Supplementary information for: Improved Quantitative Crystal-Structure Comparison using Powder Diffractograms via Anisotropic Volume Correction

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S1 Target Structures

Table S1: CCDC Identifiers for the BT6 target structures.

Compound	Form	Identifier
XXII	–	1451239
XXIII	A	1447522
XXIII	B	1447523
XXIII	C	1447524
XXIII	D	1447525
XXIII	E	1447526
XXIV	–	1447530
XXV	–	1447527
XXVI	–	1447529

S2 Dataset

S2.1 Lists removed from all BT6 submissions

Table S2: Lists of BT6 submissions removed prior to analysis.

Target-Group-List	Reason
XXII-G03-L2	structural duplicate of L1
XXV-G03-L2	structural duplicate of L1
XXII-G07-L2	structural duplicate of L1
XXIII-G07-L2	structural duplicate of L1
XXV-G07-L2	structural duplicate of L1
XXII-G12-L1	numerous issues
XXII-G12-L2	structural duplicate of L1
XXVI-G14-L2	structural duplicate of L1
XXII-G25-L2	structural duplicate of L1
XXIII-G25-L2	structural duplicate of L1

G14 submitted lists containing structures with $Z' = 1$ only, and a mix of $Z' = 1$ and $Z' = 2$, for compounds XXIII and XXVI. Only the list with the Z′ value matching the target was used in each case to avoid double counting. Thus, comparisons with targets XXIIIA, XXIIIB, and XXIIID used XXIII-G14-L1 (only $Z' = 1$). Comparisons with targets XXIIIC, and XXIIIE used XXIII-G14-L2 (mix of $Z' = 1$ and $Z' = 2$).

S2.2 Data processing

Many groups submitted lists with problematic symmetry descriptions or errors in unit cell angles for the assigned crystal systems. Corrections were made following lists:

- XXII-G04-L1: symmetry descriptions (add `_symmetry_equiv_pos_site_id` between `loop_` and `_symmetry_equiv_pos_as_xyz`)
- XXV-G04-L1: symmetry descriptions (add `_symmetry_equiv_pos_site_id` between `loop_` and `_symmetry_equiv_pos_as_xyz`)
- XXVI-G04-L1: symmetry descriptions (add `_symmetry_equiv_pos_site_id` between `loop_` and `_symmetry_equiv_pos_as_xyz`)
- XXII-G05-L1: symmetry descriptions (add `loop_` and re-order elements in `_symmetry_equiv_pos_as_xyz`)
- XXIII-G05-L1: symmetry descriptions (add `loop_` and re-order elements in `_symmetry_equiv_pos_as_xyz`)
- XXIV-G05-L1: symmetry descriptions (add `loop_` and re-order elements in `_symmetry_equiv_pos_as_xyz`)
- XXV-G05-L1: symmetry descriptions (add `loop_` and re-order elements in `_symmetry_equiv_pos_as_xyz`)
- XXVI-G05-L1: symmetry descriptions (add `loop_` and re-order elements in `_symmetry_equiv_pos_as_xyz`)
- XXII-G06-L1: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXII-G06-L2: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXIII-G06-L2: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXV-G06-L2: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXVI-G06-L2: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXII-G08-L2: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXII-G20-L1: symmetry descriptions (missing, wrong space group H-M notation)
- XXII-G23-L1: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXII-G25-L1: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXIII-G25-L1: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXIV-G25-L1: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles
- XXV-G25-L1: unit cells given a monoclinic space group without two right angles and/or an orthorhombic space group without all right angles

S3 Cell Transformation Matrices

Transformation matrices used in the structure screening:

Acute-angle triclinic cells:

$$\begin{bmatrix}-1 & 1 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}1 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}1 & -1 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 1 & 0\\ -1 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}$$

$$\begin{bmatrix}1 & 0 & 0\\ 1 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}0 & 1 & 0\\ -1 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ -1 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}0 & -1 & 0\\ 1 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}$$

$$\begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 1 & 0 & -1\end{bmatrix}\ \begin{bmatrix}0 & 0 & 1\\ 0 & -1 & 0\\ -1 & 0 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ -1 & 0 & 1\end{bmatrix}\ \begin{bmatrix}0 & 0 & -1\\ 0 & -1 & 0\\ 1 & 0 & -1\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 1\\ 0 & -1 & 0\\ 0 & 0 & 1\end{bmatrix}\ \begin{bmatrix}1 & 0 & -1\\ 0 & -1 & 0\\ 1 & 0 & 0\end{bmatrix}\ \begin{bmatrix}1 & 0 & -1\\ 0 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 1\\ 0 & -1 & 0\\ -1 & 0 & 0\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 1\\ 0 & 0 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & -1\\ 0 & 1 & 0\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & -1\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 1\\ 0 & -1 & 0\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 1 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & -1 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & -1\end{bmatrix}$$

Obtuse-angle triclinic cells:

$$\begin{bmatrix}1 & 1 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}1 & 1 & 0\\ -1 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & -1 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 0\\ 1 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}0 & -1 & 0\\ 1 & 1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}1 & 0 & 0\\ -1 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}0 & 1 & 0\\ -1 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 1 & 0 & 1\end{bmatrix}\ \begin{bmatrix}0 & 0 & -1\\ 0 & -1 & 0\\ 1 & 0 & 1\end{bmatrix}\ \begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ -1 & 0 & -1\end{bmatrix}\ \begin{bmatrix}0 & 0 & 1\\ 0 & -1 & 0\\ -1 & 0 & -1\end{bmatrix}$$

$$\begin{bmatrix}1 & 0 & 1\\ 0 & -1 & 0\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}1 & 0 & 1\\ 0 & -1 & 0\\ -1 & 0 & 0\end{bmatrix}\ \begin{bmatrix}-1 & 0 & -1\\ 0 & -1 & 0\\ 0 & 0 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & -1\\ 0 & -1 & 0\\ 1 & 0 & 0\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & 1\\ 0 & 0 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & 1\\ 0 & -1 & 0\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & -1\\ 0 & 0 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & -1\\ 0 & 1 & 0\end{bmatrix}$$

$$\begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 1 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & -1 & -1\end{bmatrix}\ \begin{bmatrix}-1 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & -1\end{bmatrix}$$

Only the 12 matrices in the two left-most columns are used for monoclinic cells, as they become symmetric with the results from using the matrices in the two right-most columns in the monoclinic crystal system.

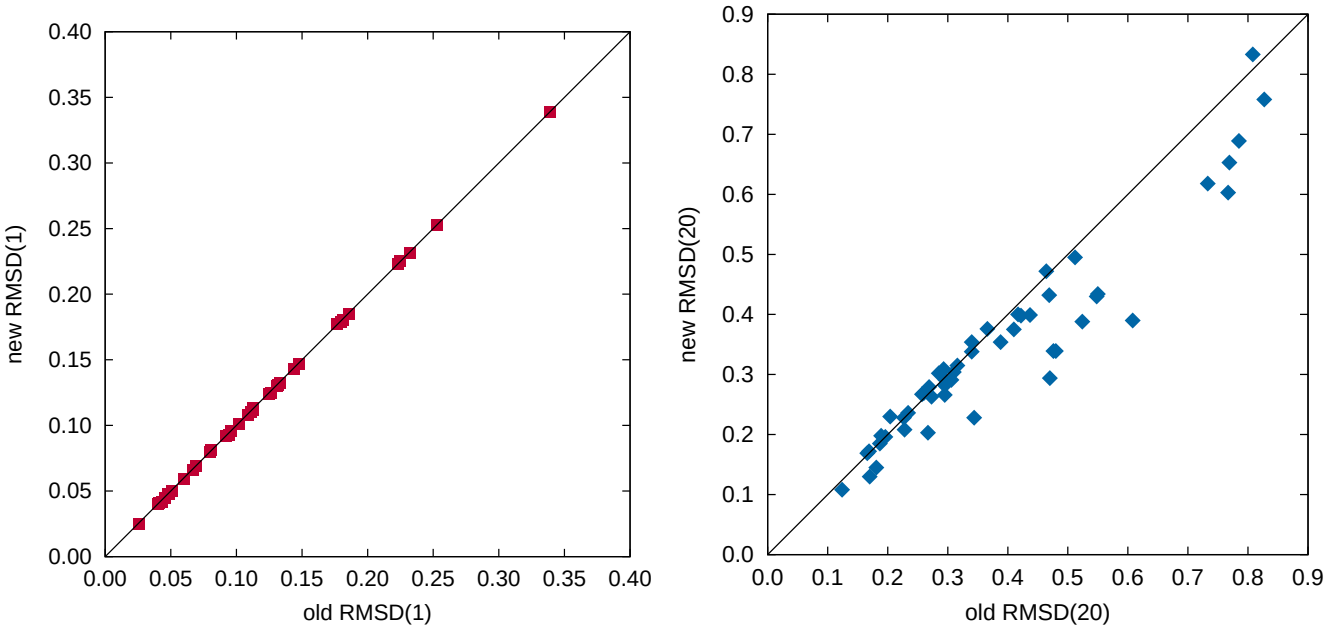
While some of these transformation matrices do not yield a determinant of 1, `critic2` is able to convert them to an appropriate transformation matrix. Alternative matrices than those shown here (other than the det=1 equivalents) are not viable as they will yield a unit cell that either 1) changes an angle from acute to obtuse or vice versa, 2) dramatically increases an axis length, or both simultaneously. Note that Niggli-reduced cells will have an obtuse angle for the non-right angle of a monoclinic cell, and will have all acute or all obtuse angles for a triclinic cell. Changing one angle from acute to obtuse (or vice versa) generates an incompatible unit cell for the developed volume correction.

Table S3: Transformation matrices applied to six structures identified as matches in BT6 in order to apply the anisotropic volume correction properly.

Structure	Transformation matrix		
XXIIIB-G09-L1-E13	[-1 0 0]	[-1 1 0]	[0 0 -1]
XXIIIB-G13-E88	[-1 0 0]	[-1 1 0]	[0 0 -1]
XXIIIB-G15-E13	[-1 0 0]	[-1 1 0]	[0 0 -1]
XXIIID-G06-L1-E73	[1 0 0]	[0 1 1]	[0 -1 0]
XXV-G05-L1-E01	[1 0 0]	[-1 -1 0]	[0 0 -1]
XXVI-G06-L1-E08	[-1 0 0]	[-1 1 0]	[0 0 -1]

S4 RMSD Drift from BT6 Results

Figure S1: Comparison of RMSD values reported in BT6 with those obtained in this work using the current version of Mercury. Results are shown for the unique structure matches, with the exceptions of XXIIID-G06-L1-E73 and XXIIID-G09-L1-E66, as their RMSD values were not reported in BT6.



S5 Dependence on COMPACK Options

Table S4: COMPACK results for structures submitted for compound XXIII that had a 180° rotation of the carboxylic acid group relative to the target. Tolerances are for both distances (%) and angles (°).

Structure	RMSD(1)	VC-RMSD(1)	Raw-RMSD(20)	Tolerance	VC-RMSD(20)	Tolerance
Ignoring H-atom and bond counts						
XXIIIA-G09-L1-E19	0.185	0.202	0.551	20	0.295	20
XXIIIB-G06-L1-E26	0.162	0.155	0.442	20	0.183	20
XXIIIB-G09-L1-E46	0.187	0.174	0.434	20	0.188	20
XXIIIB-G14-L1-E89	0.089	0.080	0.192	20	0.090	20
XXIIID-G06-L1-E73	0.220	0.261	0.747	20	0.321	20
XXIIID-G06-L1-E75	0.220	0.261	0.747	20	0.321	20
XXIIID-G09-L1-E66	0.239	0.211	0.603	20	0.269	20
Including H-atom and bond counts						
XXIIIA-G09-L1-E19	0.641	0.640	0.823	30	0.673	45
XXIIIB-G06-L1-E26	0.633	0.622	0.754	65	0.629	65
XXIIIB-G09-L1-E46	0.637	0.622	0.747	40	0.625	40
XXIIIB-G14-L1-E89	0.625	0.624	0.648	50	0.625	50
XXIIID-G06-L1-E73	0.651	0.651	0.967	65	0.679	60
XXIIID-G06-L1-E75	0.651	0.651	0.967	65	0.679	60
XXIIID-G09-L1-E66	0.658	0.639	0.860	40	0.661	40

S6 Example Output Tables

Table S5: Example `vc-pwdf` output of structures that pass the unit-cell dimension criteria, when given a 10% deviation allowance from the reference structure.

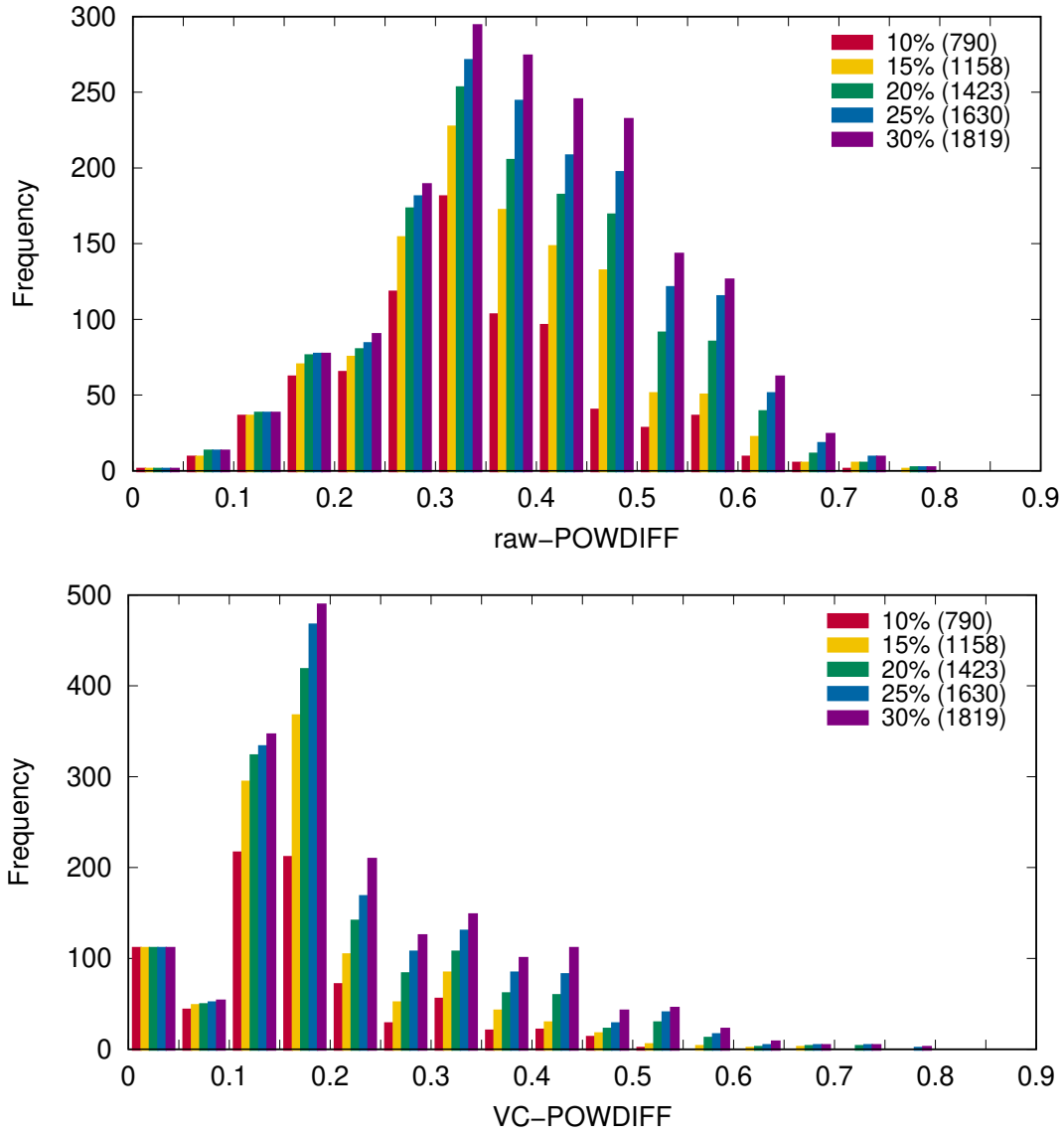
structure	POWDIFF	a	b	c	alpha	beta	gamma	volume	cryst_syst	spgrp
xx01_n.cif	0.1020773	6.804	11.999	12.542	106.60	90	90	981.2685	monoclinic	P2_1/c
xx47_n.cif	0.2202693	6.841	12.384	12.653	108.49	90	90	1016.6664	monoclinic	P2_1/c
xx71_n.cif	0.3565806	6.909	12.387	13.206	116.23	90	90	1013.8525	monoclinic	P2_1/c
xx10_n.cif	0.4136432	7.197	11.567	12.142	90	95.31	90	1006.4558	monoclinic	P2_1/c
xx22_n.cif	0.4316918	6.369	12.347	13.411	96.86	90	90	1047.0647	monoclinic	P2_1/c
xx07_n.cif	0.4443281	7.202	10.952	12.716	97.51	90	90	994.3874	monoclinic	P2_1/c
xx11_n.cif	0.5544066	6.891	11.806	12.444	94.76	90	90	1008.8917	monoclinic	P2_1/c
xx12_n.cif	0.5583085	6.889	11.807	12.452	94.86	90	90	1009.1846	monoclinic	P2_1/c
xx89_n.cif	0.6110274	7.173	11.948	12.254	103.50	90	90	1021.1873	monoclinic	P2_1/c

Table S6: Example `vc-pwdf` output of structures that have undergone volume correction, ranked by VC-POWDIFF comparison to the target structure.

structure	POWDIFF
xx01_n_VC.res	0.0040872
xx47_n_VC.res	0.0196081
xx22_n_VC.res	0.2152266
xx12_n_VC.res	0.3274327
xx11_n_VC.res	0.3274816
xx89_n_VC.res	0.3918757
xx71_n_VC.res	0.4240894
xx07_n_VC.res	0.4399329

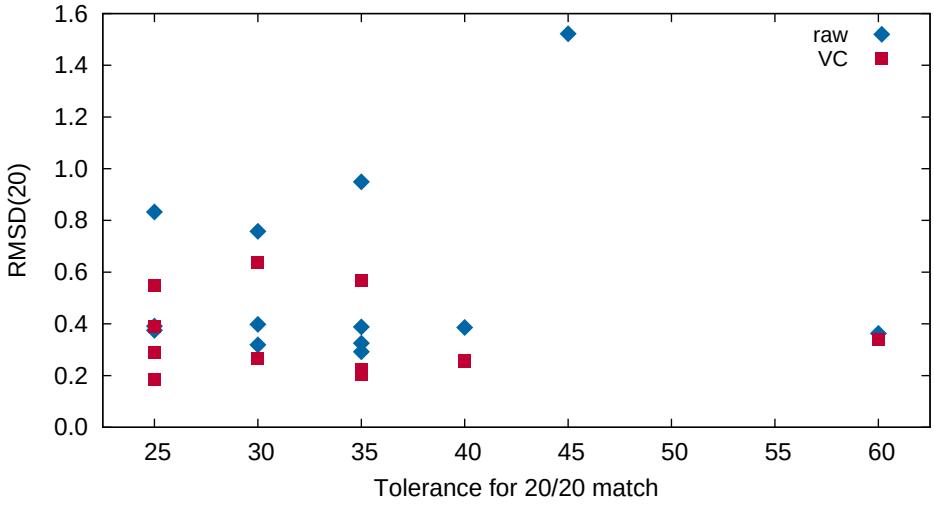
S7 Effect of VC-POWDIFF Tolerance

Figure S2: Histograms of POWDIFF values for structures that pass step (3) of our computational algorithm, with different volume and cell-length tolerances selected. Results are shown for the sets of structures before (top) and after (bottom) anisotropic volume correction.



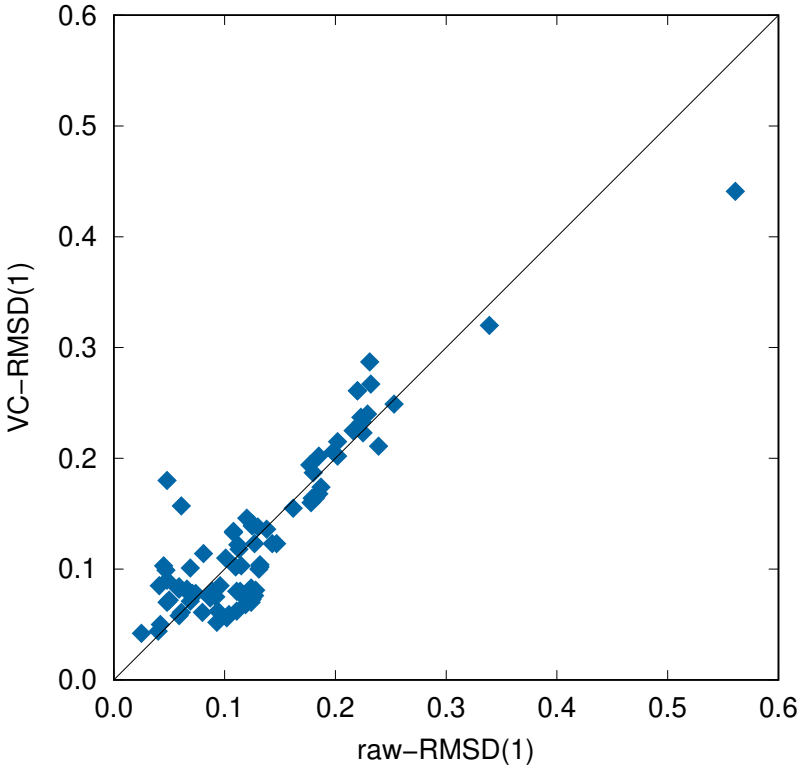
S8 Effect of RMSD Tolerance

Figure S3: RMSD(20) values (before and after volume correction) as a function of the tolerance required to obtain a 20/20 molecule match with COMPACK. Results are only shown for cases in which the tolerances had to be increased beyond their default values (20% and 20°) to obtain a match. Increments of 5% and 5° were used when raising the tolerances.



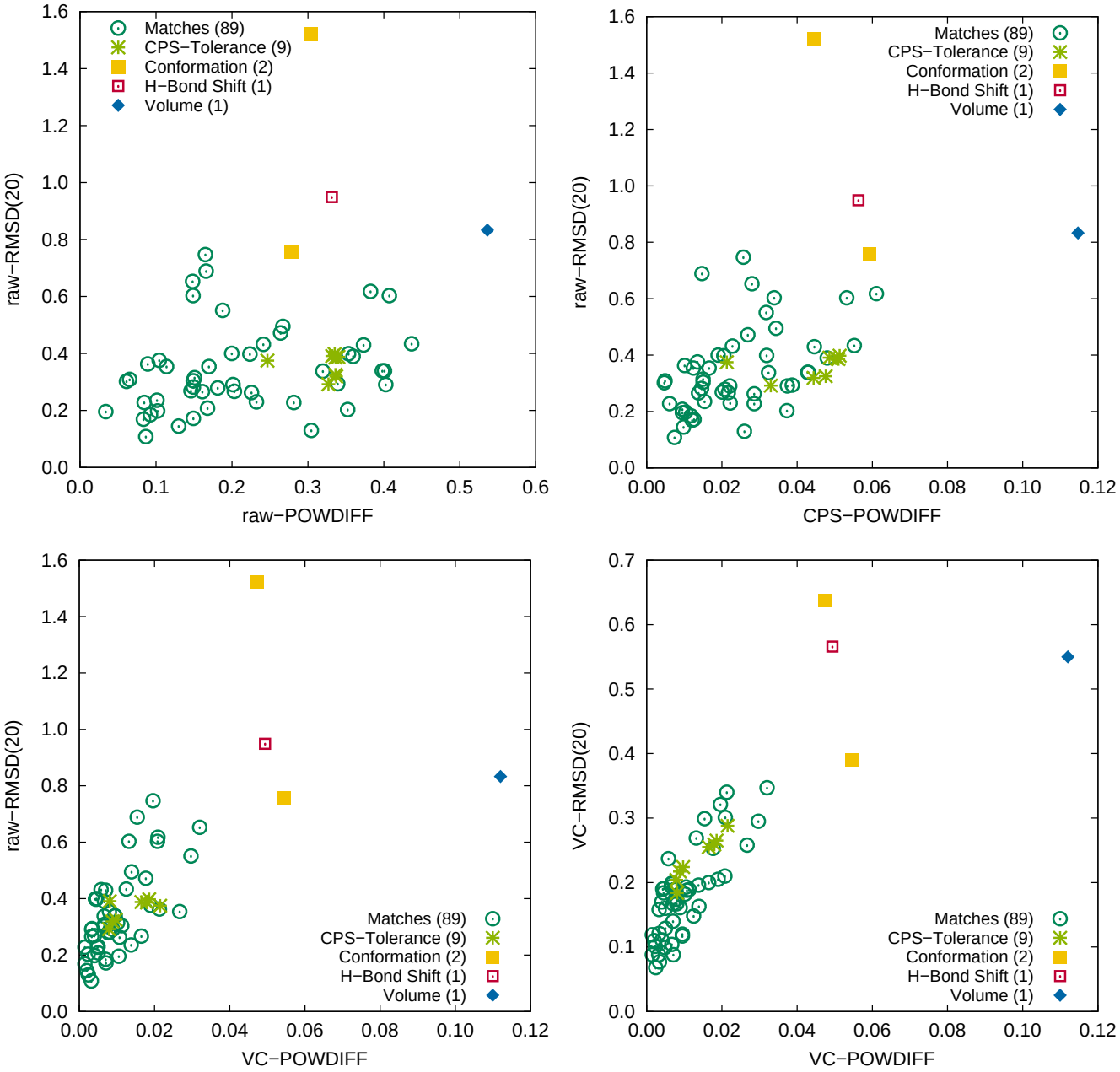
S9 Effect of Volume Correction on RMSD(1)

Figure S4: RMSD(1) values for molecules before and after anisotropic volume correction. The $y = x$ line is shown to highlight the roughly even numbers of structures where the RMSD(1) increases/decreases after volume correction.



S10 Correlations between RMSD(20) and POWDIFF Values

Figure S5: Correlations between various RMSD(20) and POWDIFF values for the 113-structure dataset.



S11 Results for the Set of 113 Structures

Table S7: Summary of results for the 113-structure set. For each structure, we indicate if it was a BT6 match (Yes/No). We additionally categorize each structure according to the labels used in Figures 3-5 in the manuscript. RMSDs are given in Å, tolerances in % and degrees. ΔV is the percent volume difference between the candidate and target structures, which is equivalent in magnitude (opposite in sign) to the percent volume correction. RMSD(1) values are only given for structures with $Z' = 1$.

Structure	BT6 Match	Category	RMSD(1)	VC-RMSD(1)	Raw-RMSD(20)	Tolerance	VC-RMSD(20)	Tolerance	Raw-POWDIFF	CPS-POWDIFF	VC-POWDIFF	ΔV
XXII-G03-L1-E03	Y	match	0.042	0.050	0.203	20	0.101	20	0.3523	0.0373	0.0023	-4.17
XXII-G03-L1-E56	N	XXII polytype	0.087	0.074	–	–	–	–	0.3229	0.0287	0.0171	-2.10
XXII-G04-L1-E01	Y	match	0.059	0.058	0.198	20	0.111	20	0.1021	0.0104	0.0041	2.73
XXII-G04-L1-E47	N	XXII polytype	0.059	0.084	–	–	–	–	0.2203	0.0355	0.0196	6.44
XXII-G05-L1-E04	Y	match	0.050	0.072	0.279	20	0.189	20	0.1813	0.0208	0.0077	-0.39
XXII-G05-L1-E77	N	XXII polytype	0.061	0.157	–	–	–	–	0.3592	0.0430	0.0406	1.63
XXII-G07-L1-E09	Y	match	0.112	0.122	0.196	20	0.193	20	0.0339	0.0095	0.0105	0.44
XXII-G07-L1-E91	N	XXII polytype	0.127	0.123	–	–	–	–	0.2313	0.0293	0.0191	2.29
XXII-G09-L1-E02	Y	Volume	0.048	0.180	0.833	25	0.550	25	0.5363	0.1147	0.1120	14.72
XXII-G13-L1-E01	Y	match	0.081	0.114	0.236	20	0.196	20	0.1013	0.0154	0.0138	1.26
XXII-G14-L1-E02	Y	match	0.040	0.044	0.130	20	0.068	20	0.3045	0.0260	0.0024	4.40
XXII-G14-L1-E42	N	XXII polytype	0.074	0.078	–	–	–	–	0.2931	0.0435	0.0238	5.34
XXII-G15-L1-E06	Y	match	0.066	0.082	0.291	20	0.158	20	0.4025	0.0374	0.0033	-1.72
XXII-G17-L1-E08	Y	match	0.110	0.102	0.267	20	0.200	20	0.2031	0.0217	0.0165	3.21
XXII-G18-L1-E06	Y	match	0.041	0.085	0.269	20	0.170	20	0.1461	0.0201	0.0040	1.27
XXII-G18-L1-E91	N	XXII polytype	0.058	0.083	–	–	–	–	0.1200	0.0211	0.0284	2.74
XXII-G18-L2-E02	Y	match	0.048	0.070	0.230	20	0.129	20	0.2323	0.0222	0.0050	5.38
XXII-G18-L2-E19	N	XXII polytype⋆	0.055	0.081	–	–	–	–	0.3217	0.0398	0.0236	7.18
XXII-G20-L1-E04	Y	match	0.101	0.110	0.185	20	0.167	20	0.0927	0.0118	0.0070	2.49
XXII-G21-L1-E03	Y	match	0.045	0.103	0.338	20	0.198	20	0.3197	0.0324	0.0066	0.48
XXII-G21-L1-E39	N	XXII polytype	0.047	0.099	–	–	–	–	0.1510	0.0248	0.0274	3.04
XXII-G23-L1-E52	N	XXII polytype	0.069	0.101	–	–	–	–	0.2564	0.0408	0.0345	-5.23
XXII-G23-L2-E13	N	XXII polytype	0.061	0.061	–	–	–	–	0.0607	0.0137	0.0199	-1.11
XXII-G25-L1-E03	Y	match	0.025	0.042	0.169	20	0.119	20	0.0835	0.0121	0.0015	3.10
XXII-G25-L1-E18	N	XXII polytype	0.069	0.071	–	–	–	–	0.2522	0.0368	0.0230	4.11
XXIIIA-G03-L1-E23	Y	match	0.180	0.187	0.354	20	0.258	20	0.1139	0.0124	0.0267	1.98
XXIIIA-G05-L1-E83	Y	match	0.177	0.194	0.689	20	0.299	20	0.1660	0.0147	0.0154	2.73
XXIIIA-G09-L2-E19	N	missed match	0.185	0.202	0.551	20	0.295	20	0.1877	0.0318	0.0297	8.68
XXIIIA-G14-L1-E26	Y	match	0.069	0.077	0.145	20	0.110	20	0.1299	0.0098	0.0020	-1.86
XXIIIA-G15-L1-E70	Y	match	0.231	0.287	0.653	20	0.347	20	0.1482	0.0280	0.0320	-2.25
XXIIIB-G03-L2-E75	Y	match	0.253	0.249	0.618	20	0.301	20	0.3825	0.0611	0.0209	4.44
XXIIIB-G05-L1-E20	Y	match	0.131	0.100	0.430	20	0.140	20	0.3733	0.0446	0.0070	2.35
XXIIIB-G06-L1-E26	N	duplicate match	0.162	0.155	0.442	20	0.183	20	0.4282	0.0550	0.0157	0.35
XXIIIB-G06-L1-E78	Y	match	0.147	0.123	0.434	20	0.148	20	0.4366	0.0552	0.0125	0.04
XXIIIB-G09-L1-E13	Y	match	0.143	0.123	0.495	20	0.163	20	0.2670	0.0344	0.0139	7.28
XXIIIB-G09-L1-E46	N	duplicate match	0.187	0.174	0.434	20	0.188	20	0.2229	0.0311	0.0174	7.44
XXIIIB-G13-L1-E88	Y	conformation	0.339	0.320	0.758	30	0.390	25	0.2783	0.0593	0.0546	9.19
XXIIIB-G14-L1-E02	Y	match	0.092	0.075	0.228	20	0.099	20	0.2814	0.0286	0.0048	-3.50
XXIIIB-G14-L1-E89	N	duplicate match	0.089	0.080	0.192	20	0.090	20	0.2629	0.0227	0.0039	-3.23
XXIIIB-G15-L1-E13	Y	match	0.179	0.164	0.603	20	0.210	20	0.4071	0.0532	0.0208	-1.23
XXIIIB-G15-L1-E21	N	duplicate match	0.216	0.225	0.455	20	0.248	20	0.3885	0.0411	0.0126	-1.67
XXIIIB-G18-L1-E01	Y	match	0.132	0.104	0.339	20	0.120	20	0.3980	0.0428	0.0095	-1.91
XXIIIB-G18-L1-E05	N	duplicate match	0.182	0.164	0.285	20	0.179	20	0.3609	0.0307	0.0075	-2.46
XXIIIB-G18-L2-E02	Y	match	0.132	0.102	0.339	20	0.117	20	0.4008	0.0430	0.0095	-2.03
XXIIIB-G23-L1-E11	Y	CPS-tolerance	0.223	0.237	0.388	35	0.255	40	0.3400	0.0506	0.0165	-7.53
XXIIIB-G23-L1-E14	N	CPS-tolerance	0.224	0.233	0.386	40	0.259	40	0.3364	0.0510	0.0180	-7.75
XXIIIB-G23-L1-E17	N	CPS-tolerance	0.229	0.240	0.398	30	0.265	30	0.3352	0.0513	0.0186	-7.74
XXIIIB-G23-L1-E26	N	CPS-tolerance	0.178	0.160	0.391	25	0.184	25	0.3320	0.0486	0.0081	-7.41
XXIIIB-G23-L1-E31	N	duplicate match	0.114	0.080	0.393	20	0.110	20	0.3175	0.0475	0.0052	-6.97
XXIIIB-G23-L1-E32	N	duplicate match	0.120	0.072	0.421	20	0.092	20	0.3196	0.0474	0.0054	-7.17
XXIIIB-G23-L1-E34	N	duplicate match	0.120	0.073	0.417	20	0.094	20	0.3195	0.0472	0.0054	-7.15
XXIIIB-G23-L1-E36	N	duplicate match	0.120	0.074	0.419	20	0.094	20	0.3182	0.0469	0.0055	-7.13
XXIIIB-G23-L1-E37	N	duplicate match	0.122	0.077	0.402	20	0.100	20	0.3211	0.0476	0.0053	-7.14
XXIIIB-G23-L1-E38	N	duplicate match	0.111	0.080	0.405	20	0.108	20	0.3154	0.0466	0.0048	-6.95
XXIIIB-G23-L1-E39	N	duplicate match	0.121	0.076	0.412	20	0.097	20	0.3206	0.0474	0.0055	-7.10

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Structure	BT6 Match	Category	RMSD(1)	VC-RMSD(1)	Raw-RMSD(20)	Tolerance	VC-RMSD(20)	Tolerance	Raw-POWDIFF	CPS-POWDIFF	VC-POWDIFF	ΔV
XXIIIB-G23-L1-E42	N	duplicate match	0.124	0.072	0.437	20	0.091	20	0.3160	0.0466	0.0056	-7.06
XXIIIB-G23-L1-E44	N	duplicate match	0.125	0.073	0.447	20	0.094	20	0.3163	0.0457	0.0059	-6.92
XXIIIB-G23-L1-E45	N	duplicate match	0.120	0.075	0.408	20	0.096	20	0.3204	0.0474	0.0054	-7.06
XXIIIB-G23-L1-E46	N	duplicate match	0.119	0.068	0.423	20	0.089	20	0.3245	0.0474	0.0055	-7.01
XXIIIB-G23-L1-E47	N	duplicate match	0.121	0.076	0.425	20	0.098	20	0.3167	0.0457	0.0051	-6.99
XXIIIB-G23-L1-E52	N	duplicate match	0.123	0.072	0.434	20	0.095	20	0.3228	0.0467	0.0057	-6.92
XXIIIB-G23-L1-E56	N	duplicate match	0.123	0.076	0.428	20	0.096	20	0.3188	0.0459	0.0053	-6.95
XXIIIB-G23-L1-E57	N	duplicate match	0.123	0.075	0.416	20	0.096	20	0.3214	0.0466	0.0052	-6.96
XXIIIB-G23-L1-E59	N	duplicate match	0.127	0.076	0.426	20	0.095	20	0.3227	0.0469	0.0055	-6.96
XXIIIB-G23-L1-E61	N	duplicate match	0.124	0.070	0.425	20	0.090	20	0.3278	0.0479	0.0056	-6.97
XXIIIB-G23-L2-E01	Y	match	0.124	0.083	0.390	20	0.104	20	0.3595	0.0480	0.0067	-5.62
XXIIIB-G23-L2-E02	N	duplicate match	0.104	0.059	0.349	20	0.078	20	0.3190	0.0465	0.0045	-6.31
XXIIIB-G23-L2-E03	N	duplicate match	0.102	0.056	0.368	20	0.076	20	0.3175	0.0452	0.0044	-6.32
XXIIIB-G23-L2-E04	N	duplicate match	0.094	0.062	0.330	20	0.090	20	0.3052	0.0439	0.0038	-6.28
XXIIIB-G23-L2-E05	N	duplicate match	0.119	0.075	0.413	20	0.104	20	0.3600	0.0471	0.0052	-5.64
XXIIIB-G23-L2-E06	N	duplicate match	0.111	0.062	0.395	20	0.088	20	0.3331	0.0445	0.0046	-5.94
XXIIIB-G23-L2-E07	N	duplicate match	0.128	0.081	0.411	20	0.105	20	0.3746	0.0485	0.0072	-5.42
XXIIIB-G23-L2-E08	N	duplicate match	0.115	0.103	0.334	20	0.132	20	0.3534	0.0485	0.0048	-6.28
XXIIIB-G23-L2-E15	N	CPS-tolerance	0.202	0.215	0.325	35	0.224	35	0.3362	0.0476	0.0097	-6.52
XXIIIB-G23-L2-E19	N	CPS-tolerance	0.198	0.206	0.319	30	0.217	35	0.3372	0.0444	0.0088	-6.23
XXIIIB-G25-L1-E02	Y	match	0.093	0.052	0.294	20	0.077	20	0.3392	0.0387	0.0034	-4.48
XXIIIB-G25-L1-E10	N	CPS-tolerance	0.202	0.202	0.292	35	0.204	35	0.3270	0.0330	0.0079	-4.21
XXIIIC-G14-L2-E06	Y	match	–	–	0.208	20	0.160	20	0.1678	0.0095	0.0050	-3.38
XXIIIC-G14-L2-E25	N	conformation	–	–	–	–	–	–	0.2305	0.0197	0.0357	-3.11
XXIIID-G03-L1-E75	Y	CPS-tolerance	0.225	0.223	0.375	25	0.288	25	0.2467	0.0213	0.0215	3.98
XXIIID-G06-L1-E73	Y	match	0.220	0.261	0.747	20	0.321	20	0.1650	0.0257	0.0196	0.95
XXIIID-G06-L1-E75	N	duplicate match	0.220	0.261	0.763	20	0.321	20	0.1650	0.0257	0.0196	0.95
XXIIID-G09-L1-E66	Y	match	0.239	0.211	0.603	20	0.269	20	0.1487	0.0339	0.0132	7.00
XXIIID-G14-L1-E11	Y	match	0.130	0.138	0.432	20	0.237	20	0.2413	0.0228	0.0058	-2.68
XXIIID-G18-L1-E85	Y	match	0.108	0.134	0.400	20	0.191	20	0.1997	0.0190	0.0046	-0.94
XXIIID-G18-L1-E99	N	duplicate match	0.120	0.146	0.349	20	0.175	20	0.0842	0.0115	0.0092	-0.02
XXIIID-G18-L2-E44	Y	match	0.108	0.133	0.398	20	0.184	20	0.2236	0.0205	0.0045	-1.36
XXIIID-G25-L1-E14	Y	match	0.113	0.118	0.399	20	0.190	20	0.3535	0.0319	0.0043	-3.62
XXIV-G14-L1-E02	Y	match	–	–	0.172	20	0.088	20	0.1492	0.0126	0.0071	-0.34
XXV-G05-L1-E01	Y	match	–	–	0.472	20	0.253	20	0.2640	0.0269	0.0177	0.68
XXV-G05-L1-E02	N	duplicate match	–	–	0.432	20	0.234	20	0.1875	0.0226	0.0159	0.86
XXV-G05-L1-E03	N	duplicate match	–	–	0.425	20	0.228	20	0.1821	0.0218	0.0155	0.89
XXV-G06-L1-E08	N	missed match	–	–	0.363	60	0.340	60	0.0892	0.0101	0.0213	-1.98
XXV-G14-L1-E06	Y	match	–	–	0.108	20	0.088	20	0.0866	0.0074	0.0032	-2.30
XXV-G15-L1-E01	Y	match	–	–	0.354	20	0.167	20	0.1697	0.0166	0.0080	0.18
XXV-G15-L1-E24	N	H-bond shift	–	–	0.949	35	0.566	35	0.3314	0.0563	0.0494	4.20
XXV-G18-L1-E01	Y	match	–	–	0.315	20	0.182	20	0.1507	0.0150	0.0102	-0.54
XXV-G18-L2-E01	Y	match	–	–	0.304	20	0.189	20	0.1491	0.0150	0.0113	-1.07
XXV-G21-L1-E02	Y	match	–	–	0.291	20	0.161	20	0.2013	0.0221	0.0089	-5.22
XXV-G23-L1-E02	Y	match	–	–	0.263	20	0.188	20	0.2258	0.0286	0.0107	-6.27
XXV-G25-L1-E01	Y	match	–	–	0.282	20	0.174	20	0.1492	0.0146	0.0080	-2.11
XXVI-G06-L1-E08	Y	match	0.185	0.168	0.376	20	0.205	20	0.1043	0.0135	0.0190	2.52
XXVI-G06-L1-E14	N	duplicate match	0.182	0.165	0.384	20	0.200	20	0.1043	0.0133	0.0175	2.49
XXVI-G06-L1-E16	N	duplicate match	0.182	0.165	0.375	20	0.200	20	0.1030	0.0132	0.0175	2.49
XXVI-G06-L2-E01	Y	match	0.096	0.085	0.266	20	0.121	20	0.1611	0.0138	0.0033	-4.03
XXVI-G06-L2-E02	N	duplicate match	0.059	0.082	0.250	20	0.127	20	0.1418	0.0126	0.0037	-3.96
XXVI-G06-L2-E03	N	duplicate match	0.071	0.078	0.262	20	0.132	20	0.1528	0.0115	0.0036	-4.01
XXVI-G06-L2-E04	N	duplicate match	0.048	0.090	0.234	20	0.146	20	0.1272	0.0097	0.0054	-4.04
XXVI-G06-L2-E05	N	duplicate match	0.138	0.136	0.376	20	0.177	20	0.1880	0.0195	0.0057	-3.76
XXVI-G14-L1-E01	Y	match	0.080	0.061	0.228	20	0.088	20	0.0845	0.0061	0.0015	-1.90
XXVI-G14-L1-E03	N	duplicate match	0.232	0.267	0.770	20	0.401	20	0.1409	0.0183	0.0208	-1.58
XXVI-G14-L1-E06	N	conformation	0.561	0.441	1.522	45	0.637	30	0.3037	0.0444	0.0473	-2.20
XXVI-G18-L1-E02	Y	match	0.125	0.139	0.302	20	0.194	20	0.0612	0.0047	0.0066	0.25
XXVI-G18-L2-E01	Y	match	0.125	0.141	0.309	20	0.199	20	0.0653	0.0049	0.0067	-0.04

⋆ This structure has a space group of Pc, while the other polytype structures are all $P2_1/c$, and can only be identified if the space-group option is deselected in the structure screening.