	4	5	1	10	4.30–4.40	0	0	0	0



(c) Constrained by atom connectivity number (defined as CCW; 25400 matches):

RMS Range	Proper	Improper	Either	TOTAL	RMS Range	Proper	Improper	Either	TOTAL
0.00–0.10	4334	3351	719	8404	2.60–2.70	5	3	2	10
0.10–0.20	3098	2319	347	5764	2.70–2.80	3	4	3	10
0.20–0.30	1689	1149	150	2988	2.80–2.90	3	0	0	3
0.30–0.40	1092	736	140	1968	2.90–3.00	3	1	0	4
0.40–0.50	848	606	108	1562	3.00–3.10	2	0	1	3
0.50–0.60	653	446	88	1187	3.10–3.20	1	1	0	2
0.60–0.70	433	309	67	809	3.20–3.30	2	0	2	4
0.70–0.80	315	228	46	589	3.30–3.40	2	0	1	3
0.80–0.90	264	147	45	456	3.40–3.50	2	1	0	3
0.90–1.00	186	111	26	323	3.50–3.60	2	0	1	3
1.00–1.10	125	83	19	227	3.60–3.70	0	0	0	0
1.10–1.20	116	77	19	212	3.70–3.80	0	1	0	1
1.20–1.30	73	47	15	135	3.80–3.90	0	0	1	1
1.30–1.40	77	54	7	138	3.90–4.00	0	0	0	0
1.40–1.50	62	34	10	106	4.00–4.10	0	0	0	0
1.50–1.60	47	29	6	82	4.10–4.20	1	0	1	2
1.60–1.70	37	36	10	83	4.20–4.30	0	0	0	0
1.70–1.80	19	29	5	53	4.30–4.40	1	0	0	1
1.80–1.90	27	19	3	49	4.40–4.50	0	1	0	1
1.90–2.00	23	27	7	57	4.50–4.60	0	0	1	1
2.00–2.10	12	11	4	27	4.60–4.70	0	0	0	0
2.10–2.20	17	12	3	32	4.70–4.80	1	0	0	1
2.20–2.30	21	8	2	31	4.80–4.90	0	0	0	0
2.30–2.40	10	8	2	20	4.90–5.00	0	0	1	1
2.40–2.50	13	8	1	22	5.00–5.10	0	0	1	1
2.50–2.60	10	9	1	20					

* Also ABOPUC: RMS = 12.5397



S2. Details of the results listings

- Three listings are provided:

  unconstrained.txt (25926 lines)
  type.txt (25926 lines)
  connectivity.txt (25400 lines)

- Format per line:

  {0},{1}:{0},{2}:{3}:{4}:{5}:{6}:{7}

  {0} = CSD refcode
  {1} = molecule 1 index
  {2} = molecule 2 index
  {3} = number of atoms
  {4} = molecule 1 site symmetry
  {5} = molecule 2 site symmetry
  {6} = optimal RMS value
  {7} = operator code: 1 = proper, -1 = improper, 0 = either

  Molecule index numbers are arbitrary, but are consistent in the three lists