

## Supplementary information for the manuscript

### “Fast energy minimization of the CCDC drug-subset structures by molecule-in-cluster computations allows independent structure validation and model completion”

by

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Content:

- a. List of 53 Drug Subset<sup>1</sup> structures with atoms or molecules on special positions not considered in our GFN2-xTB<sup>2</sup> computations
- b. List of disordered structures where two separate conformers were optimized
- c. List of structures where optimization failed or was not performed due to missing atoms combined with structural complexity.
- d. List of 708 optimized structures. When `_m` is added to the refcode it means that the molecule were either not within the unit cell, or needed moving to bring cation and anion close together.
- e. List of 690 RMSD values for most of the optimized structures that serve as an additional cross validation and confirm that the optimized structure agrees with the experimental one. These were computed between the optimized and the original refcode coordinates, using the non-hydrogen atom coordinates only. The flagged entries were checked and corrected afterwards. This illustrates the power of combining quantum chemical optimization with experiment.
- f. Computer-generated list of 732 plots of ASU-in-cluster geometry optimizations, displaying energy versus individual optimization cycle, re-generating the cluster four times each time

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Table 1: List of 53 Drug Subset<sup>1</sup> structures with atoms or molecules on special positions not considered in our GFN2-xTB<sup>2</sup> computations

1. ACXMAC\_water\_on\_special\_position
2. AMALAC\_1\_molecule\_on\_special\_position
3. ASATOD\_mol\_on\_special\_position
4. AWUWIY01\_water\_on\_special\_position
5. BETXON\_water\_on\_special\_position
6. BINZIH\_cl\_on\_special\_position
7. BOKHAM02\_biphenyl\_on\_special\_position
8. BRPRBZ\_molecule\_on\_special\_position
9. CAASCO02\_Ca\_on\_special\_position
10. CATDAE\_mol\_on\_special\_position
11. CIGCIG\_molecule\_on\_special\_position
12. CYCLIZ10\_molecule\_on\_special\_position
13. CYPHEP\_water\_on\_special\_position
14. EPUDIE\_dioxane\_on\_special\_position
15. GIHWOJ\_mol\_on\_special\_position
16. GUCSEC\_solvent\_on\_special\_position
17. HIHF EK\_water\_on\_special\_position
18. JINGIW01\_chloride\_on\_special\_position
19. JOHFUJ\_mol\_on\_special\_position
20. JUBFER\_molecule\_on\_special\_position
21. JUKWAN\_molecule\_on\_special\_position
22. KADKIJ\_on\_special\_position
23. KANXIG\_h\_molecule\_on\_special\_position
24. KHD BEZ\_h\_K\_on\_special\_position
25. L CYSTI14\_molecule\_on\_special\_position
26. LIKVEI\_acn\_on\_special\_position
27. LOYCUZ\_solvent\_on\_special\_position
28. MAAZNB\_h-molecule\_on\_special\_position
29. MAVGAS\_counterion\_on\_special\_position
30. NEQVEL\_mol\_on\_special\_position
31. NOJKON\_cofomer\_on\_special\_position
32. OGEREY\_sulphate\_on\_special\_position
33. OGUTOB\_cofomer\_on\_special\_position
34. OJUQAN\_cofomer\_on\_special\_position
35. ORACUH\_solvent\_on\_special\_position
36. QIGCEO05\_molecule\_on\_special\_position
37. QUOLSO\_on\_special\_position
38. RIGTOS01\_molecule\_on\_special\_position
39. SALHIW\_chloride\_on\_special\_position
40. SIMJUU\_mol\_on\_special\_position
41. SIXZOO02\_molecule\_on\_special\_position
42. TIWXOM01\_molecule\_on\_special\_position
43. VIKLUX\_fumaric\_a\_on\_special\_position

44. WAXZEC\_cofomer\_on\_special\_position
45. WECGUI\_water\_on\_special\_position
46. XOGDEE\_solvent\_on\_special\_position
47. XOVBIU\_molecule\_on\_special\_position
48. YAWROF\_molecule\_on\_special\_position
49. YOWTAH01\_molecule\_on\_special\_position
50. YOYSUC\_molecule\_on\_special\_position
51. ZAZLER\_cofomer\_on\_special\_position
52. ZZZDRQ01\_molecule\_on\_special\_position
53. ZZZVZA05\_molecule\_on\_special\_position

Table 2: List of 24 disordered structures contained in the Drug Subset that were optimized using two conformers. These were thus present twice, denoted REFCODE\_1 and REFCODE\_2 in the following list of 732 optimized structures.

1. BEQGIN
2. BULCUG03
3. DIKWEA
4. DULKAX
5. FMDURD02
6. HAFNOR
7. IHOZOW
8. ILUSAL
9. JOWCAB02
10. KABZES
11. LCYSTN28
12. LERJID
13. MIFZIK
14. MUCDUK
15. NIQVIT
16. NUYSEG
17. PCLPMS
18. SEBPEU01
19. SIWCEG
20. SOYMID
21. TADZAZ03
22. VIGDAR
23. WETPOB
24. YIGPIO02

Table 3: List of structures where optimization failed or was not performed due to missing atoms, disorder, and/or combined with structural complexity.

1. ACXMAC
2. ADENTP<sup>3</sup>
3. AMASIS
4. BAGVUA
5. CEFMEN\_h
6. DAHREJ
7. FUFJUL<sup>4</sup>
8. IDIVOG<sup>5</sup>
9. JINGIW01
10. LUQREW
11. LUXYOU<sup>6</sup>
12. NAQLAU<sup>7</sup>
13. NUYSEG
14. NACGLY03\_h
15. OGIZEJ<sup>8</sup>
16. RUWHEX
17. SUCHOL12
18. SUDXAQ
19. TEZZUV\_h
20. TMTUBC\_h
21. TUCMEJ<sup>9</sup>
22. TUSHIZ<sup>10</sup>
23. YICMUS<sup>11</sup>
24. ZEFNOP

Table 4: List of 708 optimized structures. 732 structures are listed, because the 24 disordered structures appear twice, one for each optimized conformer.

1. ABABIQ\_r
2. ACEROR
3. ACHOLC
4. ACPRET03
5. ACSALA14
6. ACTDGU10\_h
7. ADENOS10
8. ADPOSM01\_h
9. ADRTAR
10. AHILOU
11. AIPBAR\_h
12. AKENOU
13. AKOFUD
14. AMAVEP
15. AMAVIT
16. AMAVOZ
17. AMBZCL
18. AMCAPR11
19. AMEQAK
20. AMEVET
21. AMMCHC11
22. AMOXCT10\_h
23. AMPCIH01
24. AMYTAL10\_h
25. ANIXAX
26. ANSTER10
27. ANTPYR
28. APUYOA02
29. ARFCYT10
30. ARFUAD
31. ARISOK\_h
32. ASPARM06
33. ASPART10
34. ATDZSA03
35. AXAKOA
36. BAFVOT
37. BAHDET
38. BASCUT\_h
39. BEDLUR
40. BEDMIG04
41. BENWUO
42. BEQGIN\_1
43. BEQGIN\_2
44. BEWKUJ15
45. BEZJIA

46. BIDFUQ  
47. BIHGUV  
48. BIHYEW10  
49. BIKHIN01  
50. BILJEN  
51. BIOTIN12  
52. BIRKES10  
53. BISMEV11  
54. BIXFOD\_h  
55. BIXGIY03\_h  
56. BIYSEH07  
57. BOCYAV  
58. BOLBOV  
59. BOMDUC  
60. BOVDUM  
61. BPYZDO21\_h  
62. BUBYII  
63. BUFPAV  
64. BUGJOC  
65. BUHCIQ\_h  
66. BULCUG03\_1  
67. BULCUG03\_2  
68. BZPENK01  
69. BZTRMS\_h  
70. CABCU06  
71. CAGWOW  
72. CAGWUC\_h  
73. CAGXUD  
74. CAKYOE  
75. CALDAU\_h  
76. CANDOM10\_h  
77. CANDUR  
78. CANFED  
79. CARPEQ\_h  
80. CATBOP  
81. CAVVUQ02  
82. CEKBEZ  
83. CELCIF  
84. CEPGLY\_h  
85. CEPHHM10\_h  
86. CETHNA\_h  
87. CEYHUJ01\_h  
88. CFHPRG  
89. CHEBAR01  
90. CIDDEZ  
91. CIHHIK01  
92. CIMETD02  
93. CINSEZ



94. CIPWUT\_h  
95. CIRTIG01\_h  
96. CISKUL  
97. CITREC01  
98. CITYIN10  
99. CIVFOC10  
100. CIYRIL\_h  
101. CLAMBU  
102. CLDZPA01  
103. CLEMAS02  
104. CLMPCL02  
105. CLONDC11  
106. CLPNXA  
107. COCHCL01  
108. COQWOU02  
109. CORYIR10\_h  
110. COTYEP  
111. COTYOA02  
112. COTYOA  
113. COVPIN03  
114. COXYOE  
115. COYSAK  
116. CPHNZP  
117. CPPBGC  
118. CPTAZP\_h  
119. CPTZAP\_h  
120. CREATH01  
121. CUBHUE  
122. CUYCEF01  
123. CUYDOQ\_w\_h  
124. CXMCYT  
125. CYPROT10  
126. DABJAR  
127. DACMOR01  
128. DAPSUO05  
129. DAQCII  
130. DARGOT03  
131. DAUNMY\_h  
132. DAXYUX01\_h  
133. DBEZPO01\_h  
134. DEFZEU  
135. DEMXUO  
136. DEQYIH  
137. DESNAR  
138. DEWHOC  
139. DEXMET11  
140. DEXPOX\_h  
141. DFIMZP01

142. DIAZOX  
143. DIGOXN10  
144. DIJWOJ  
145. DIKWEA\_1  
146. DIKWEA\_2  
147. DINXIJ  
148. DIRCIS  
149. DIVHOF02\_h  
150. DIWQIJ  
151. DIYYOB  
152. DIZPAM11  
153. DIZWAK\_h  
154. DLPROM02  
155. DLSERN31  
156. DMANTL07  
157. DMTYRS\_h  
158. DOLJIX\_h  
159. DOQBUI  
160. DPHPZL  
161. DPYALC  
162. DUDGAL  
163. DUJFAQ  
164. DUJPOO  
165. DUKTOS\_h  
166. DULKAX\_1  
167. DULKAX\_2  
168. DUNGAV  
169. DUNXAL\_h  
170. DUTRUF10  
171. DUVZOJ02\_h  
172. DXMTAS  
173. EDALEC\_m  
174. EFAXAM  
175. EFEHOO  
176. EFEMUX01  
177. EGINEP  
178. EHOXEE\_h  
179. EJEQAL  
180. ELIZAC  
181. ELOVAE01  
182. ELOVOS  
183. EMIQEY  
184. ENEBOQ  
185. EPHPMO  
186. EQONOP  
187. ESOURCE11  
188. ESTRIO  
189. ESTRON14

190. ETBBAR02  
191. ETCYPY01  
192. ETEXIK02  
193. ETHACN\_h  
194. ETHDPH05  
195. ETHUSS03  
196. ETPRGN\_h  
197. EVAFUD  
198. EXAQEA  
199. EXAQIE  
200. EXAQOK  
201. FABVAF01  
202. FAHFVAV01  
203. FAHMAC  
204. FAJKUW  
205. FAJMAE  
206. FANNEN\_h  
207. FARRUM02  
208. FAXYAG  
209. FDOURD01  
210. FEBHUP02  
211. FEFNEK  
212. FEMBII  
213. FETGAN  
214. FHMANE  
215. FIDYIA01  
216. FIFDON\_h  
217. FIKFIP  
218. FILGEM03\_h  
219. FIMNIY  
220. FIMTAW  
221. FINWEE\_h  
222. FISLIE  
223. FITPIH02  
224. FIXGAU01  
225. FIXNUV  
226. FIZWAM\_h  
227. FMDURD02\_1  
228. FMDURD02\_2  
229. FOGVIG02  
230. FOHLIY01  
231. FOLCAH03  
232. FOPYUE\_h  
233. FOQREK  
234. FORGAU01  
235. FOSPEA  
236. FOYMAH  
237. FPRTOD10

238. FUFTIK  
239. FUGSEF  
240. FUHGOE  
241. FUMKEF  
242. FUPDOJ  
243. FUPFAX\_h  
244. FUQMOU01  
245. FUWNIU  
246. FUXMOA01  
247. GABFOE\_h  
248. GAHHOM01  
249. GAKWIY\_h  
250. GALDEC01  
251. GAMFAC  
252. GAQTAU01  
253. GARFEK  
254. GEGJAD  
255. GEHXEX  
256. GERXAE  
257. GICHEG  
258. GICVUJ01\_h  
259. GIDLUB  
260. GILHAL  
261. GIMYEG  
262. GIXXOB  
263. GLCROL01  
264. GLUCIT  
265. GLUTAM02  
266. GLUTAS05  
267. GLYCIN99  
268. GODTIC  
269. GOHSUS  
270. GOLWIN  
271. GOPDUK01  
272. GORKUV01  
273. GRISFL02  
274. GUBLAS  
275. GUNKEH  
276. GUYGOX03\_h  
277. HAFNOR\_1  
278. HAFNOR\_2  
279. HAKJIM  
280. HANEDP10  
281. HAXHET\_h  
282. HCCYHG\_h  
283. HEPHCL10  
284. HERGOM\_h  
285. HEYGEX

286. HIJFAH  
287. HISHEX  
288. HISTPA15  
289. HMXBZP  
290. HOQHUQ  
291. HOTTER  
292. HUCHEU02  
293. HUHZEP  
294. HXVITD  
295. HYDLAZ01  
296. IBUNOJ  
297. ICRFRB10  
298. IDOXUR01  
299. IFOSAY  
300. IGAZUM\_h  
301. IHOZOW\_1  
302. IHOZOW\_2  
303. IHUHAW\_h  
304. IKACUT  
305. ILUSAL\_1  
306. ILUSAL\_2  
307. IMEHOY  
308. INAHZC\_h  
309. INOMUV  
310. IPILUQ  
311. IPMEPL  
312. IPRAMI\_h  
313. IQILAW  
314. IQISAE  
315. IQUMAI  
316. IVEGIA\_h  
317. IVUQIZ05  
318. IWOCON  
319. JAKGEH  
320. JAMRIY  
321. JAVCIS10  
322. JAZCET  
323. JEBNUZ\_h  
324. JIWPEL01  
325. JIWQAI03  
326. JODZUX  
327. JOHKUM  
328. JOPSUE  
329. JORJUX  
330. JOSWAP01\_h  
331. JOWCAB02\_1  
332. JOWCAB02\_2  
333. JUPDAB

334. JUYLEW  
335. JUYZOS  
336. KABGUR  
337. KABZES\_1  
338. KABZES\_2  
339. KAGCIE  
340. KASMOH  
341. KAXSEJ  
342. KCANRO  
343. KEBGAB01  
344. KEBVES\_h  
345. KEHBAA  
346. KEMZIL01  
347. KEYSOW  
348. KIDRAR01  
349. KIDWAW  
350. KIJMEX  
351. KIKWUW  
352. KIMDER  
353. KIPLEC  
354. KIWQUC  
355. KNMYSL  
356. KOFNIC  
357. KORSAL02\_h  
358. KORYUL  
359. KUGWIS\_h  
360. KUQDAC01\_h  
361. KURJAK  
362. KUTJIU  
363. LADTIT  
364. LAKZII  
365. LALNIN03  
366. LANLET  
367. LAQBAI  
368. LAQSON01  
369. LARGPH06  
370. LATPIH  
371. LATQAA  
372. LATSOQ01\_h  
373. LAYCET01  
374. LCYSTN28\_1  
375. LCYSTN28\_2  
376. LDOPAS03  
377. LEBLUB  
378. LERJID\_1  
379. LERJID\_2  
380. LESVEM  
381. LEXQIQ

382. LEZREO\_h  
383. LINTUX\_h  
384. LOPZEX  
385. LORCAW\_h  
386. LOSLEL  
387. LOWKOX\_h  
388. LTXPSE\_h  
389. LUDDUJ  
390. MACKUX  
391. MACXPR10  
392. MAFLAI\_h  
393. MCPRPL01  
394. MELATN01  
395. MELFIT09  
396. MEQCOB  
397. METHCL01  
398. MEXSEP  
399. MEYGII  
400. MHOCUM01  
401. MIFPOI  
402. MIFZIK\_1  
403. MIFZIK\_2  
404. MIGQID  
405. MIHZUA  
406. MIMOSN\_h  
407. MIRACD\_h  
408. MNIMET02  
409. MOKXIU  
410. MOKXOA  
411. MOPHAC  
412. MORPHM01  
413. MOSXUO  
414. MOVLOZ  
415. MOVYAY01\_h  
416. MOXAZO\_h  
417. MPIXPS\_h  
418. MPZPAM  
419. MTEPAM  
420. MTHPRG  
421. MUBPAB  
422. MUCDUK\_1  
423. MUCDUK\_2  
424. MUGKAA01  
425. MUYVAE\_h  
426. MVERIQ01  
427. NADREN  
428. NAJPOE  
429. NAKGOY

430. NALCYS10  
431. NAMDPC01\_m  
432. NANNUN  
433. NAPHZL10\_h  
434. NARBOY  
435. NAZLAC02  
436. NDNHCL01  
437. NEPHCL  
438. NEQGUM  
439. NEQHEY  
440. NESKED  
441. NETIND01  
442. NEVMOR  
443. NHPBZO\_h  
444. NICOAM05  
445. NIHMOH01  
446. NIKROP  
447. NILXOV\_m  
448. NIQVIT\_1  
449. NIQVIT\_2  
450. NIRRAH\_h  
451. NIVBIO\_h  
452. NOBDUF  
453. NOKGAX  
454. NORGES01  
455. NORMET\_h  
456. NUJDAX\_w  
457. NUPQEW  
458. NUYHUK  
459. NUYSEG\_1  
460. NUYSEG\_2  
461. OBEQAN01  
462. OCAHAC  
463. OFAZUQ  
464. OFEJOA  
465. OFILEW  
466. OGIXIN  
467. OMAKOE01  
468. OPOGAD  
469. OPOQER  
470. ORNHCL12  
471. OROZAX  
472. OXYTET01\_h  
473. PABHIJ01  
474. PAJNUJ  
475. PANCUR  
476. PBUMSL\_h  
477. PBUMSL



478. PCLPMS\_1  
479. PCLPMS\_2  
480. PEBGUC02  
481. PEDWOM  
482. PEKFAN  
483. PERPAZ  
484. PETHID\_h  
485. PEXKOS01  
486. PEYGOQ  
487. PGDEDO  
488. PHEPHR  
489. PICVUU01  
490. PIGSOO  
491. PILOCP01  
492. PIMKOL  
493. PIMOZD  
494. PINDON  
495. PIPAMP  
496. PIPCIL\_h  
497. PIRENA10\_w  
498. PIWLEM02  
499. PMEPEN01  
500. POBKOG  
501. POFORM\_m  
502. POGKOM  
503. PRAZAM\_h  
504. PRGDOL02  
505. PROCPH  
506. PROGLE20\_h  
507. PROGST12  
508. PUFGUU  
509. PUQGUF  
510. PUVMAU  
511. PUVRIH  
512. PYRXCL01  
513. PYRZIN23  
514. QABCII  
515. QABTOD01  
516. QATNEF01  
517. QECHOV03  
518. QEMLIE  
519. QETZUL  
520. QICMEU\_h  
521. QIFKEX01  
522. QIJPAC  
523. QIJZOY  
524. QIQKEI  
525. QIQLIL

526. QOMKUA  
527. QQQAEJ02  
528. QQQAUG04  
529. QQQBSS01\_h  
530. QUBQIO01  
531. QURWOQ02  
532. QUZWOY  
533. RALMIA  
534. RALMOG01  
535. RASTAG\_m  
536. RAVPUB  
537. RBFLAV10\_h  
538. REBCIL  
539. REDNIX  
540. REZBII  
541. RIGDES  
542. RILQOU  
543. RINTIT  
544. RIQFOO  
545. RIWKOX  
546. ROKNUB  
547. ROQLOA  
548. RSERPNO1  
549. RUKBOP  
550. RUKQOF  
551. RUTGOE  
552. RUTGUK  
553. RUWBAM  
554. RUYZAO  
555. SAFNIW  
556. SAHSOJ\_h  
557. SAJFIT  
558. SAJNOG\_h  
559. SAQYIR  
560. SATHOL  
561. SAWFIF\_h  
562. SAXFED  
563. SAXQIT  
564. SAZLAG  
565. SAZNOW\_m  
566. SEBPEU01\_1  
567. SEBPEU01\_2  
568. SEBPEU01  
569. SENJIF  
570. SEQKAA02  
571. SEQNIL  
572. SESKUY01  
573. SETSOA

574. SFDMOX05\_h  
575. SIFGOD  
576. SIJWUF  
577. SIKLIH07  
578. SIWCEG\_1  
579. SIWCEG\_2  
580. SLFNMB02  
581. SLFNMC20\_h  
582. SLFNMG01  
583. SLFSXZ12  
584. SOBBUG\_h  
585. SONKEM  
586. SOPSEV  
587. SOYMID\_1  
588. SOYMID\_2  
589. SUJXUR  
590. SUTHAZ37  
591. SUTWIO  
592. SUVGUL  
593. SUWNUT  
594. TADLIU02  
595. TADZAZ03\_1  
596. TADZAZ03\_2  
597. TAJFOZ\_h  
598. TANDET  
599. TAYFUV\_h  
600. TAZZUP  
601. TEPSAM\_h  
602. TESTON10  
603. TETCYH12  
604. TEZZEE  
605. TFPROM10  
606. THCLCS\_h  
607. THGUAN10  
608. TIJMII  
609. TIPWAQ\_h  
610. TITHYN10\_h  
611. TIYQAU01  
612. TMPHCL01  
613. TOKSES\_h  
614. TOPXED\_m  
615. TOXXIN\_h  
616. TOYJOG  
617. TOYSUX  
618. TRHTRT\_h  
619. TUBOBM\_h  
620. TULRIB\_m  
621. TUQGET

622. TUTDOD  
623. TUZCOI  
624. UCUVET  
625. UGIYEP  
626. UHUQUK  
627. UKAKIA  
628. UKIFIE\_h  
629. UMOMAL  
630. UPUKOH  
631. UQAPEJ  
632. URAVUG  
633. UREA0H12  
634. USOCOV  
635. UXIXUV  
636. VAMBOA01  
637. VAWPIT  
638. VAWQEQ  
639. VAYJOW  
640. VAYXOI  
641. VEMRAI  
642. VEVQAQ  
643. VICXOV  
644. VIDJEX01  
645. VIFQIL  
646. VIGDAR\_1  
647. VIGDAR\_2  
648. VOGCAV\_h  
649. VOXDUH  
650. VUCDUS  
651. VUCJEI  
652. VUJRUO\_h  
653. VUXPUZ  
654. WACHIR\_h  
655. WADPIC  
656. WADTIG  
657. WAHJAR  
658. WAJYUC  
659. WALPIJ  
660. WASGAA\_h  
661. WAWVOH  
662. WEHYEO  
663. WELGAV  
664. WEMGEC  
665. WEQHEF01\_h  
666. WERVEU02  
667. WETLOY  
668. WETPOB\_1  
669. WETPOB\_2

670. WEXQAS01  
671. WEZCOT  
672. WIBZEM  
673. WINJAE\_m  
674. WINWUL02  
675. WIPYOL  
676. WOQDAH  
677. WOYPAB  
678. WURPUU  
679. WUTHEA01  
680. XANTOX\_h  
681. XAPTAK01  
682. XAQNOU  
683. XATJAF  
684. XAVTOF02  
685. XAYGEJ01  
686. XAZRUN  
687. XEJKUS  
688. XEZTON01  
689. XICRUY  
690. XIJKIK01  
691. XIRHOX  
692. XOCXUI01  
693. XOGMOX  
694. XOJNOB  
695. XOSGUH  
696. XOZRUZ  
697. XULRUT  
698. YACGUE\_h  
699. YACHAL\_h  
700. YACTEC01  
701. YALWIS  
702. YALYUH  
703. YAPZEU  
704. YARXEW  
705. YIGPIO02\_1  
706. YIGPIO02\_2  
707. YIGRAI  
708. YIKNUD  
709. YIYRAZ  
710. YODXAR  
711. YOKQAQ  
712. YUKVAD  
713. YURSUB\_h  
714. ZAPLEJ  
715. ZAPXOF  
716. ZEMJOQ  
717. ZENREP

718.	ZIDLED
719.	ZIKJOS
720.	ZIMBOO
721.	ZIVKEU
722.	ZIZRUX01
723.	ZOGSOD
724.	ZOXSEK
725.	ZUHFIR
726.	ZUQMIJ_h
727.	ZZZECG01
728.	ZZZPNG01
729.	ZZZPUS19
730.	ZZZRCG01_h
731.	ZZZSHG01
732.	ZZZTSE03

refcode	rmsd		Tanimoto_rmsd
ABABIQ_ro		0.10962	0.99925
ACERORo		0.05292	0.99956
ACHOLCo		0.14007	0.99662
ACPRET03o		0.06479	0.99975
ACSALA14o		0.03692	0.99975
ACTDGU10_ho		0.19352	0.99882
ADENOS10o		0.04381	0.9998
ADPOSM01_ho		1.29284	0.86729
ADRTARo		0.09257	0.99897
AHILOUo		0.16949	0.99922
AIPBAR_ho		0.08951	0.99859
AKENOUo		0.18442	0.9992
AKOFUDo		0.08304	0.99952
AMAVEPo		0.07934	0.99939
AMAVITo		0.06364	0.99952
AMAVOZo		0.07694	0.99961
AMBZCLo		0.06669	0.99966
AMCAPR11o		0.12386	0.99818
AMEQAKo		0.04025	0.9999
AMEVETo		0.08915	0.99963
AMMCHC11o		0.11217	0.99804
AMOXCT10_ho		0.11275	0.99918
AMPCIH01o		0.0806	0.99957
AMYTAL10_ho		0.04831	0.99968
ANIXAXo		0.05647	0.99966
ANSTER10o		0.04046	0.99986
ANTPYRo		0.05262	0.99958
APUYOAO2o		0.09924	0.99951
ARFCYT10o		0.05835	0.99958
ARFUADo		0.07592	0.99936
ASPARM06o		0.05009	0.99932
ASPART10o	Initially two hydrogen atoms missing, corrected		n/a
ATDZSA03o		0.07522	0.99932
AXAKOAO		0.1522	0.99817
BAFVOTo		0.03027	0.99984
BAHDETo		0.141	0.99835
BASCUT_ho		0.12558	0.99771
BEDLURo		0.07748	0.99973
BEDMIG04o		0.22336	0.99477
BENWUOo		0.04949	0.99977
BEQGIN_1o		0.12694	0.999
BEQGIN_2o		0.35614	0.99218
BEWKUJ15o		0.06383	0.99954
BEZJIAo		0.06415	0.99969
BIDFUQo		0.07285	0.99984
BIHGUVo		0.16461	0.99736
BIHYEW10o		0.06408	0.99946
BIKHIN01o		0.02317	0.99985
BILJENo		0.1137	0.99888

BIOTIN12o	0.06949	0.9996
BIRKES10o	0.16381	0.9985
BISMEV11o	0.04256	0.99959
BIXFOD_ho	0.13603	0.99784
BIXGIY03_ho	0.04319	0.99981
BIYSEH07o	0.08263	0.9995
BOCYAVo	0.08305	0.99951
BOLBOVo	0.09515	0.99982
BOMDUCo	0.077	0.99955
BOVDUMo	0.29245	0.99613
BPYZDO21_ho	0.12853	0.9985
BUBYIlo	0.05154	0.99965
BUFPAVo	0.10324	0.99892
BUGJOCo	0.04629	0.99985
BUHCIQ_ho	0.08469	0.99936
BULCUG03_1o	0.02467	0.99977
BULCUG03_2o	0.02469	0.99977
BULCUG03_3o	0.02482	0.99977
BULCUG03_4o	0.02461	0.99977
BULCUG03_5o	0.02368	0.99979
BULCUG03_6o	0.02401	0.99979
BULCUG03_7o	0.02402	0.99979
BULCUG03_8o	0.02402	0.99979
BZTRMS_ho	0.10244	0.99912
CABCUD06o	0.08292	0.99955
CAGWOWo	0.07614	0.99937
CAGWUC_ho	1.78426	0.73287
CAGXUDo	0.0887	0.99931
CAKYOEo	0.04337	0.99982
CALDAU_ho	0.11941	0.99946
CANDOM10_ho	0.11674	0.99914
CANDURo	0.07844	0.99919
CANFEDo	0.07756	0.99938
CARPEQ_ho	0.43989	0.99003
CATBOPo	0.07741	0.9994
CAVVUQ02o	0.57497	0.96508
CEKBEZo	0.0827	0.99958
CELCIFo	0.10233	0.99961
CEPGLY_ho	0.25241	0.99651
CEPHHM10_ho	0.11777	0.9993

Considerable changes in optimized structure. Input structure without H. Ion shifted considerably. OK

CETHNA_ho		n/a
CFHPRGo	0.13751	0.99874
CHEBAR01o	0.06957	0.99936
CIDDEZo	0.07596	0.99908
CIHHIK01o	0.13656	0.99844
CIMETD02o	0.12948	0.9985
CINSEZo	0.103	0.99948
CIPWUT_ho	0.10846	0.99881
CIRTIG01_ho	0.27882	0.99536



CISKULo		0.22902	0.99825
CITYIN10o		0.10905	0.99888
CIVFOC10o		0.05992	0.99944
CIYRIL_ho		0.04875	0.9998
CLAMBUo		0.15218	0.99837
CLDZPA01o		0.10356	0.99883
CLEMAS02o		0.14308	0.99845
CLMPCL02o		0.08617	0.9993
CLONDC11o		0.12006	0.99792
CLPNXAo		0.03572	0.99994
COCHCL01o		0.06109	0.99969
COQWOU02o		0.09949	0.99934
CORYIR10_ho		0.09474	0.99895
COTYEPo		0.0406	0.99978
COTYOA02o		0.11046	0.99806
COTYOAo		0.13901	0.99807
COVPIN03o		0.09276	0.99938
COXYOEo		0.12382	0.99864
COYSAKo		0.05711	0.99969
CPHNZPo		0.09412	0.99913
CPPBGCo		0.22256	0.99566
CPTAZP_ho		1.38006	0.92718
CPTZAP_ho		0.08739	0.99924
CREATH01o		0.08448	0.99819
CUBHUEo		0.06637	0.99934
CUYCEF01o		0.08657	0.99948
CUYDOQ_w_ho		0.04818	0.9997
CXMCYTo		0.0866	0.99912
CYPROT10o		0.04715	0.99985
DABJARo		0.07619	0.99959
DACMOR01o		0.26037	0.99386
DAPSUO05o		0.05112	0.99973
DAQCIIo		0.069	0.99971
DARGOT03o		0.08415	0.99971
DAUNMY_ho		0.14928	0.99895
DAXYUX01_ho		0.16565	0.99835
DBEZPO01_ho		0.06578	0.99968
DEFZEUo		0.08982	0.99946
DEMXUOo		0.08621	0.99882
DEQYIHo		0.04534	0.9998
DESNARo	0.131, OK		
DEWHOCo		0.04765	0.99976
DEXMET11o		0.07047	0.99964
DEXPOX_ho		0.15367	0.99794
DFIMZP01o		0.07801	0.99939
DIAZOXo		0.03537	0.99981
DIGOXN10o		0.12445	0.99977
DIJWOJo		0.12776	0.99942
DINXIJo		0.21488	0.99885
DIRCISo		0.12426	0.99935

DIVHOF02_ho	0.61576	0.97992
DIWQIJJo	0.11525	0.99955
DIYYOBo	0.0617	0.99953
DIZPAM11o	0.0451	0.99979
DIZWAK_ho	0.06928	0.99973
DLPROM02o	0.04439	0.9994
DLSERN31o	0.08911	0.99712
DMANTL07o	0.0237	0.99991
DMTYRS_ho	0.04613	0.99969
DOLJIX_ho	0.34664	0.98908
DOQBUIo	0.0951	0.9995
DPHPZLo	0.1102	0.99879
DPYALCo	0.17146	0.99758
DUDGALo	0.05584	0.9997
DUJFAQo	0.15444	0.99903
DUKTOS_ho	1.61333	0.81462
DULKAX_1o	0.11129	0.99945
DULKAX_2o	0.26958	0.99677
DUNGAVo	0.08791	0.99926
DUNXAL_ho	0.15772	0.99927
DUTRUF10o	0.11135	0.99943
DUVZOJ02_ho	0.11271	0.99845
DXMTASo	0.09835	0.99931
EDALEC_mo	P-XRD structure with considerable differences to optimized one, OK n/a	
EFAXAMo	0.13809	0.99973
EFEHOOo	0.07661	0.99979
EFEMUX01o	0.04681	0.99973
EGINEPo	0.09409	0.99945
EHOXEE_ho	0.13647	0.99865
EJEQALo	0.10494	0.99933
ELIZACo	0.10226	0.99918
ELOVAE01o	0.02879	0.99989
ELOVOSo	0.05711	0.99986
EMIQEYo	0.2706	0.99666
ENEBOQo	0.15034	0.9975
EPHPMOo	0.06313	0.99935
EQONOPo	0.23767	0.99532
ESOURE11o	0.02618	0.99994
ESTRIOo	0.05159	0.99978
ESTRON14o	0.05059	0.99977
ETBBAR02o	0.07399	0.99919
ETCYPY01o	0.04293	0.99968
ETEXIK02o	0.08854	0.99925
ETHACN_ho	0.73812	0.96026
ETHDPH05o	0.12333	0.99665
ETHUSS03o	0.06435	0.99965
ETPRGN_ho	0.56779	0.97142
EVAFUDo	0.04249	0.99983
EXAQEAo	0.10733	0.99908
EXAQIEo	0.05257	0.99972

EXAQOKo		0.04498	0.9998
FABVAF01o		0.15763	0.99829
FAHFVAV01o		0.10849	0.9992
FAHMACo		0.10082	0.99926
FAJKUWo		0.16041	0.99864
FAJMAEo		0.13122	0.99893
FANNEN_ho	0.0853, OK		n/a
FARRUM02o		0.05746	0.99985
FAXYAGo		0.19805	0.99821
FDOURD01o		0.06256	0.99956
FEBHUP02o		0.047	0.99988
FEFNEKo		0.0782	0.99954
FEMBIIo		0.11881	0.9994
FETGANo		0.07326	0.99981
FHMANEo		0.05817	0.99969
FIFDON_ho		0.06325	0.99976
FIKFIPo		0.06422	0.99955
FILGEM03_ho		0.05022	0.99972
FIMNIYo		0.16089	0.99756
FIMTAWo		0.10236	0.99905
FINWEE_ho		0.18695	0.99874
FISLIEo		0.21804	0.99415
FITPIH02o		0.02886	0.99984
FIXGAU01o		0.07751	0.99942
FIXNUVo		0.30538	0.99066
FIZWAM_ho		2.1554	0.81824
FMDURD02_1o		0.09604	0.99903
FMDURD02_2o		0.46354	0.97838
FOGVIG02o		0.0862	0.99924
FOHLIY01o		0.05938	0.9995
FOLCAH03o		0.16186	0.99918
FOPYUE_ho		0.14679	0.99949
FOQREKo		0.03568	0.99985
FORGAU01o		0.08504	0.99952
FOSPEAo		0.09092	0.99767
FOYMAHo		0.0536	0.99928
FPRTOD10o		0.07823	0.99955
FUFTIKo		0.08343	0.99892
FUGSEFo		0.09305	0.99927
FUHGOEo		0.07015	0.99957
FUMKEFo		0.07401	0.99953
FUPDOJo		0.08922	0.99958
FUQMOU01o		0.24981	0.99438
FUWNIUo		0.10236	0.9988
FUXMOA01o		0.04601	0.99983
GABFOE_ho		0.30211	0.9963
GAKWIY_ho		0.12795	0.99926
GALDEC01o		0.02062	0.99989
GAMFACo		0.09087	0.99907
GAQTAU01o		0.02325	0.99993

GARFEKo	0.13618	0.99857
GEHXEXo	0.03755	0.99986
GERXAEo	0.19917	0.99801
GICHEGo	0.34667	0.99164
GICVUJ01_ho	0.07365	0.99977
GIDLUBo	0.02568	0.99987
GILHALo	0.0747	0.99979
GIMYEGo	0.10895	0.99963
GIXXOBo	0.06733	0.99986
GLCROL01o	0.01897	0.99988
GLUCITo	0.24703	0.99105
GLUTAM02o	0.15289	0.99577
GLUTAS05o	0.18215	0.99777
GLYCIN99o	0.14877	0.98915
GODTICo	0.0445	0.99982
GOHSUSo	0.0917	0.99934
GOLWINo	0.0422	0.99989
GOPDUK01o	0.16992	0.99851
GORKUV01o	0.58293	0.9524
GRISFL02o	0.07489	0.9995
GUBLASo	0.15622	0.99878
GUNKEHo	0.06835	0.99976
GUYGOX03_ho	0.2156	0.99652
HAFNOR_1o	0.30616	0.99625
HAFNOR_2o	0.36496	0.99469
HAKJIM_ho	H was initially missing. Corrected.	n/a
HANEDP10o	0.08547	0.99937
HAXHET_ho	0.11878	0.99948
HCCYHG_ho	0.11827	0.99735
HEPHCL10o	0.03082	0.99988
HERGOM_ho	0.12258	0.99945
HEYGEXo	0.03909	0.99978
HIJFAHo	0.1539	0.99919
HISHEXo	0.06325	0.99958
HISTPA15o	0.04951	0.99962
HMXBZPo	0.04678	0.99979
HOQHUQo	0.01123	0.99994
HOTTERo	0.08056	0.99939
HUCHEU02o	0.12968	0.99947
HUHZEPo	0.06862	0.9995
HXVITDo	0.04126	0.99994
HYDLAZ01o	0.0484	0.99955
IBUNOJo	0.05303	0.9997
ICRFRB10o	0.04168	0.99987
IDOXUR01o	0.05415	0.99967
IFOSAYo	0.06216	0.99957
IHOZOW_1o	0.21223	0.99743
IHOZOW_2o	0.32726	0.99394
IHUHAW_ho	0.26596	0.99691
IKACUTo	0.02813	0.99984

ILUSAL_1o		0.07959	0.99962
IMEHOYo		0.08374	0.99922
INAHZC_ho		0.07816	0.99878
INOMUVo		0.06678	0.99967
IPILUQo		0.07306	0.99963
IPMEPLo		0.01962	0.99993
IPRAMI_ho		0.13013	0.99856
IQILAWo		0.07373	0.99981
IQISAEo		0.18946	0.99777
IQUMAIo		0.11398	0.99908
IVUQIZ05o		0.06183	0.99964
IWOCONo		0.06021	0.99976
JAKGEHo		0.06924	0.9996
JAMRIYo		0.06701	0.99886
JAZCETo		0.35546	0.99744
JEBNUZ_ho		0.23532	0.9968
JIWPEL01o		0.11087	0.99912
JIWQAI03o		0.07602	0.99961
JODZUXo		0.39612	0.99392
JOHKUMo		0.13805	0.99907
JOPSUEo		0.05955	0.99956
JORJUXo		0.08261	0.99942
JOSWAP01_ho		0.11319	0.99913
JOWCAB02_1o		0.10776	0.9996
JOWCAB02_2o		0.25153	0.99784
JUPDABo		0.06133	0.99934
JUYLEWo		0.03238	0.99987
JUYZOSo		0.07788	0.99952
KABGURo		0.0979	0.99901
KABZES_1o		0.23063	0.9959
KABZES_2o		0.23489	0.99574
KAGCIEo		0.14225	0.99896
KASMOHo		0.0831	0.9992
KAXSEJo		0.03113	0.9999
KEBGAB01o		0.08246	0.99864
KEBVES_ho		0.63653	0.98137
KEHBAAo		0.15385	0.99903
KEMZIL01o		0.00245	0.99998
KEYSOWo		0.20762	0.99651
KIDRAR01o		0.07301	0.99964
KIDWAWo		0.14639	0.99876
KIJMEXo		0.08174	0.99949
KIKWUWo		0.13292	0.99887
KIMDERo		0.11794	0.99939
KIPLECo		0.11329	0.99933
KIWQUCo	0.162, OK		n/a
KNMYSLo		0.13311	0.99912
KOFNICo		0.09246	0.99903
KORSAL02_ho		0.06568	0.9981
KORYULo		0.04068	0.99984

KUGWIS_ho	0.08963	0.99925
KUQDAC01_ho	0.1885	0.99785
KURJAKo	0.10878	0.9978
KUTJIUo	0.08488	0.99933
LADTITo	0.03506	0.99984
LAKZIIo	0.18684	0.99841
LALNIN03o	0.10104	0.99573
LANLETo	0.06283	0.99966
LAQBAlO	0.04132	0.99984
LAQSON01o	0.13359	0.99921
LARGPH06o	0.12111	0.99816
LATPIHo	0.11703	0.99898
LATQA Ao	0.10556	0.99925
LAYCET01o	0.05042	0.99974
LCYSTN28_1o	0.11336	0.9957
LCYSTN28_2o	0.03481	0.99959
LDOPAS03o	0.04774	0.99975
LESVEMo	0.07517	0.99978
LEXQIQo	0.0951	0.99949
LINTUX_ho	0.03153	0.99988
LOPZEXo	0.25765	0.9973
LORCAW_ho	0.06848	0.99958
LTXPSE_ho	0.10068	0.99883
LUDDUJo	0.17077	0.99745
MACKUXo	0.09777	0.99951
MACXPR10o	0.06703	0.99969
MCPRPL01o	0.06725	0.99936
MELATN01o	0.06661	0.99966
MELFIT09o	0.19868	0.99899
MEQCOBo	0.09652	0.99973
METHCL01o	0.15682	0.99557
MEXSEPo	0.03772	0.99986
MEYGIIo	0.11699	0.99808
MHOCUM01o	0.09383	0.99938
MIFPOIo	0.02687	0.99994
MIFZIK_1o	0.16046	0.99618
MIFZIK_2o	0.17576	0.99543
MIGQIDo	0.06523	0.99955
MIHZUAo	0.09869	0.99935
MIMOSN_ho	0.06378	0.99953
MIRACD_ho	0.48916	0.98407
MNIMET02o	0.07684	0.99879
MOKXIUo	0.1871	0.99858
MOKXOAo	0.08621	0.99959
MOPHACo	0.06137	0.99935
MORPHM01o	0.0489	0.99968
MOSXUOo	0.02285	0.99991
MOVLOZo	0.27855	0.97669
MOVYAY01_ho	0.182	0.99844
MOXAZO_ho	0.06206	0.99896

MPIXPS_ho	0.503, molecule was shifted, OK	n/a	
MPZPAMo		0.04426	0.99983
MTEPAMo		0.07018	0.99975
MTHPRGo		0.06835	0.99967
MUBPABo		0.07506	0.99956
MUCDUK_1o		0.11722	0.99888
MUCDUK_2o		0.89743	0.93625
MUGKAA01o		0.04067	0.99975
MUYVAE_ho		0.11963	0.99838
MVERIQ01o		0.06224	0.99971
NADRENo		0.02977	0.99987
NAJPOEo		0.1776	0.99881
NAKGOYo		0.04871	0.99956
NALCYS10o		0.11783	0.99719
NAMDPC01_mo	0.0249, OK	n/a	
NANNUNo		0.08421	0.99934
NARBOYo		0.16148	0.99692
NAZLAC02o		0.1739	0.99891
NDNHCL01o		0.08564	0.9994
NEPHCLo		0.03218	0.99979
NEQGUMo		0.15798	0.99872
NEQHEYo		0.1168	0.99932
NESKEDo		0.07268	0.99958
NETIND01o		0.04863	0.99981
NEVMORo		0.0407	0.99973
NHPBZO_ho		0.11397	0.99874
NICOAM05o		0.0205	0.99989
NIHMOH01o		0.1863	0.99801
NIKROPo		0.12923	0.99824
NILXOV_mo	Molecules shifted into unit cell, OK	n/a	
NIQVIT_1o		0.10167	0.99947
NIQVIT_2o		0.3545	0.99358
NIRRAH_ho		0.20923	0.99832
NIVBIO_ho		0.27073	0.99835
NOBDUFo		0.23058	0.99871
NOKGAXo		0.09112	0.99906
NORGES01o		0.02757	0.99994
NUJDAX_wo		0.10144	0.9988
NUPQEWo		0.08552	0.9997
NUYHUKo		0.04418	0.99988
OBEQAN01o		0.06784	0.9997
OCAHACo		0.06806	0.99971
OFAZUQo		0.17568	0.99792
OFEJOAo		0.03568	0.99989
OFIEWo		0.05666	0.99982
OGIXINo		0.01673	0.99991
OPOGADo		0.02419	0.99995
OPOQERo		0.02804	0.99992
ORNHCL12o		0.06706	0.99916
OROZAXo		0.08453	0.99938

OXYTET01_ho		0.12604	0.99881
PABHIJ01o		0.06994	0.9994
PAJNUJo		0.04815	0.9998
PANCURo		0.11263	0.99954
PBUMSLo		0.20896	0.99732
PBUMSL_ho		0.20896	0.99732
PCLPMS_1o		0.28432	0.99551
PCLPMS_2o		0.16634	0.99848
PEBGUC02o		0.105	0.99895
PEDWOMo		0.109	0.99939
PEKFANo		0.10696	0.99897
PERPAZo		0.08545	0.9996
PETHIDo		0.06759	0.99946
PETHID_ho		0.06759	0.99946
PEXKOS01o	0.0552 wo Cl-ion, OK		n/a
PEYGOQo		0.11195	0.99883
PGDEDOo		0.03546	0.9999
PHEPHRo		0.05242	0.99962
PICVUU01o		0.10304	0.99959
PIGSOOo		0.0394	0.99984
PILOCP01o		0.21653	0.9943
PIMKOLo		0.05709	0.99963
PIMOZDo		0.19124	0.99879
PINDONo		0.05678	0.99963
PIPAMPo		0.13724	0.99935
PIPCIL_ho		0.55519	0.98834
PIRENA10_wo		0.07397	0.99962
PIWLEM02o		0.04117	0.9999
PMEPEN01o		0.06593	0.99971
POBKOGo		0.11535	0.99945
POGKOMo		0.17417	0.99936
PRAZAM_ho		0.10019	0.99901
PRGDOL02o		0.04603	0.99985
PROCPHo		0.10914	0.99901
PROGLE20_ho		0.36106	0.9923
PROGST12o		0.05848	0.99974
PUFGUJo		0.10077	0.99899
PUQGUFo	0.0778 wo K-ion, OK		n/a
PUVMAUo		0.06904	0.99902
PUVRIHo		0.05053	0.99974
PYRXCL01o		0.0443	0.99964
PYRZIN23o		0.02084	0.99989
QABCIIo		0.13095	0.9995
QABTOD01o		0.04561	0.9999
QATNEF01o		0.09152	0.99963
QECHOV03o		0.02692	0.99981
QEMLIEo		0.08323	0.99964
QETZULo		0.16113	0.99813
QICMEU_ho		1.3643	0.91064
QIFKEX01o		0.28505	0.99635



QIJPACo	0.11878	0.99904
QIJZOYo	0.07371	0.99977
QIQKEIo	0.06937	0.99966
QIQLILo	0.14224	0.99728
QOMKUAo	0.13853	0.99918
QQQAEJ02o	0.12456	0.99753
QQQAUG04o	0.17424	0.99649
QQQBSS01_ho	0.18443	0.9971
QUBQIO01o	0.04653	0.99979
QURWOQ02o	0.07866	0.99916
QUZWOYo	0.14467	0.99846
RALMIAo	0.11174	0.99918
RALMOG01o	0.09553	0.99944
RAVPUBo	0.11706	0.99963
RBFLAV10_ho	0.05375	0.99979
REBCILo	0.06858	0.99984
REDNIXo	0.02118	0.99997
REZBILo	0.07094	0.99952
RIGDESo	0.05105	0.9997
RILQOUo	0.12598	0.99853
RINTITo	0.05982	0.99986
RIQFOOo	0.02523	0.99988
RIWKOXo	0.05359	0.99966
ROKNUBo	0.115	0.99955
ROQLOAo	0.02756	0.99994
RSERPNO1o	0.06414	0.99988
RUKBOPo	0.04324	0.9998
RUKQOFo	0.06983	0.99977
RUTGOEo	0.10642	0.99846
RUTGUKo	0.13208	0.99574
RUWBAMo	0.11541	0.99934
RUYZAOo	0.14751	0.99765
SAFNIWo	0.18995	0.99778
SAHSOJ_ho	0.0844	0.9995
SAJFITo	0.07058	0.9997
SAJNOG_ho	0.12709	0.99927
SAQYIRo	0.11339	0.99948
SATHOLo	0.08193	0.99944
SAWFIF_ho	0.15208	0.99892
SAXFEDo	0.1566	0.99931
SAXQITo	0.09258	0.99911
SAZLAGo	0.07774	0.99948
SAZNOW_mo	1.04061	0.94459
SEBPEU01o	0.07161	0.99924
SENJIFo	0.11156	0.99932
SEQKAA02o	0.08854	0.99922
SEQNILo	0.08365	0.99974
SESKUY01o	0.10766	0.99919
SETSOAo	0.10801	0.99885
SFDMOX05_ho	0.07209	0.99954

SIFGODo		0.04594	0.99988
SIJWUFo		0.02562	0.99982
SIKLIH07o		0.06758	0.99951
SIWCEG_1o		0.58071	0.98471
SIWCEG_2o	2 <sup>nd</sup> disorder component, OK		n/a
SLFNMB02o		0.07372	0.99938
SLFNMC20_ho		0.4365	0.98495
SLFNMG01o		0.05218	0.99961
SOBBUG_ho		0.09966	0.99864
SONKEMo		0.07659	0.99973
SOPSEVo		0.12329	0.99735
SOYMID_1o		0.12783	0.99931
SOYMID_2o		0.12481	0.99934
SUTHAZ37o		0.09876	0.99887
SUTWIOo		0.16617	0.99835
SUVGULo		0.07814	0.99964
SUWNUTo		0.04281	0.99978
TADLIU02o		0.06383	0.99979
TAJFOZ_ho		0.15295	0.99876
TANDETo		0.06101	0.9991
TAYFUV_ho		0.17324	0.99783
TAZZUPo		0.06631	0.99955
TEPSAM_ho		0.05485	0.9994
TESTON10o		0.01998	0.99996
TETCYH12o		0.65366	0.97227
TEZZEEo		0.05745	0.99973
TFPROM10o		0.11861	0.99898
THCLCS_ho		0.27221	0.99678
THGUAN10o		0.03158	0.99978
TIJMIIo		0.08151	0.99919
TIPWAQ_ho		0.29034	0.99419
TITHYN10_ho		0.09802	0.99944
TIYQAU01o		0.08499	0.99966
TMPHCL01o		0.09478	0.99928
TOPXED_mo		0.11378	0.99893
TOXXIN_ho		0.2012	0.99729
TOYJOGo		0.16045	0.99874
TOYSUXo		0.30231	0.99469
TUBOBM_ho		0.30468	0.9957
TULRIB_mo	0.0138 for main molecule, OK		n/a
TUQGETo		0.30116	0.98274
TUTDODo		0.06265	0.99971
TUZCOIo		0.05442	0.99976
UCUVETo		0.07066	0.9996
UGIYEPo		0.07854	0.99971
UHUQUKo		0.0986	0.9997
UKAKIAo		0.10855	0.99912
UMOMALo		0.06128	0.99982
UPUKOHo		0.08006	0.99923
UQAPEJo		0.09666	0.9995

URAVUGo		0.11861	0.99939
UREAOH12o		0.04305	0.99903
USOCOVo		0.12698	0.99947
UXIXUVo		0.04642	0.99966
VAMBOA01o		0.1859	0.99881
VAWPITo		0.102	0.99851
VAWQEQo		0.07488	0.99957
VAYJOWo		0.2376	0.99689
VAYXOIo		0.1061	0.99945
VEMRAIo		0.10869	0.99951
VEVQAQo		0.08667	0.99955
VICXOVo		0.1236	0.99919
VIDJEX01o		0.15361	0.99784
VIFQILo		0.10361	0.99928
VIGDAR_1o		0.22684	0.99679
VIGDAR_2o		0.23294	0.99662
VOGCAV_ho		0.08841	0.99982
VOXDUHo		0.13282	0.99819
VUCDUSo		0.24421	0.99307
VUCJElO		0.11824	0.99928
VUJRUE_ho		0.05639	0.99989
VUXPUZo		0.09748	0.99861
WACHIR_ho		0.08044	0.99977
WADPICo		0.0886	0.99954
WADTIGo		0.06208	0.99981
WAHJARo		0.10273	0.99955
WAJYUCo		0.11277	0.99959
WALPIJo		0.10863	0.99899
WASGAA_ho		0.08781	0.99945
WAWVOHo		0.10572	0.99955
WEHYEOo		0.08654	0.99942
WELGAVo		0.08137	0.99968
WEMGECo		0.05612	0.99951
WEQHEF01_ho		0.67036	0.96789
WERVEU02o		0.093	0.99923
WETLOYo		0.08313	0.99949
WETPOB_1o	0.054, disordered, OK		n/a
WETPOB_2o	0.082, disordered, OK		n/a
WEXQAS01o		0.07044	0.99958
WEZCOTo		0.07175	0.99956
WIBZEMo		0.1187	0.99944
WINJAE_mo	0.0284, shifted due to cation, OK		n/a
WINWUL02o		0.08977	0.99933
WIPYOLo		0.10867	0.99904
WOQDAHo		0.07312	0.99947
WOYPABo		0.07603	0.99967
WUTHEA01o	Moved molecules in unit cell, higher Z structure, OK		n/a
XANTOX_ho		0.18893	0.99512
XAPTAK01o		0.03314	0.99986
XAQNOUo		0.09623	0.99885

XATJAFo		0.08216	0.99953
XAYGEJ01o		0.11048	0.99911
XAZRUNo		0.10032	0.99901
XEJKUSo		0.07451	0.99888
XEZTON01o		0.09007	0.99943
XICRUYo		0.12032	0.99851
XIJKIK01o		0.04537	0.99898
XIRHOXo		0.13245	0.99699
XOCXUI01o		0.06183	0.99972
XOGMOXo		0.14906	0.99565
XOJNOBo		0.13887	0.99889
XOSGUHo		0.07944	0.99978
XOZRUZo		0.24582	0.99525
XULRUTo		0.06772	0.99975
YACGUE_ho		0.32192	0.99121
YACHAL_ho		0.09409	0.99937
YACTEC01o		0.06532	0.99944
YALWISo		0.04813	0.99989
YALYUHo		0.0736	0.99963
YAPZEUo		0.03839	0.99989
YARXEWo		0.05939	0.99986
YIGRAIo		0.06347	0.99961
YIKNUDo		0.11619	0.99887
YODXARo		0.13084	0.99879
YOKQAQo		0.0937	0.99852
YUKVADo		0.04393	0.99989
YURSUB_ho		0.12828	0.99937
ZAPLEJo		0.11601	0.9995
ZAPXOFo		0.16955	0.99574
ZEMJOQo		0.05147	0.99984
ZENREPo		0.15334	0.99939
ZIDLEDo		0.07708	0.99964
ZIKJOSo		0.0599	0.99949
ZIMBOOo		0.077	0.99857
ZIVKEUo		0.09763	0.99907
ZOGSODo		0.22119	0.99727
ZOXSEKo		0.1117	0.99914
ZUHFIRo		0.08305	0.99935
ZUQMIJ_ho	0.105, OK		n/a
ZZPUS19o		0.14205	0.99801
ZZRRCG01_ho		0.09679	0.99942
ZZTSE03o		0.04035	0.9998













































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































































